PHY-892 Quantum Material's Theory, from perturbation theory to dynamical-mean field theory (lecture notes).

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1. PREAMBLE

1.1 Aim

The main part of this book can be used as a graduate-level course that takes the student who is familiar with elementary quantum mechanics and statistical mechanics to research-level. This book is about the language that is necessary to understand the physics of large assemblies of interacting particles. This book is thus about *physical principles*, as well as *mathematical formalism*.

In quantum mechanics in general, what we normally call the "Physics" is very much tied to the calculational tools. If you think of the wave function of a system with N degrees of freedom, it gives one complex number for any given specified value of the N degrees of freedom. What can you tell from this? In principle everything, but in practice the size of the space over which this complex number is defined grows exponentially with the number of degrees of freedom and it is not very illuminating. As usual in quantum mechanics, we need to focus on observables, i.e. expectation values, or if you want, averages in a quantum state. In addition, when we work at finite temperature, we need to take thermal averages over states. The average density at a point, that we can extract from the wave function, is an example of observable that has physical content. Similarly, the average of the product of the density at a point, times the density at some other point and some other time has meaning. It is a correlation function, that tells us how a density perturbation will propagate, how changing the density at one point influences density at another point. Furthermore, this correlation function is measurable and, as usual in quantum mechanics, by focusing on observables, much is gained.

By analogy with the case of density correlation functions, in quantum mechanics we can look at amplitudes, namely we can ask what is the amplitude for an electron to go from one point at one time to another point at another time. This is a correlation function, the Green's function, that, in conjunction to perturbation theory, behaves in the way that is closest to the concept of a particle that propagates and interacts with other particles.

In fact, without perturbation theory, describing the "Physics" often becomes impossible, or extremely difficult. Other emergent concepts that come out of these calculational tools are that of self-energy and vertex functions. Self-energy will, in a way, play the same role as viscosity in ordinary hydrodynamics and vertex the role of collision amplitude. They are quantities where much of our ignorance about the exact solution to the problem can be hidden. Identifying these hidding places, is part of what it means to understand the physics of a problem. We work part with images, part with formalism, but in quantum mechanics, often the images or physical intuitions are meaningless without the formalism.

This book is thus both about calculational tools and about the physics that comes out of these tools.

In a way this book is about applications of field-theory to Many-Body physics. There are many classic books on this subject. (?? Add comments on other books)

In any book on this topic, one needs to discuss the notions of Green's functions, self-energy, vertex functions, spectral weights, sum rules etc. that have withstood the test of time and are the basis, in fact the language of this field. On the

other hand, most classic books focus on perturbation theory to do calculations that relate to experiments. Indeed, the original methods of many-body theory that were born in Quantum Electrodynamics, as treated by Feynman, Tomonaga and Schwinger, were based on perturbation theory. In that context, the more physically transparent methods of Feynman became widespread. However, in the last decades, non-perturbative approaches have become necessary to describe phenomena that are characteristic of strong interactions, such as the interaction-induced metal-insulator transition, the so-called Mott transition. It is in this context that the methods of Schwinger display their power.

There are many subtle points in Many-Body theory that I try to point out explicitly in various remarks spread throughout the book. These subtleties are often glanced over in many books: violation of the Pauli exclusion principle by certain approximations, limitations of various approximations for the self-energy with regards to sum rules, how irreversibility arises in the limit of an infinite system, etc...

1.2 In broad strokes, adiabatic continuity and broken symmetry

Summarizing this book in broad strokes, it introduces the general notions associated with Green's functions and explains both the Feynman and Schwinger approaches to compute them. The Coulomb gas is discussed in a way that makes natural the non-perturbative treatment of the Hubbard model by the two-particle self-consistent approach. In the Schwinger approach, the dynamical-mean-field theory of the Mott transition becomes natural. There is thus in this book an emphasis on Schwinger's methods and non-perturbative approaches that is not found in many other books. Functional integral methods would be another useful method to discuss non-perturbative problems. Solitons, tunneling can be treated elegantly with functional integrals. This approach is thus introduced, mostly in the last part of this book, but it is not necessary to understand the main topics. Dealing with both Feynman's and Schwinger's approach without getting lost in formalism is already difficult enough.

The Coulomb gas and the Hubbard model are the two models that serve as paradigms throughout this book. The Coulomb gas is useful to understand screening and simple metals. The Hubbard model becomes natural once screening is understood and is a paradigm for interaction-induced metal-insulator transitions (Mott transition) high-temperature superconductors and for many other materials that exhibit strong correlations.

These two models allow us to illustrate very general key *principles* that are behind assemblies of many particles. One of them is *adiabatic continuity*. It is possible to describe a "phase", say the normal state of a metal, by starting from a simple Hamiltonian with known properties, such as that of band electrons, and including interactions with perturbation theory. This is the subject of many parts of this book, in particular those related to the Coulomb gas. In the presence of interactions, "quasiparticles" are adiabatically connected to our notion of free electrons. But they are not the same as free electrons. In studying this, we understand the limitations of the ordinary band theory of solids. The quasiparticles we have in mind, are those of the Fermi-liquid theory, put forward by Landau in the 1960's.

But eventually, perturbation theory breaks down and interactions lead to phase

transitions, in other words to new phases of matter that are *not* adiabiatically connected to the original Hamiltonian. At phase transitions, the free energy has mathematical singularities that cannot be treated by perturbation theory. These new phases can very often be connected to a new Hamiltonian, that must sometimes be "guessed", a Hamiltonian that breaks some of the symmetries present in the original phase. The Stoner approach to the Hubbard model description of ferromagnetism is an easy way approach the main underlying principle of importance, namely that of *broken symmetries*.

Adiabatic continuity and broken symmetry are the two most important basic principles of condensed matter physics, according to P.W. Anderson. The all important example of superconductivity, perhaps the deepest example of broken symmetry, is also treated taking the jellium model to justify attractive electron-phonon interactions.

Why broken symmetries? Because "More is different", as emphasized by P.W. Anderson [11]. Suppose we give ourselves the Hamiltonian that should suffice to describe all homogeneous substances at room temperature and normal pressure. It consists in the sum over individual kinetic energies, plus pairwise interactions between constituents, plus spin-orbit interactions (a relativistic effect that can be deduced from perturbation theory). The energy scales involved are of the order of 10 to 100 eV. All physics at these energy scales and less should be contained in that Hamiltonian. But the challenge we are facing is enormous. Suppose we write down the Hamiltonian for a piece of aluminum. It is a superconductor at a few degrees Kelvin, or if you want at energies of the order of about 10^{-4} eV. This means that to predict from first principles the presence of superconductivity in aluminum, we need a precision of 10^5 to 10^6 in a calculation that involves a macroscopic number of degrees of freedom, say 10^{23}. The difference in time scales and length scales between the atoms and a piece of matter are similarly enormous. What we need to proceed are new concepts, new principles, new laws if you want, that "emerge" from the basic theory.

I have used this expression"emergent" a number of times above without ever specifying what I meant. Entropy and irreversibility and even absolute temperature are concepts that emerge when an extremely large number of particles is present in a piece of matter, the subject of statistical mechanics. Another simple example of an emergent phenomenon is the Fermi surface. An aluminium atom has a discrete absorption spectrum. Yet, a piece of aluminium meral is shiny. Its abosroption spectrum is completly different. In particular, it can absorb radiation of arbitrary small energy instead of the minimum energy we have in the atom. It is because we now have a Fermi surface. Another emergent property related to the Fermi surface is topology. What to I mean by that. The band structure, or electronic structure, is defined on a torus in wave-vector space and the wave function describing several bands can be thought of as a vector that lives on that torus. Upon transporting that vector on that torus, one discovers that certain electronic structures have non-trivial topology. This is a subject in itself that I will not touch in this book, except to show that Green's functions can detect that non-trivial topology. There are a number of books on the topic of topology in condensed matter. (?? books)

Other emergent properties in broken symmetry states include collective modes known as Goldstone modes and Mermin-Wagner theorem, both of which can be illustrated with the simple ferromagnetic example.

The concept of broken symmetry is necessary to study an emergent phenomenon such as superconductivity. And before that concept emerges, other conceptual steps had to be taken: the Born-Oppenheimer approximation, the introduction of collective quantum coordinates such as phonons, density functional theory to obtain a first guess at the structure of electronic energy levels, Migdal's approx-

imation for electron-phonon interaction... Once in the broken symmetry states, new collective modes appear. For example, when the symmetry that is broken is continuous, then Goldstone's theorem shows that collective modes appear. The modes restore the symmetry in the infinite wavelength limit. Remarkably, one can argue that different states of matter in general, and broken symmetries in particular, each correspond to a new universe, containing its own interacting elementary particles, spin wave and phonons being simple examples. In this way, the field of quantum materials, or condensed matter physics if you want, is extremely rich.

Despite what I have said above, much progress has been made in recent years in devising first-principle methods that start with the full Hamiltonian and make materials-specific predictions. These methods are based on bringing together ideas from density functional theory and calculations on model Hamiltonians. While I focus on model Hamiltonians in this book, the methods that are present are also useful in these first-principle "realistic materials" calculations, including modern treatments that combine dynamical mean-field theory with density functional methods. Model Hamiltonians hide the presence of other energy scales in effective parameters, for example hopping integrals and screened electron-electron interactions. Physics is indeed a question of scale. Even though we know the basic laws of Physics, say at the level of quarks and gluons, much of the structure of the laws at this level are of no relevance for atomic Physics. Exchange of gluons between quarks in the atomic nucleus will influence the difference between energy levels of the atom, but in such a minute way that it is essentially insignificant. These details are for all practical purposes irrelevant. In some sense this is a consequence of the structure of quantum mechanics itself. The influence of physics at a high energy scale on physics at a lower energy scale that is well separated from the former can be estimated with perturbation theory. More generally, the "renormalization group" tells us how to construct effective theories that depend on the scale. The Coulomb gas and the Hubbard model that we study in detail in this book are effective models that we do not fully justify from a completely first-principles approach.

Note that indifference to details about higher energy scales, or shorter distances if you wish, also occurs in purely classical mechanics. Ordinary hydrodynamics, as contained in the Navier-Stokes equation, is a theory that is valid for a very broad class of liquids. The specific atomic details will come in for example in determining the specific value of viscosity for example, but the concept of viscosity is a notion that emerges at long wave lengths and large time scales. Examples of emergent concepts that come out of these calculational tools that we develop here are those of self-energy and vertex functions. The imaginary part of these quantities, in a way, play the same role as viscosities in ordinary hydrodynamics.

1.3 Contents

The first part of this book begins with the elementary example of a classical, driven damped harmonic oscillator. With this simple example, one can illustrate what happens when we focus on a single degree of freedom in contact with many others whose detailed motion we do not care about: frequency is renormalized, absorption occurs over a finite frequency range, and the real and imaginary parts of the response are related by Kramers-Kronig relations. One can even introduce the analog of a Green's function, the polarisation operator, the fluctuation-dissipation theorem and work out explicitely examples that show how irreversibility arises as

a consequence of interactions with an infinite number of degrees of freedom. We will even be able to introduce the concept of hybridization.

The second part is about general properties of correlation functions and their relation to experiments. It is shown that scattering experiments measure fluctuations whereas transport experiments measure dissipation. But there is a deep relation between fluctuations and dissipation. In this part of the book, it is shown that correlation functions obey properties, such as the one just mentioned, that are extremely general and do not depend on any explicit calculation of these correlations functions. Causality, Kramers-Kronig relations, Lehmann representation, sum rules are important exact results that are introduced and that guide us throughout this book. General properties that follow from symmetry are also introduced. The famous Kubo formula for conductivity allows one to discuss Drude weight and the fundamental differences between an insulating gap and a superconducting gap for example.

The Green's function appears explicitly in part III as an alternate approach to one-body physics as described by the Schrödinger equation. The Green's function is explained as a special case of correlation functions, obeying sum rules, Kramers-Kronig relations and the like. Perturbation theory gives glimpse of what Feynman diagrams are about. It is even possible to discuss self-energy rather simply. The impurity averaging method allows one to introduce more complicated Feynman diagrams and general resummation methods. The Feynman path integral as an alternate way of computing the Green's function appears naturally.

Second quantization is introduced only in the fourth part that focuses on the one-particle Green's function at finite temperature. This late introduction of second quantization is in line with the general idea that one should allow you to separate what is a general property of correlation functions from the machinery nessary to compute these correlation functions. The definition is motivated formally and through the link with angle-resolved photoemission spectroscopy. Perturbation theory makes time-ordered products a natural concept so that the Matsubara Green's function does not appear so strange. Its link to the retarded Green function is established through both the Lehmann representation and analytic continuation along a contour in imaginary time. Its imaginary-time boundary conditions follow from the same procedure as that which gave the fluctuation-dissipation theorem for correlation functions. The physical meaning of Green's function and how they naturally lead to the concept of quasiparticles is discussed. The section ends with three general theorems that are useful in many-body theory, namely Wick's theorem, the linked cluster theorem and Feynman's variational principle.

The Coulomb gas treated in the long fifth part is a classic subject that cannot be avoided. This is where perturbation theory and diagrams make their first appearance. You can choose two roads. Either the classic Feynman approach or the functional derivative approach of Schwinger and Martin. Although less intuitive, the latter approach has the virtue of being more natural for non-perturbative approches. For example, the link between irreducible vertices and functional derivatives of the self-energy appears naturally. Similarly, certain consistency relations, for example between self-energy and density fluctuations, are quite natural. Collective modes are discussed with simple phenomenological approaches before they are treated in full detail with many-body methods in the random phase approximation (RPA). As usual, the best self-energy for the electron gas is obtained after the collective modes are under control. This leads to the so-called GW approximation, a special case of Hedin's equations that are also introduced.

The sixth part takes us to a topic of current interest, namely interacting fermions on a lattice. Density functional theory is the starting point. Then the Hubbard model is introduced and solved approximately following the two step process of

the electron gas, namely find the collective modes, then the self-energy. This is the procedure followed by the two-particle self-consistent (TPSC) method. Sum rules play a more prominent role in this non-perturbative approach than in the case of the electron gas. They allow one to find renormalized vertices whose physical description goes back to Kanamori and Brückner. TPSC cures many limitations of RPA: RPA violates the Pauli exclusion principle, which is a severe limitation for a one-band model on a lattice. RPA also leads to phase transitions in two dimensions that violate the Mermin Wagner theorem. Benchmark Monte Carlo calculations show that TPSC is more accurate than other known methods in the weak to intermediate correlation limit. The hallmark of strong correlations is the Mott transition. Dynamical Mean-Field Theory (DMFT) is the best method to describe this. That method is presented in the last section of Part VI.

Broken symmetry is a key concept of many-particle physics. Part VII is devoted to various examples. Stoner ferromagnetism is the simplest one. Antiferromagnetism is another one. The latter allows us to discuss the pseudogap in electron-doped cuprates. The Hubbard Stratonovich transformation is a common tool in many-body physics that is introduced in this part of the book. Phonons make their debut as a prelude to the theory of superconductivity. As for other phase transitions, the Bardeen Cooper Schrieffer (BCS) theory of superconductivity is introduced as an instability of the normal state and then studied in the broken symmetry state. The Bogoliubov transformation is introduced in a way that makes the phase of the order parameter appear naturally. Note that mean-field theory in this part of the book is presented in several different ways. The Green's function effective medium point of view is useful to understand the Eliashberg-Migdal theory of superconductivity even if this theory is not treated in detail here.

Before we conclude with Part IX, which is a short version of the book for the advanced student or the expert, Part VIII discusses alternate approaches to Many-Body theory, leading to a broader perspective on the field. It introduces the Luttinger-Ward functional and the self-energy functional approach to DMFT. Coherent-state functional integrals are explained. The book could have been based on that approach: As emphasized by Feynman, there is often no unique starting point in Physics. While some may be more fundamental, it is hard to know from the start which is best. As stated by Feynman, contrary to the axiomatic approach of the Greeks, the Babylonian approach, where one has many tools and possible starting points, is often useful since some problems are easier to handle in one approach than in the other.

1.4 Summary

This is work in progress. Many-body physics is an open frontier. Everyday new materials lead to new surprises, new phases, new phenomena appear, and often new calculational tools must be developed. This course is about the foundations. Much of it will be like learning spelling and grammar, but rest assured, there are great novels, great stories to be read while you grasp the rules of this language. And whether you are a theorist or an experimentalist, this language is indispensable. It is behind the calculations, but it is also behind the interpretation of the experiments, it is behind the workings of nature.

To the lecturer:

This book is partly a set of lecture notes and partly a monography. In lecture notes, one aims at pedagogy. A monography should give a complete overview of a

specific field, but for the student it is often overcomplete and not very pedagogical. The two styles are difficult to reconcile. The following guide should help the lecturer focus on the sections and chapters of this book that are essential for a first encounter with that field. (??? To come)

- The introduction introduces the language of correlation functions in the very simple context of the harmonic oscillator.**??** If it is skipped, then the student will need to go back to some of the formulas later.
- Section 7.2 on the detailed cross-section calculation can be skipped on first reading.

Part I

Classical hamonic oscillator to introduce basic mathematical tools and concepts

In many-body physics, we are concerned with the behavior of a an electron, or of the local density, or in general of some observable. What complicates the problem is the effect of all other particles, namely of the environment, on the quantity we are interested in. Focusing on a single observable, we have to average over the coordinates of all other particles. We will see that this leads us naturally to the calculation of correlation functions.

You are probably eager to learn about Green's functions, Feynman diagrams and all that. And indeed, sometimes, the first thing you hear about in many-body physics is Green functions. You find out all sort of properties of that object, such as analyticity, spectral representations, irreversibility and so on. But in fact, many of these concepts are not special to Green's functions. Hence, before I drag you through Green's functions, I consider in this introductory chapter the simplest case of a many-body system, namely a classical harmonic oscillator coupled to an environment.[149] You will wonder why all this formalism for something as simple as the harmonic oscilator. I ask you to look at it the other way. This simple example will allow me to introduce in this very simple context much of the machinery we need for the many-body problem and almost all the undergraduate mathematics that we need. This will refresh our memory and demystify much of what will come later. To understand the physics hidden behing the mathematics, in many cases you will be able to return to the harmonic oscillator. We will encounter for example the Kramers-Kronig relations that follow simply from causality and have wide applicability in all of physics.

In the case of the harmonic oscillator, we are used to represent the environment by a damping constant, whose role will be played by the self-energy later. Taking the damping constant as just a number is sometimes a good approximation even for more complicated many-body systems. We will see however that there are limitations to the representation of the environment by a single number. For deep reasons, the damping constant should be frequency dependent. More specifically, we will see that certain sum rules are not satisfied with a frequency independent damping constant. And by the way, we will also see what sum rules are and why they are important as the few results that are known exactly in many cases. Sum-rules will come back very often in this book.

We will show that the response to an external force can be described by a response function (susceptibility) that is the analog of a propagator, or Green function. This susceptibility describes the dissipation and obeys a very important theorem, the fluctuation-dissipation theorem. So the susceptibility is related to a correlation function. Its poles have special significance, as they do for Green's functions. We will see how irreversibility emerges in the limit where the oscillator is connected to an infinite bath. We will even encounter the concept of hybridization that arises in quantum impurity problems. These are all very general results that we will see again and again in this book. This introduction is inspired by lecture notes of Paul Martin [150].

2. THE DAMPED, DRIVEN, HARMONIC OSCILLATOR

Back to basics. This is where we go back in time to undergraduate days of the harmonic oscillator and Fourier transforms. You are perhaps not so familiar with the consequences of causality on analytic properties of functions that describe the response to external forces. That is where we will introduce Kramers-Kronig relations.

2.1 The driven harmonic oscilator

Take a simple one-dimensional harmonic oscillator in a bath described by the displacement x from equilibrium, as illustrated in Fig.(2-1).

It is described by the equation of motion

$$m\frac{d^2x}{dt^2} = -kx + F^{int}(t) \tag{2.1}$$

where m is the mass, k is the spring constant and $F^{int}(t)$ represents the effect of all other particles on the system. Experiment teaches us that on average, the effect of all other particles may be approximated by a force that depends linearly on velocity. More specifically, we write

$$\left\langle F^{int}(t)\right\rangle_{n.e.} = -m\gamma\frac{dx}{dt}. \tag{2.2}$$

The average on the left $\langle\rangle_{n.e.}$ is a non-equilibrium average. It is over a time that is long enough that we do not see the individual collisions, but short enough that the oscillator does not have time to relax completely. To keep the notation simple, we do not put an average on the coordinate x. Here γ has units of frequency, or inverse relaxation time. We then have to solve the equation of motion

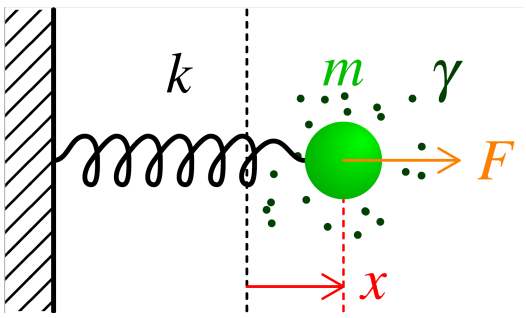


Figure 2-1 Damped forced harmonic oscillator in one dimension. The mass is m the spring constant k. It interacts with an environment that is modeled by a damping constant γ.

$$m\frac{d^2x}{dt^2} = -m\gamma\frac{dx}{dt} - kx \tag{2.3}$$

which we do using the usual trick for linear equations. Namely, we posit

$$x = Ae^{-i\omega t} \tag{2.4}$$

which gives us the equation for ω,

$$-m\omega^2 - i\omega m\gamma + k = 0. \tag{2.5}$$

With the usual definition $\omega_0^2 = k/m$, we have

$$-\omega^2 - i\omega\gamma + \omega_0^2 = 0 \tag{2.6}$$

whose solution is

$$\omega = -i\frac{\gamma}{2} \pm \omega_R \; ; \; \omega_R = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}. \tag{2.7}$$

As you can see, the natural frequency ω_0 is modified by the presence of damping. We assume that the oscillator is not overdamped, namely $\omega_0^2 > \frac{\gamma^2}{4}$. The resulting displacement for free motion is

$$x(t) = e^{-\gamma t/2}\left(A\cos\omega_R t + B\sin\omega_R t\right) \tag{2.8}$$

where the constants A and B are determined from the initial conditions on the position and on the velocity.

Remark 1 *This example illustrates that it is impossible to include damping without also changing the resonance frequency. In the jargon, we say that the frequency is renormalized by interactions with an evironment. .*

In many body-physics, we want to know how a physical system responds to an external probe, for example light, sound, magnetic field etc. Let us thus add an external driving force

$$m\frac{d^2x}{dt^2} + m\gamma\frac{dx}{dt} + kx = F(t). \tag{2.9}$$

Taking again a single harmonic motion, we end up with the equation

$$\left(-\omega^2 - i\omega\gamma + \omega_0^2\right)x(\omega) = \frac{1}{m}F(\omega). \tag{2.10}$$

The solution of this equation will give us $x(\omega)$ as a function of $F(\omega)$ from which we can extract the solution $x(t)$ which is appropriate once the transients, obtained from the solution of the equation with $F(t) = 0$ above, have been damped out.

2.2 Interlude: A reminder of some definitions and theorems on Fourier transforms and integrals of functions of a complex number

I seem obsessed with Fourier transforms and frequency. Why is that? If I were a communication engineer trying to use a carrier frequency for radio that would seem

more natural. Well, it is very natural for us as well because in quantum mechanics, frequency is assocciated with energy, Planck's constant $\hbar$ helping. When we send a photon or a neutron of a given energy to probe a piece of material, we are sending it at a given frequency. So that is one of the reasons it is so important. I will also use the opportunity of this mathematical chapter to remind you of some theorems on complex variables that we will need.

The time and frequency components are defined by

$$\int_{-\infty}^{\infty} e^{i\omega t} x(t)\, dt = x(\omega) \tag{2.11}$$

$$\int_{-\infty}^{\infty} e^{-i\omega t} x(\omega) \frac{d\omega}{2\pi} = x(t) \tag{2.12}$$

whose consistency is garanteed by the result

$$\int_{-\infty}^{\infty} e^{i\omega t} dt = 2\pi\delta(\omega) = \mathcal{T}\delta_{\omega,0}. \tag{2.13}$$

Here, $\mathcal{T}\delta_{\omega,0}$ is not really rigorous, but it tells us that if we had a discrete set of frequencies defined over a periodic time interval $\mathcal{T}$, the same $\mathcal{T}$ as that used above, then the integral would be equal to $\mathcal{T}$ time a Kronecker delta function, defined by

$$\begin{aligned} \delta_{\omega,0} &= 1 \text{ if } \omega = 0 \\ &= 0 \text{ otherwise.} \end{aligned} \tag{2.14}$$

One of the important theorems is the convolution theorem which states that the Fourier transform of a convolution is the product of the Fourier transforms

$$\int_{-\infty}^{\infty} dt\; e^{i\omega t} \left(\int_{-\infty}^{\infty} dt' \gamma(t-t') f(t') \right) = \gamma(\omega) f(\omega). \tag{2.15}$$

Also, Parseval's identity takes the form

$$\int_{-\infty}^{\infty} \gamma(-t) f(t)\, dt = \int_{-\infty}^{\infty} \gamma(\omega) f(\omega) \frac{d\omega}{2\pi}. \tag{2.16}$$

or, more commonly

$$\int_{-\infty}^{\infty} \gamma(t) f(t)\, dt = \int_{-\infty}^{\infty} \gamma(\omega) f(-\omega) \frac{d\omega}{2\pi}. \tag{2.17}$$

Proof. To prove the convolution theorem, it suffices to use the Fourier representation of $\gamma(t-t')$ and of $f(t')$

$$\begin{aligned} \int_{-\infty}^{\infty} dt e^{i\omega t} \left(\int_{-\infty}^{\infty} dt' \gamma(t-t') f(t') \right) &= \int_{-\infty}^{\infty} dt e^{i\omega t} \left(\int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega'(t-t')} \gamma(\omega') \right. \\ &\quad \left. \times \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} e^{-i\omega'' t'} f(\omega'') \right). \end{aligned}$$

Performing the integral over t on the right-hand side gives $2\pi\delta(\omega-\omega')$ while the integral over t' gives $2\pi\delta(\omega'-\omega'')$. With these two delta functions, we can do the the integrals over ω' and ω'' trivially and obtain the result.

Parseval's identity follows by taking $\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}$ on both sides of the convolution theorem and noting that on the left-hand side $\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}$ gives $\delta(t)$. The alternate form of the theorem is more commonly used. You can proove it easily for yourself. ■

Remark 2 *I pay tribute to the usual bad habit of physicists by denoting with the same symbol γ the function in both time and frequency space. Only the argument tells us where we are. Clearly, $\gamma(t)$ and $\gamma(\omega)$ are different functions of, respectively, t and ω.*

Two other important theorems for functions of a complex variable that we will need are

a) *Cauchy's theorem* stating that this integral over a closed contour vanishes

$$\oint f(z)\,dz = 0 \tag{2.18}$$

if $f(z)$ has no singularity inside the contour, in other words if it is analytic (holomorphic inside the contour).

b) *The residue theorem*, that states that if $f(z)$ is analytic, then the following contour integral over a closed contour encircling z_0 is given by

$$\oint \frac{f(z)}{z-z_0} dz = 2\pi i\, f(z_0) \tag{2.19}$$

where $f(z_0)$ is called the residue. Using integration by parts

$$\oint \frac{f(z)}{(z-z_0)^n} dz \tag{2.20}$$

can be related to derivatives of $f(z)$ evaluated at z_0.

2.3 The effect of damping can be retarded. Where we encounter the consequences of causality and the Kramers-Kronig relations

At very high frequency, or very short time, there is no time to interact with the environment and the damping should disappear. In other words, the most general damping is frequency dependent. This reflects retardation, namely the fact that the position may depend on what happened in the environment much earlier, not just instantaneously. We have seen that in the presence of damping, the frequency is renormalized in a way that depends on damping. There is a generalization of this in the presence of a frequency-dependent damping: there is a corresponding frequency-dependent renormalization. This is embodied in the Kramers Kronig relation Eqs. (2.31) and (2.32) that are the important results of this section.

Expressed in the time domain, retardation means that the internal force coming from the environment depends on what happened on previous times. Stated as an equation, we have

$$m\frac{d^2x}{dt^2} + m\int_{-\infty}^{\infty} dt'\gamma(t-t')\frac{dx}{dt'} + kx = F(t). \tag{2.21}$$

In frequency space, the convolution theorem allows us to write

$$\left(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2\right) x(\omega) = \frac{1}{m} F(\omega). \tag{2.22}$$

As I said above, if $\gamma(\omega)$ has a real and an imaginary part, the imaginary part will renormalize ω_0 and the real part will give dissipation. The resonance frequency will be modified by both the real and the imaginary parts of $\gamma(\omega)$.

Causality implies that the damping force coming from the environment cannot depend on the future. Mathematically, this means that

$$\gamma(t-t') = 0 \text{ if } t-t' < 0. \tag{2.23}$$

This result has an elegant counter part in frequency space. The analytic continuation of $\gamma(\omega)$ in the complex plane is holomorphic everywhere in the upper half-plane, a complicated way of saying it does not have poles there. We will say say that $\gamma(\omega)$ is analytic in the upper complex ω half-plane.

Proof. Consider the expression

$$\gamma(t) = \int_{-\infty}^{\infty} e^{-i\omega t}\gamma(\omega)\frac{d\omega}{2\pi}. \tag{2.24}$$

If $\gamma(\omega)$ is analytic in the upper half-plane, then we can satisfy the constraint that if $t<0$ then $\gamma(t)=0$. Indeed, assume that ω has both a real, ω_1, and an imaginary, ω_2, part. With $\omega = \omega_1 + i\omega_2$ we can complete the contour in the upper half-plane, *i.e.* take , $\omega_2 > 0$, and use Cauchy's theorem to obtain $\gamma(t<0)=0$.

To prove this in the other direction, note from the definition and from the fact that $\gamma(t)=0$ for $t<0$ that

$$\gamma(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\gamma(t)\,dt \tag{2.25}$$

$$= \int_{0}^{\infty} e^{i\omega t}\gamma(t)\,dt. \tag{2.26}$$

If ω is in the upper half plane, $e^{i\omega t} = e^{i\omega_1 t - \omega_2 t}$ with $\omega_2 > 0$ and the factor $e^{-\omega_2 t}$ makes the integral converge for $t>0$. For this to be true on the real axis as well, where $\omega_2 = 0$, all we need is that the Fourier transform exists. Given all this, there cannot be poles. ■

Definition 1 *A function that is analytic in the upper half-pane is called"retarded", as suggested by the fact that the effect comes after the cause. A function that is analytic in the lower-half plane is called "advanced" because the effect occurs before the cause. Not very physical in the latter case, but mathematically well defined, and even useful as we shall see.*

Using analyticity in the upper half-plane, we can derive the Kramers-Kronig relations that have wide applicability in physics and engineering since they relate real and imaginary parts of response functions, such as impedance when we talk about electrical circuits. The integral

$$\oint \frac{d\omega'}{2\pi}\frac{\gamma(\omega')-\gamma(\omega=\infty)}{\omega'-\omega} = 0 \tag{2.27}$$

vanishes on the contour illustrated in Fig. (2-2). Indeed, the contour has two parts, and assuming that $\gamma(\omega')-\gamma(\omega=\infty)$ vanishes at least like a small power of ω' in the upper half-plane, the two parts add up to zero since we can complete the contour in the upper half-plane and there is no singularity there.

The contour on the infinitesimal half-circle is easy to do. It suffices to take a half-circle around the singularity and to go to cylindrical coordinates with $(z-\omega) = R\ e^{i\theta}$. Since γ has no singularity in the upper half-plane, $\lim_{R\to 0}\gamma\left(\omega + Re^{i\theta}\right) = \gamma(\omega)$ and the integral is

$$\lim_{R\to 0} -\int_{-\pi}^{0}\frac{\left(Re^{i\theta}\right)id\theta}{2\pi}\frac{\gamma\left(\omega+Re^{i\theta}\right)-\gamma(\infty)}{Re^{i\theta}} = -\frac{i}{2}\left(\gamma(\omega)-\gamma(\infty)\right) \tag{2.28}$$

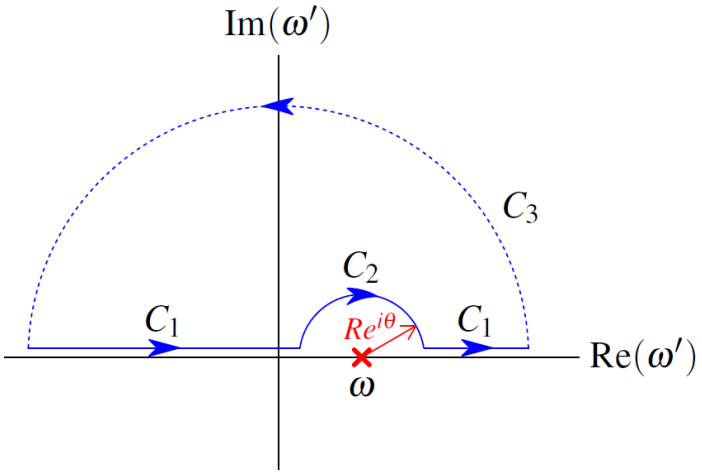


Figure 2-2 Integration contour in the ω' complex plane used to prove the Kramers-Kronig relations. The integral has two contributions, one on the real axis C_1 that stops short of the singularity at ω and a semi-circle C_2 around the singularity. We will always work with functions that vanish sufficiently fast at infinity that the integral over C_2 vanishes. This is related to Jordan's lemma in complex analysis. When the contour is completed with C_3, there is no singularity inside the contour since the function is analytic in the upper half-plane. Hence the integral vanishes.

The minus sign above comes from the differential because the integral is done in the anti-trigonometric direction. The rest of the integral is, by definition, a principal-part integral. Using this, the vanishing of the integral because of causality Eq. 2.27 can then be rewritten as

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{\gamma\left(\omega'\right)-\gamma\left(\infty\right)}{\omega'-\omega}\frac{d\omega'}{2\pi}-\frac{i}{2}\left(\gamma\left(\omega\right)-\gamma\left(\infty\right)\right)=0 \tag{2.29}$$

where $\mathcal{P}$ denotes the principal part.

If we write explicitly as $\gamma'\left(\omega\right)$ the real part of $\gamma\left(\omega\right)$ and as $\gamma''\left(\omega\right)$ its imaginary part,

$$\gamma\left(\omega\right)=\gamma'\left(\omega\right)+i\gamma''\left(\omega\right) \tag{2.30}$$

the imaginary and real parts of this equation give us, respectively, the following two results that are known as the Kramers-Kronig relations

$$\boxed{\mathcal{P}\int_{-\infty}^{\infty}\frac{\gamma''\left(\omega'\right)-\gamma''\left(\infty\right)}{\omega'-\omega}\frac{d\omega'}{\pi}=\gamma'\left(\omega\right)-\gamma'\left(\infty\right)} \tag{2.31}$$

$$\boxed{-\mathcal{P}\int_{-\infty}^{\infty}\frac{\gamma'\left(\omega'\right)-\gamma'\left(\infty\right)}{\omega'-\omega}\frac{d\omega'}{\pi}=\gamma''\left(\omega\right)-\gamma''\left(\infty\right).} \tag{2.32}$$

This is a very important result that applies to all causal response functions, such as optical conductivity, impedance of an electrical circuit, you name it. It means that if I know for all frequencies either the real or the imaginary part of a response functions, I can find the missing one with the Kramers-Kronig relations.

In practice then, if we know for example $\gamma''\left(\omega'\right)-\gamma''\left(\infty\right)$, we define the so-called spectral representation

$$\boxed{\gamma\left(z\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\gamma''\left(\omega'\right)-\gamma''\left(\infty\right)}{\omega'-z}} \tag{2.33}$$

where z is a complex variable. Taking $z = \omega + i\eta$ in the limit $\eta \to 0$ [1] we find

$$\gamma^R(\omega) = \lim_{\eta \to 0} \gamma(\omega + i\eta) \tag{2.34}$$

the causal, or retarded function $\gamma^R(\omega) = \gamma'(\omega) + i\gamma''(\omega)$ with real and imaginary parts that obey the Kramers-Kronig relation. To see that, it suffices to use the Sokhatsky-Weierstrass formula

$$\boxed{\lim_{\eta \to 0^+} \frac{1}{\omega \pm i\eta} = \lim_{\eta \to 0} \frac{\omega \mp i\eta}{\omega^2 + \eta^2} = \lim_{\eta \to 0} \left(\frac{\omega}{\omega^2 + \eta^2} \mp \frac{i\eta}{\omega^2 + \eta^2} \right)} \tag{2.35}$$

$$\boxed{\lim_{\eta \to 0^+} \frac{1}{\omega \pm i\eta} = \mathcal{P}\left(\frac{1}{\omega}\right) \mp i\pi\delta(\omega)} \tag{2.36}$$

which has meaning only when appearing in an integral, which is how we will use it. You can look at the first remark below and do Exercise (6.0.1).

Correspondingly, the advanced function is

$$\gamma^A(\omega) = \lim_{\eta \to 0} \gamma(\omega - i\eta). \tag{2.37}$$

It has poles only in the upper half of the complex plane because $\gamma''(\omega)$ in the spectral representation Eq. 2.33 is real. This function is acausal, in other words, the effect always happen before the cause.

Remark 3 *Another argument for the Sokhatsky-Weierstrass formula is the following. Using Cauchy's residue theorem in the following integral, we find*

$$\lim_{\eta \to 0^+} \int_{-\infty}^{\infty} \frac{\gamma(\omega') - \gamma(\infty)}{\omega' - \omega - i\eta} \frac{d\omega'}{2\pi} = i\left(\gamma(\omega) - \gamma(\infty)\right). \tag{2.38}$$

because there is only one pole in the upper half-plane and it is at $\omega + i\eta$ if $\gamma(\omega')$ is causal so that its extension in the upper half-plane is analytic. We can set $\lim_{\eta \to 0} \gamma(\omega + i\eta) = \gamma(\omega)$ without problem because, again, $\gamma(\omega)$ is analytic in the upper half-plane. We recover the previous two equations (2.31) and (2.32) by using the Sokhatsky-Weierstrass formula. Indeed, our integral in Eq.(2.38) then becomes

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{\gamma(\omega') - \gamma(\infty)}{\omega' - \omega} \frac{d\omega'}{2\pi} + \frac{1}{2} i\left(\gamma(\omega) - \gamma(\infty)\right) = i\left(\gamma(\omega) - \gamma(\infty)\right). \tag{2.39}$$

which, using the definition $\gamma(\omega) = \gamma'(\omega) + i\gamma''(\omega)$ and taking the real and imaginary parts of previous equation, recovers the Kramers Kronig relation Eqs. (2.31) and (2.32). Given that these two equations have already been proven, we can see the last derivation as a proof that the Sokhatsky-Weierstrass formula is consistent with what we know from Kramers-Kronig. Working backwards, we can start from the first equation (2.38), assume that Kramers Kronig are satisfied and deduce that Sokhatsky-Weierstrass formula must be true.

Remark 4 *While strictly speaking all frequencies contribute, in practice the integrand shows that the real part at a given frequency is mainly determined by the imaginary part in a close frequency range and vice-versa.*

Remark 5 *Each of (2.31) and (2.32) is called a Hilbert transform. Like Fourier transforms, we see that, apart from a sign, the Hilbert transform of a Hilbert transform is the identity, in other words the Hilbert transform is an involution. One can see the Hilbert transform as the unique way of extending a function of a real variable, say $\gamma''(\omega)$, into a function equal to $\gamma(\omega) = \gamma'(\omega) + i\gamma''(\omega)$ on the real axis that is analytic when extended in the complex half-plane.*

[1] We will always take η as a real, positive infinitesimal.

Remark 6 *The absorption, here described by $\gamma'(\omega)$, always decays to zero with frequency at high frequency. This will become clearer later, but it is intuitively clear that there is no eigenmode available to absorb energy at high enough frequency.*

Remark 7 *Numerics: To evaluate a Hilbert transform numerically, one way to avoid the singularity is to do part of the job analytically. For example, you can write*

$$\mathcal{P}\int_a^b \frac{f(\omega')}{\omega'-\omega}\frac{d\omega'}{\pi} = \int_a^b \frac{f(\omega')-f(\omega)}{\omega'-\omega}\frac{d\omega'}{\pi} + f(\omega)\,\mathcal{P}\int_a^b \frac{1}{\omega'-\omega}\frac{d\omega'}{\pi} \tag{2.40}$$

where the limits a and b have to be chosen large enough that the result converges and where the principal part has been removed in front of the first integral since it does not have any singularity as long as $f(\omega)$ is differentiable once. The last integral can be performed analytically so that the final result is

$$\mathcal{P}\int_a^b \frac{f(\omega')}{\omega'-\omega}\frac{d\omega}{\pi} = \int_a^b \frac{f(\omega')-f(\omega)}{\omega'-\omega}\frac{d\omega}{\pi} + \frac{1}{\pi}f(\omega)\ln\left|\frac{\omega-b}{\omega-a}\right|. \tag{2.41}$$

It is important to recall that in the rest of these notes, starting immediately with the following section, I will mostly be concerned with response functions. For response functions, imaginary parts will generally be associated with dissipation and real parts with reactive response. There are exceptions. For example, it is the real part of the conductivity that leads to absorption, in analogy with our $\gamma'(\omega)$ here.

3. SUSCEPTIBILITY, PROPAGATOR: SOME GENERAL PROPERTIES

In this book, you will learn to "talk susceptibility". Susceptibilities are measurable quantities as we will see. In the quantum mechanical case of phonons the susceptibility will be a propagator, or a certain type of Green's function if you want. Most of the formal, exact properties of the susceptibility, or of the boson-type Green functions, are very general and easy to understand with our simple example of the harmonic oscillator. These properties include sum rules, Kramers-Kronig relation, positivity and the very important theorem that relates fluctuations to dissipation in the linear response regime.

I will introduce the retarded response function Eq. (3.4) that gives the amplitude of the response to a given external force, its spectral representation Eq. (3.18), the relation that is imposed by the fact that a passive system is necessarily dissipative Eq. 3.28 and finally the fluctuation-dissipation (or Nyquist's) theorem, that relates the dissipative response to fluctuations, as its name suggests.

3.1 Definition of the susceptibility and preview of some of its properties

Eq. (2.10), describing the response to an external force, can be written as

$$x(\omega) = \frac{1/m}{(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2)} F(\omega). \tag{3.1}$$

If we know the response to a driving force that is a delta function $\delta(t)$ in time, i.e. frequency independent, we can calculate the response for any force as we will see. It is useful to define the susceptibility, or propagator, $\chi^R(\omega)$, as follows:

$$x(\omega) = \chi^R(\omega) F(\omega) \tag{3.2}$$

$$\chi^R(\omega) \equiv \frac{1/m}{(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2)} \tag{3.3}$$

$\chi^R(\omega)$ is precisely the response to a driving force that is independent of frequency and equal to unity, which, in the time domain, is a delta function. The response is peaked around two frequencies, $\pm\omega_R$ when $\gamma(\omega)$ is taken small. The superscript R on the susceptibility reminds us that the response is "retarded", or causal if you wish.

Definition 2 *In the context of the harmonic oscillator, or more generally of a bosonic mode, one usually calls $\chi^R(\omega)$ a susceptibility. Since $\chi^R(t)$ describes the response to $\delta(t)$, mathematically it is a Green's function (also known as a propagator, for reasons we will see later).*

In the context of quantized lattice vibration, one encounters the propagator $\mathcal{D}^R(\omega)$ (which will have Bose statistics in the quantum case)

$$\boxed{\chi^R(\omega) = \mathcal{D}^R(\omega) \equiv \frac{1/m}{-\omega^2+\omega_0^2+2\omega_0\Pi^R(\omega)}} \tag{3.4}$$

where one can identify the so-called polarization operator Π^R as being equal to

$$\boxed{\Pi^R(\omega) = \frac{-i\omega\gamma(\omega)}{2\omega_0}.} \tag{3.5}$$

Definition 3 *It is usual to define*

$$\chi^R(\omega) = \chi'(\omega) + i\chi''(\omega) \tag{3.6}$$

where $\chi'(\omega)$ and $\chi''(\omega)$ are both real functions of a real variable ω.

Remark 8 *Since $\chi^R(\omega)$ is causal, it is real and imaginary parts must obey Kramers-Kronig relations, just like $\gamma(\omega)$.*

There are many properties of $\chi^R(\omega)$ that are worth noting:

- $\chi^R(\omega)$ represents the response to a driving force, hence it is causal and is thus analytic in the upper-half of the complex frequency plane. It has poles in the lower half-plane only, as one can check in the simple case where γ is a constant by referring to our previous results with the free oscillator, Eq.(2.5).
- The poles of $\chi^R(\omega)$ describe the response independently of the driving force. For example, at $\gamma(\omega) = 0$, the poles are at the natural frequency of the oscillator, ω_0. A pole corresponds to an infinite response to an infinitesimal force, hence they represent the collective modes of the system. If the pole is in the complex plane, then the imaginary part represents damping. This is a very general result that will come back over and over again.
- If $\gamma = 0$, we still want oscillations to damp out at infinity. That forces us to take $\omega \longrightarrow \omega + i\eta$ with η a positive infinitesimal part, consistent with what we found earlier from causality. The susceptibility $\chi^R(\omega)$,which contains both real and imaginary parts of the response, must be an analytic function in the upper half plane. Another way to see that is with the spectral representation

$$\chi^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - (\omega + i\eta)}. \tag{3.7}$$

  When there is no damping, $\chi''(\omega')$ is just a delta function since energy is absorbed only at the resonnant frequency.
- For rather deep reasons related to sum rules, $\gamma(\omega)$ cannot be frequency independent, as will be demonstrated in exercice (6.0.3). It vanishes at infinity, as I will show in the specific example of the Caldeira-Leggett model. Which leads us to the next property.
- Note that at high frequency, the response is that of a free particle, $\chi^R(\omega) = \mathcal{D}^R(\omega) \approx \frac{1}{-m\omega^2}$.When we derive the results quantum mechanically, we will see that a few of the coefficients of the expansion in powers of $1/\omega^{2n}$ can often be calculated exactly.
- In a section 3.3 below, we will see that $2k_BT\omega\chi''(\omega) = \omega^2 S_{xx}(\omega)$ where $S_{xx}(\omega)$ is an even function of ω that represents fluctuations.

- In the quantum mechanical case, we will see that even though $S_{xx}(\omega)$ is not even or odd with respect to a change of sign of ω, $\chi''(\omega)$ itself remains odd.
- $\omega\chi''(\omega) > 0$. This follows from the positivity of the dissipation, as will be seen in Sec. 3.3
- As we discuss in the quantum mechanical derivation Sec. 10.3, $\chi''(\omega)$ itself is odd, namely $\chi''(\omega) = -\chi''(-\omega)$. The latter statement is consistent with a) the positivity of dissipation, $\omega\chi''(\omega) > 0$, and b) with the fact that $\gamma(\omega)$ cannot change sign if causality is to be respected (See Eq.(3.29))

3.2 Real-time version of the retarded susceptibility

Eq.(3.2) $x(\omega) = \chi^R(\omega) F(\omega)$ for the response to an external force is, using the convolution theorem, equivalent to

$$x(t) = \int_{-\infty}^{\infty} dt' \chi^R(t-t') F(t'). \tag{3.8}$$

Because $\chi^R(t)$ is causal, its Fourier transform must be analytic in the upper half-plane and have a spectral representation of the form

$$\boxed{\chi^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - (\omega + i\eta)},} \tag{3.9}$$

or, equivalently it must satisfy the Kramers Kronig formulas (2.31) and (2.32)

$$\boxed{\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi''(\omega)}{\omega' - \omega}\frac{d\omega}{\pi} = \chi'(\omega)} \tag{3.10}$$

$$\boxed{-\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi'(\omega)}{\omega' - \omega}\frac{d\omega}{\pi} = \chi''(\omega).} \tag{3.11}$$

Definition 4 *The spectral representation for the retarded susceptibility is Eq.(3.9).*

Let us now have a look at what $\chi^R(\omega)$ looks like in time. This will be useful when we do linear response theory in the quantum case. We just need to work out the Fourier transform

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\chi''(\omega')}{\omega' - (\omega + i\eta)}. \tag{3.12}$$

If t is less than zero, we must complete the contour in the upper half-plane since it is there that $e^{-i\omega t}$ is convergent, and we obtain zero because of the absence of poles in that half-plane. If t is larger than zero, we must complete the contour in the lower half-plane and there is a single pole there. This means that, using the residue theorem Eq. (2.19)

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi^R(\omega) = \left[\frac{2\pi i}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} e^{-i(\omega' - i\eta)t} \chi''(\omega')\right] \theta(t) = 2i\chi''(t)\theta(t) e^{-\eta t} \tag{3.13}$$

or

$$\boxed{\chi^R(t) = 2i\chi''(t)\theta(t) e^{-\eta t}.} \tag{3.14}$$

This vanishes at infinite time. In other words, we can write the retarded response Eq. (3.8) in real time in the form

$$x(t) = 2i \int_{-\infty}^{\infty} dt' \chi''(t-t')\,\theta(t-t')\,e^{-\eta(t-t')} F(t')\,. \tag{3.15}$$

Remark 9 *We can interpret the infinitesimal damping as the physical statement that a force at time t' cannot influence the response at a time t infinitely larger than t' in any physical system that interacts ever so weakly with its environment.*

Remark 10 *Another way that is often used to justify the above results is to take time t finite and η infinitesimal in such as way that $\eta t \to 0$. Then $e^{-\eta(t-t')}$ becomes $e^{\eta t'}$ and it is as if the force $e^{\eta t'} F(t')$ was "turned on" adiabatically from $t' = -\infty$ (where we cannot set $\eta t'$ to zero).*

Remark 11 *Numerics: Fast Fourier transforms and the real-time expression Eq. (3.14) provide another convenient way of doing Kramers Kronig transformations.*

As long as we take the limit $\eta \to 0$ at the end of calculations only, it is always possible to go back and forth between functions in time and in frequency using Fourier transforms. To show this, let us start from $\chi^R(t)$ in Eq. (3.14) and find its Fourier transform

$$\chi^R(\omega) = 2i \int_{-\infty}^{\infty} dt e^{i\omega t} \chi''(t)\,\theta(t)\,e^{-\eta t} = 2i \int_0^{\infty} dt e^{i(\omega+i\eta)t} \chi''(t)\,. \tag{3.16}$$

The last expression is a Laplace transform, often used in engineering. Using the Fourier representation for χ'', it follows that

$$\begin{aligned}
\chi^R(\omega) &= 2i \int_0^{\infty} dt e^{i(\omega+i\eta)t} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t} \chi''(\omega') \\
&= 2i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t} \left. \frac{\chi''(\omega')\, e^{i(\omega+i\eta)t}}{-i(\omega' - (\omega+i\eta))} \right|_{t=0}^{t=\infty} \\
&= \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - (\omega+i\eta)}.
\end{aligned}$$

which is what we set to prove. Using the Weirstrauss-Stokhaski formula, Eq. (2.36), the last result demonstrates that

$$\operatorname{Im} \chi^R(\omega) = \chi''(\omega)\,. \tag{3.17}$$

Remark 12 *Significance of $i\eta$: One can also see the choice of $i\eta$ as a choice of initial condition for the real-time version of the equation, as can be seen from the discussion in Section 144. If we had chosen $-i\eta$ instead, we would have obtained the advanced function, as is clear from the definition of the advanced function. .*

In general, one defines a function of a complex variable

$$\boxed{\chi(z) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - z}} \tag{3.18}$$

which becomes the retarded function, $\chi^R(\omega)$ when $z = \omega + i\eta$ and the advanced function $\chi^A(\omega)$ when $z = \omega - i\eta$, in complete analogy with what we did for the damping Eq. (2.33) earlier. Note that $\chi(z)$ has a branch cut along the real axis and that the discontinuity across that branch cut is $2\chi''(\omega)$.

$$\chi^R(\omega) - \chi^A(\omega) = 2i\chi''(\omega) \tag{3.19}$$

Remark 13 *The concept of branch cut probably brings to mind the concept of Riemann sheets. Depending on $\chi''(\omega')$, the function $\chi(z)$ could be extended or not to several Riemann sheets. The concept of Riemann sheets in our context is never used.*

Definition 5 *The quantity $\chi''(\omega)$ in the context of the spectral representation is called a spectral weight.*

Remark 14 *The real-time version of the response, Eq. (3.14) shows that all the physics is contained in the spectral weight χ''.*

3.3 Positivity of the power absorbed, implies that $\omega\chi''(\omega)$ is positive

The first constraint we can impose is that the work done by the external force is positive. While for a short instant we can absorb energy from a system, entropy considerations force us to impose that on average we can only dissipate energy in the system. This will have the important consequence that $\omega\chi''(\omega) \geq 0$, as we now proceed to demonstrate. The work done by the external force is

$$dW(t) = F(t)\, dx(t) \tag{3.20}$$

so that

$$\frac{dW}{dt} = F(t)\frac{dx(t)}{dt}. \tag{3.21}$$

Taking a single harmonic component $F(t) = \mathrm{Re}\left(F(\omega)\, e^{-i\omega t}\right)$, we define the average power density $P(\omega)$ in that frequency interval by

$$P(\omega)\frac{d\omega}{2\pi} = \lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}\frac{dW}{dt}dt \tag{3.22}$$

$$= \lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}F(t)\frac{dx(t)}{dt}dt \tag{3.23}$$

where $\mathcal{T}$ is some large time over which we average. It determines the bandwidth. Substituting our expression $\mathrm{Re}\left(F(\omega)\, e^{-i\omega t}\right)$ for the force, we obtain

$$P(\omega)\frac{d\omega}{2\pi} = \mathrm{Re}\left[F(\omega)\lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}e^{-i\omega t}\frac{dx(t)}{dt}dt\right]. \tag{3.24}$$

Integrating by parts, assuming periodic boundary conditions so that the integrated term vanishes,

$$P(\omega)\frac{d\omega}{2\pi} = \mathrm{Re}\left[F(\omega)\lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}(i\omega)\left(\int_{-\mathcal{T}/2}^{\mathcal{T}/2}e^{-i\omega t}x(t)\,dt\right)\right]$$

$$P(\omega) = -\mathrm{Im}\left[F(\omega)\,\omega x^*(\omega)\right] \tag{3.25}$$

By analogy with quantization in a box,we have used $d\omega = 2\pi/\mathcal{T}$. Since $x(t)$ is real, we also used $x(-\omega) = x^*(\omega)$. Since the definition of the susceptibility Eq.(3.2) gives us $x^*(\omega) = \chi^{R*}(\omega)\, F^*(\omega)$, we find

$$P(\omega) = -\mathrm{Im}\left[F(\omega)\,\omega\chi^{R*}(\omega)\, F^*(\omega)\right] \tag{3.26}$$

$$= |F(\omega)|^2\,\omega\chi''(\omega). \tag{3.27}$$

Hence, since $P(\omega)$ is positive, the product $\omega\chi''(\omega)$ is also positive. The result

$$\boxed{\omega\chi''(\omega) \geq 0} \tag{3.28}$$

is general and important.

There is a consequence of this on the damping $\gamma(\omega)$. Our expression for the susceptibility Eq.(3.3), tells us that

$$\chi''(\omega) = \frac{1}{m} \frac{\omega\gamma'(\omega)}{\left(-\omega^2 + \omega_0^2 + \omega\gamma''(\omega)\right)^2 + \left(\omega\gamma'(\omega)\right)^2} \tag{3.29}$$

which means that

$$\boxed{\gamma'(\omega) \geq 0}$$

if we want to impose that heat cannot be transformed into work without an additional cold reservoir. An external force doing work on a system can only dissipate energy into heat, as required by the second law of thermodynamics.

Remark 15 *When γ is a constant, as in the simple phenomenological model, the positivity of γ is obvious from Eq.(2.8) for the general solution since if γ were negative, it would also have led to a displacement that amplifies without applied external force. That positivity must obviously be satisfied at all frequencies.*

Remark 16 *The definition of susceptibility, Eq. (3.6) $\chi = \chi' + i\chi''$ suggests that the response that is out of phase by $\pi/2$ with respect to the force is χ'', the imaginary part. And our experience with the simple harmonic oscillator tells us that this is where absorption occurs.*

4. DISSIPATION AND IRREVERSIBILITY EMERGE IN THE LIMIT OF AN INFINITE NUMBER OF DEGREES OF FREEDOM

Looking at the problem of coupled harmonic oscillators, we will discover in this Chapter that in the limit where there is an infinite number of oscillators, irreversibility appears. Otherwise, the motion is periodic, or quasi-periodic.[1] This is a very general result that demonstrates in a very simple context how irreversibility emerges in the limit of an infinite number of degrees of freedom. The model in Fig. (4-1) that we consider will give us Eq. (4.14) which allows us to explain how damping comes about. In practice, if we take the infinite-size limit before we take the $\eta \to 0$ limit, the response of the system will be irreversible.

4.1 Example of an oscillator attached to a bath of harmonic oscillators: A model in the Caldeira-Leggett category

This model is a classical analog of what is known as the Caldeira-Leggett[47] model [47] that was used to include the effect of dissipation on the tunneling of a macroscopic but quantum degree of freedom, namely the phase of a superconducting Josephson junction. The fermionic analog of this problem plays an important role in dynamical mean-field theory.

This is the case of a harmonic oscillator attached to a one-dimensional chain of harmonic oscillators that plays the role of a bath or of a reservoir if you wish.

[1] The periodic motion in the case of a finite number of degrees of freedom reminds us of Rabi oscillations in quantum optics, although the analogy cannot be taken litterally

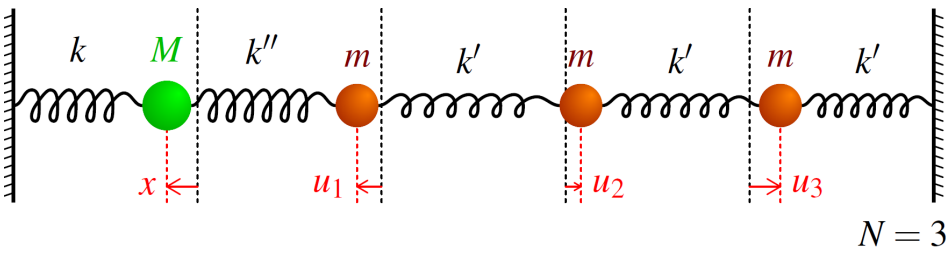


Figure 4-1 An oscillator of mass M is attached to a one-dimensional chain of oscillators that play the role of a bath. There are $N = 3$ masses in that bath in this example.

As illustrated in Fig. (4-1) a mass M is attached on the left to a wall with a spring of constant k and on the right to a one-dimensional chain of oscillators. The deviation of the mass M with respect to equilibrium is denoted by x. Each of the masses m of the one-dimensional chain of oscillators is attached to its neighbor by a spring of constant k', except for the first link between M and m that I call k'' because it will play the role of a coupling constant between the bath and the mass M. The deviation from equilibrium of the mass at position i is u_i. A force F is also applied to the mass M. The potential energy is thus

$$V\left(x,\{u_i\}\right)=-Fx+\frac{1}{2}kx^2+\frac{k''}{2}\left(x-u_1\right)^2+\frac{k'}{2}\left(u_2-u_1\right)^2+\frac{k'}{2}\left(u_3-u_2\right)^2+\ldots, \tag{4.1}$$

from which, recalling that the force on particle i is $-\partial V/\partial u_i$, we find the following equations of motion in Fourier space (taking $\omega+i\eta$ as we know we need to do for causality):

$$\begin{aligned}
-M\left(\omega+i\eta\right)^2 x &= -kx-k''\left(x-u_1\right)+F && (4.2)\\
-m\left(\omega+i\eta\right)^2 u_1 &= -k''\left(u_1-x\right)-k'\left(u_1-u_2\right) && (4.3)\\
-m\left(\omega+i\eta\right)^2 u_2 &= -k'\left(u_2-u_1\right)-k'\left(u_2-u_3\right) && (4.4)\\
&\ldots && (4.5)
\end{aligned}$$

With the definition $z=\omega+i\eta$ these equations take the following form in matrix notation:

$$\begin{bmatrix}
-Mz^2+(k+k'') & -k'' & 0 & 0 & \ldots & 0\\
-k'' & -mz^2+k'+k'' & -k' & 0 & \ldots & 0\\
0 & -k' & -mz^2+2k' & -k' & \ldots & 0\\
\ldots & \ldots & \ldots & \ldots & \ldots & \\
\ldots & \ldots & \ldots & \ldots & \ldots & \\
0 & 0 & 0 & \ldots & -k' & -mz^2+2k'
\end{bmatrix}
\begin{bmatrix} x\\ u_1\\ u_2\\ \ldots\\ \ldots\\ u_N \end{bmatrix}
=
\begin{bmatrix} F\\ 0\\ 0\\ \ldots\\ \ldots\\ 0 \end{bmatrix}. \tag{4.6}$$

Using the definition of the propagator in Eqs. (3.2) and (3.3) we rewrite the following shorthand

$$\begin{bmatrix} \mathcal{D}_0^{-1}(z) & V^T\\ V & \mathcal{D}_b^{-1}(z) \end{bmatrix}\begin{bmatrix} x\\ u \end{bmatrix}=\begin{bmatrix} F\\ 0 \end{bmatrix} \tag{4.7}$$

where $\mathcal{D}_0^{-1}(z)=-Mz^2+(k+k')$ is a scalar, V is a $N\times 1$ vector, V^T is its transpose, $\mathcal{D}_b^{-1}(z)$ is an $N\times N$ matrix for the bath, and u is a vector whose N components are u_i. The bottom block can easily be solved for u as follows in matrix notation, with Einstein summation implied

$$u^a=-\mathcal{D}_b^{ab}(z)\,V^b x. \tag{4.8}$$

Substituting in the first line we find

$$x=\left(\mathcal{D}_0^{-1}(z)-V^T\mathcal{D}_b(z)\,V\right)^{-1}F, \tag{4.9}$$

where $\left(\mathcal{D}_0^{-1}(z)-V^T\mathcal{D}_b(z)\,V\right)$ is a scalar. In the case where there are no degrees of freedom in the bath, there is a single pair of eigenfrequencies at $\mathcal{D}_0^{-1}(z)=0$, i.e. two poles infinitesimally close to the real axis at $\omega+i\eta=\pm\sqrt{(k+k'')/M}$. In the presence of the bath, there will be $N+1$ pairs of poles. We can see that more explicitly as follows.

Defining K as the real symmetric matrix of spring constants, we have

$$\mathcal{D}_b^{-1}(z)=\sqrt{m}\left(-z^2+\frac{1}{\sqrt{m}}K\frac{1}{\sqrt{m}}\right)\sqrt{m}. \tag{4.10}$$

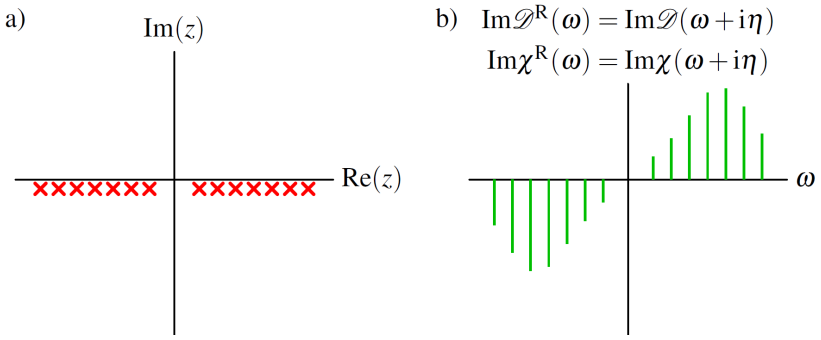


Figure 4-2 a) Poles of retarded susceptibility for $N = 6$ particles in the bath. b) The corresponding value of the imaginary part of the susceptibility on the real axis.

Let O the orthogonal matrix that diagonalizes $\frac{1}{\sqrt{m}}K\frac{1}{\sqrt{m}}$, then[2] $\frac{1}{\sqrt{m}}K\frac{1}{\sqrt{m}} = O^T D O$, and

$$\mathcal{D}_b^{-1}(z) = \sqrt{m}O^T\left(-z^2 + D\right)O\sqrt{m} \tag{4.11}$$

$$\mathcal{D}_b(z) = \frac{1}{\sqrt{m}}O^T\left(-z^2 + D\right)^{-1}O\frac{1}{\sqrt{m}} \tag{4.12}$$

so that the propagator Eq. (4.9) with the bath is now

$$\mathcal{D}(z) = \left(\mathcal{D}_0^{-1}(z) - T^T\left(-z^2 + D\right)^{-1}T\right)^{-1} \tag{4.13}$$

where we defined the $N \times 1$ vector $T = O\frac{1}{\sqrt{m}}V$. Since V has units of a spring constant and O is dimensionless, T has units of $\sqrt{k}\omega$. Labeling the eigenvalues by α, the poles in the presence of the bath are then given by the solution to

$$\boxed{-M(\omega + i\eta)^2 + (k + k'') - \sum_{\alpha=1}^{N} T_\alpha \frac{1}{-(\omega+i\eta)^2+\omega_\alpha^2} T_a = 0.} \tag{4.14}$$

Rewriting with a common denominator, you see that we are looking for the zeros of a polynomial of order $N+1$ in $(\omega + i\eta)^2$. The propagator will have $N+1$ pairs of poles located symmetrically about the imaginary axis in the lower half plane, infinitesimally close to the real axis, as illustrated in Fig.(4-2a).

Any motion of the mass M can be written as a sum of oscillations at discrete frequencies. The motion may look complicated because the frequencies may not be commensurable, but it is in principle periodic. Physically, the mass M in the presence of the bath is a finite system and a disturbance will oscillate back and forth.

To see that the imaginary part of the retarded propagator, or susceptibility, is odd in frequency, note the retarded propagator, defined by $x(\omega) = \mathcal{D}^R(\omega)F(\omega)$ can be rewritten as

$$\mathcal{D}^R(\omega) = \chi^R(\omega) = \lim_{\eta\to 0} \frac{1/M}{-(\omega + i\eta)^2 + \frac{(k+k'')}{M} - \frac{1}{M}\sum_{\alpha=1}^{N} T_\alpha \frac{1}{2\omega_\alpha}\left[\frac{1}{\omega+i\eta+\omega_\alpha} - \frac{1}{\omega+i\eta-\omega_\alpha}\right]T_a^T} \tag{4.15}$$

so that it may look like Fig.(4-2b) where I represent the weight of the delta function for some case.

[2] This notation suggests how to take into account the general case where the masses are all different. Then, m is simply a diagonal matrix.

Remark 17 *The effective equation that we obtained for the coordinate x takes into account the one-dimensional set of oscillators, that acts like a "bath" or reservoir. We have "integrated out" the bath, to obtain an equation of motion for the degree of liberty that we are interested in. The result, Eq. (4.14) contains $V\mathcal{D}_b(z)V^T$ that will be called a hybridization function in the context of the Anderson impurity problem that arises in dynamical mean-field theory. Also, $\mathcal{D}_b(z)$ is a propagator in the bath. It takes into account that a wave produced by a motion of x can go in the one-dimensional bath and come back in a retarded way later.*

Remark 18 *In mathematics, $\mathcal{D}_0^{-1}(z) - V\mathcal{D}_b(z)V^T$ is known as the Schur complement of $\mathcal{D}_0^{-1}(z)$.*

4.2 Irreversibity emerges in the limit of an infinite bath

What happens if the bath is infinite? Then, it looks as if the mass M was attached to some sort of infinite transmission line. A disturbance will propagate in the bath and never come back. This is how irreversibility arises. Mathematically, it is as if the motion was now represented by Fourier transforms instead of Fourier series.

Let us go back to our expression Eq. (4.14) for the poles of $\mathcal{D}(z)$ in the presence of the bath. If we take the number of degrees of freedom of the bath N to infinity, the poles are located at $\mathcal{D}^{-1}(z) = 0$, namely

$$M^{-1}\mathcal{D}^{-1}(\omega + i\eta) = -(\omega + i\eta)^2 + \omega_0^2 - \int_0^\infty N(\Omega^2)\frac{1}{-(\omega + i\eta)^2 + \Omega^2}d(\Omega^2) = 0 \tag{4.16}$$

where we defined the "bare" frequency $\omega_0^2 = (k + k'')/M$ and the bath density of states, in the limit $\eta \to 0$,by

$$N(\Omega^2) = \frac{1}{M}\sum_{\alpha=1}^{N}\delta(\Omega^2 - \omega_\alpha^2)T_\alpha T_a^T. \tag{4.17}$$

In the limit where the number of eigenmodes goes to infinity, the coupling to the mass M represented by $T_\alpha T_a^T$ will scale as $1/N$, in other words, the more modes there are, the smaller the coupling to any given mode if we want a well defined continuum limit. Then $\frac{1}{N}\sum_{\alpha=1}^{N}$ can be transformed to an integral, and $N(\Omega^2)$ becomes a continuous function.

Remark 19 *Another way to look at this is to return to a finite η, in other words to the Lorentzian representation of the delta function. If within a width η there are many modes ω_α, then the function $N(\Omega^2)$ appears continuous. It is with a continuous $N(\Omega^2)$ that irreversibility appears as we shall see. In other words, if we take the limit of an infinite bath before the limit $\eta \to 0$, we introduce irreversibility.*

Remark 20 *This representation in terms of sum over poles is the equivalent of the spectral representation discussed in Chapter 3.2.*

Let us continue our derivation. We will see that any damping function $\gamma(\omega)$ can be represented by an appropriately constructed infinite bath. Since

$$\frac{1}{-(\omega + i\eta)^2 + \Omega^2} = \frac{1}{2\Omega}\left(\frac{1}{\omega + i\eta + \Omega} - \frac{1}{\omega + i\eta - \Omega}\right), \tag{4.18}$$

Eq. (4.16) for the poles in the presence of an infinite bath becomes,

$$-\omega^2+\omega_0^2-\mathcal{P}\int_0^\infty \frac{N\left(\Omega^2\right)}{2\Omega}\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)2\Omega d\Omega \tag{4.19}$$

$$+i\pi\int_0^\infty \frac{N\left(\Omega^2\right)}{2\Omega}\left(\delta\left(\omega+\Omega\right)-\delta\left(\omega-\Omega\right)\right)2\Omega d\Omega=0. \tag{4.20}$$

Several things have happened here. I have used the Sokhatsky-Weierstrass formula Eq. (2.36) inside the integral, and I have removed the $+i\eta$ in the first term since it is no longer necessary, as we see from performing the last integral. Indeed, you can see that we obtain

$$-\omega^2+\omega_0^2-\mathcal{P}\int_0^\infty N\left(\Omega^2\right)\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)d\Omega \tag{4.21}$$

$$-i\pi N\left(\omega^2\right)\left(\theta\left(\omega\right)-\theta\left(-\omega\right)\right)=0 \tag{4.22}$$

where $\theta\left(\omega\right)$ is Heaviside's theta function that, I recall, equals unity for ω positive and 0 otherwise. Since we saw that $N\left(\omega^2\right)>0$, we can define

$$\pi N\left(\omega^2\right)\left(\theta\left(\omega\right)-\theta\left(-\omega\right)\right)=\omega\gamma'\left(\omega\right) \tag{4.23}$$

where $\gamma'\left(\omega\right)>0$ is a real even function. By taking an infinite number of oscillators and assuming that this leads to a smooth $N\left(\omega^2\right)$ we introduced irreversibility. Mathematically, this was achieved by going from a discrete sum to an integral. The propagator can thus be written as

$$\mathcal{D}^R\left(\omega\right)=\frac{1/M}{-\omega^2+\omega_0^2-\mathcal{P}\int_0^\infty N\left(\Omega^2\right)\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)d\Omega-i\omega\gamma'\left(\omega\right)} \tag{4.24}$$

which corresponds to our general form Eqs. (3.4) and (3.5).

The frequency dependence of the damping will depend on the nature of the bath. If we can assume that $\gamma'\left(\omega\right)$ is independent of frequency in an interval around ω_0, we see that we recover the simple damped harmonic oscillator. In reality, unless the eigenenergies of the bath can become infinite, $\gamma'\left(\omega\right)$ vanishes at infinity. That can be seen from the definition of $N\left(\Omega^2\right)$ in Eq.(4.17) and its relation to γ' in Eq.(4.23). At high enough frequency, there will be no eigenmodes in the one-dimensional bath formed by the chain of masses and springs. The renormalization of the bare frequency coming from the principal part integral will also then vanish at ω infinity, meaning that in this limit we recover free-particle behavior, as expected.

Irreversibility is discussed further in Exercise (6.0.4).

Remark 21 *Order of limits: It is very important to take the infinite volume, or infinite bath limit, before we take the $\eta\longrightarrow 0$ limit. These limits do not commute. We can physically understand that this is the proper limit by noticing that the separation of levels in a large system will always be smaller than the inverse time we have to measure accurately, or if you want to make an accurate Fourier transform.*

Remark 22 *As argued before, $\chi''\left(\omega\right)=\operatorname{Im}\chi^R\left(\omega\right)=\operatorname{Im}\mathcal{D}^R\left(\omega\right)$ is an odd function of frequency.*

Remark 23 *As we saw above, partial fractions allow us to write*

$$\begin{aligned}\int_0^\infty N\left(\Omega^2\right)\frac{1}{-\left(\omega+i\eta\right)^2+\Omega^2}d\left(\Omega^2\right) &= \int_0^\infty N\left(\Omega^2\right)\frac{1}{2\Omega}\left(\frac{1}{\omega+i\eta+\Omega}-\frac{1}{\omega+i\eta-\Omega}\right)d\left(\Omega^2\right)\\ &= \int_{-\infty}^\infty N\left(\Omega^2\right)\frac{1}{\Omega-\left(\omega+i\eta\right)}\operatorname{sgn}\left(\Omega\right)\,d\left(\Omega\right),\end{aligned} \tag{4.25}$$

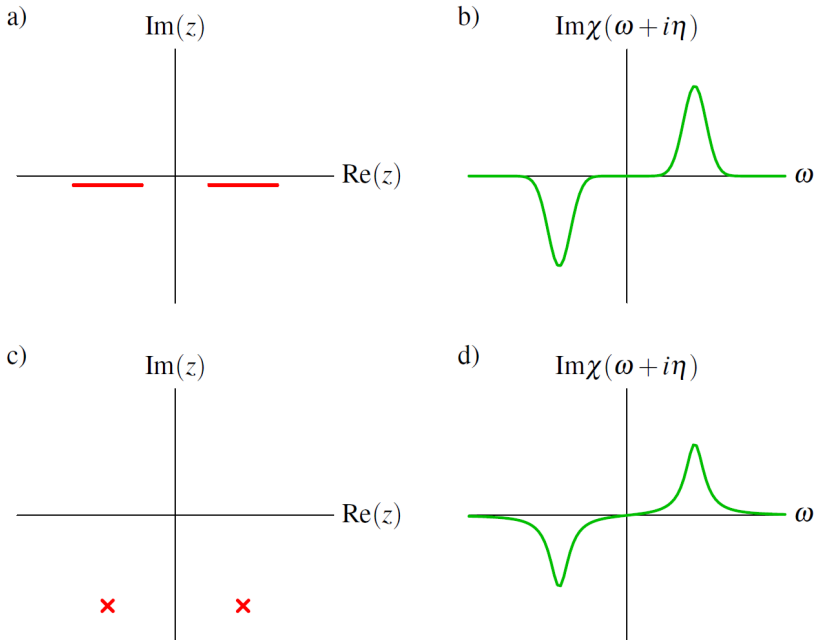


Figure 4-3 a) In the limit of an infinite bath, the retarded susceptibility $\chi^R(\omega) = \mathcal{D}^R(\omega)$ has cuts in the lower half-plane. b) The value of its imaginary part on the real axis is given by an odd continuous function. c) Pole structure of the retarded susceptibility when its imaginary part is approximated by Lorentzians as in d).

which shows the relation to the spectral representation of the damping, Eq. (2.33) since the correspondance between our starting point Eq. (4.16) and the phenomenological oscillator model Eq. (2.22) shows that the above quantity is $i\omega\gamma(\omega)$.

Remark 24 *As you can see from Eq.(4.17), unless the eigenfrequencies of the bath do not vanish at infinity,* $\gamma'(\omega)$ *vanishes at infinity in such a way that all sum rules will be satisfied, contrary to the problem encountered in exercice (6.0.3) with the simple harmonic oscillator.*

Remark 25 *The real and imaginary parts of the integral in Eq. (4.16) are related by Kramers-Kronig relations, in other words, damping and frequency renormalization are related by these relations, as we found above for* $\gamma(\omega)$ *in Sec. (2.3) above.*

Remark 26 *It is important to notice that the results above imply that any* $\gamma(\omega)$ *can be mimicked by an appropriately built infinite bath.*

Remark 27 *Fig. (4-3a) shows that in the infinite size limit, the poles of infinitesimally below the real axis collapse into a branch cut. The corresponding imaginary part of the susceptibility in Fig. (4-3b) is a continuous function. If we decide to approximate this continuous function by two Lorentzians, as in Fig. (4-3d) then the pole structure changes. There are now only two isolated poles far below the real axis as in Fig. (4-3c). The fact that the poles are no longer close to the real axis is often not a problem. We are just approximating continuous function representing the imaginary part of the susceptibility differently. However, the Lorentzian approximation has problems at high frequency so that sum rules can be violated.*

Remark 28 *We will encounter a similar problem for the so-called quantum impurity. The non-interacting bath will also be described by a "hybridization function"*

which will be the analog of

$$\int_0^\infty N\left(\Omega^2\right)\frac{1}{-\left(\omega+i\eta\right)^2+\Omega^2}d\left(\Omega^2\right)=\sum_{\alpha=1}^{N}T_\alpha\frac{1}{-\left(\omega+i\eta\right)^2+\omega_\alpha^2}T_a^T\ . \tag{4.26}$$

4.3 *Fluctuations and dissipation are related

There is a very deep relation between fluctuations and the damping observed in response to an external force, as long as that response is linear in the external force. That is what we discuss here. There are marked differences with the quantum case in the derivation I am going to give, although it is possible to obtain more closely related derivations. The quantum result we will reduce to the classical one in the limit $\hbar\omega \ll k_BT$, as expected for the classical limit of a simple undamped classical harmonic oscillator.

Experimentalists can measure the electrical noise of a resistor for example. In such a case, they would characterize the noise by taking the modulus square of the Fourier transform of the signal. They can repeat the measurement several times and average that modulus square over measurements, which for us corresponds to taking a thermal average, represented here by the symbol $\langle\ \rangle$. This is the usual canonical ensemble thermal average you are used to, the one that leads to the equipartition theorem for variables entering quadratically in the Hamiltonian. There are other ways correlation functions of this type can be measured, as we will see in the next chapter.

I will want to use the equipatition theorem. Since whatever the nature of the bath, the kinetic energy will enter quadratically in the Hamiltonian, it is the velocity of the mass M that we will be interested in.

In short, the measurement mentioned above corresponds to the following correlation function

$$\begin{aligned}\left\langle \dot{x}\left(\omega\right)\dot{x}\left(-\omega\right)\right\rangle &= \left\langle \dot{x}\left(\omega\right)\dot{x}^*\left(\omega\right)\right\rangle &(4.27)\\ &= \left\langle \int_{-\infty}^{\infty}e^{i\omega t}\frac{dx\left(t\right)}{dt}dt\int_{-\infty}^{\infty}e^{-i\omega t'}\frac{dx\left(t'\right)}{dt}dt'\right\rangle &(4.28)\\ &= \mathcal{T}\int_{-\infty}^{\infty}e^{i\omega\left(t-t'\right)}\left\langle \dot{x}\left(t\right)\dot{x}\left(t'\right)\right\rangle d\left(t-t'\right). &(4.29)\end{aligned}$$

To obtain the above result, we have changed integration variables to $t-t'$ and $\left(t+t'\right)/2$ and used the fact that in equilibrium we have time-translation invariance. This transforms the integral over $\left(t+t'\right)/2$ into the total time $\mathcal{T}$. Using time translational invariance $\left\langle \dot{x}\left(t\right)\dot{x}\left(t'\right)\right\rangle = \left\langle \dot{x}\left(t-t'\right)\dot{x}\left(0\right)\right\rangle$.

Remark 29 *A famous fluctuation-dissipation theorem is that by Nyquist that relates the voltage fluctuations, measured as above, to resistance. More specifically,* $\left\langle V\left(\omega\right)V\left(-\omega\right)\right\rangle = \mathcal{T}\ 2R\ k_BT$. *where* $V\left(\omega\right)$ *is a measured fluctuating voltage and* $V\left(-\omega\right)=V^*\left(\omega\right)$ *since* $V\left(t\right)$ *is real.*

The final result we are looking for is

$$\boxed{\frac{M}{\mathcal{T}}\left\langle \dot{x}\left(\omega\right)\dot{x}\left(-\omega\right)\right\rangle = S_{\dot{x}\dot{x}}\left(\omega\right)=\frac{2k_B\mathcal{T}}{\omega}\chi''_{\dot{x}\dot{x}}\left(\omega\right)} \tag{4.30}$$

//To compute the integral we change integration variable and divide it in two parts

$$\left\langle \dot{x}\left(\omega\right)\dot{x}\left(-\omega\right)\right\rangle = \mathcal{T}\int_0^\infty e^{i\omega t}\left\langle \dot{x}\left(t\right)\dot{x}\left(0\right)\right\rangle dt+\mathcal{T}\int_{-\infty}^{0}e^{i\omega t}\left\langle \dot{x}\left(t\right)\dot{x}\left(0\right)\right\rangle dt. \tag{4.31}$$

In the first integral, we can replace $\dot{x}(t)$ by $\int_0^t \chi^R_{\dot{x}\dot{x}}(t')\,\dot{x}(0)\,dt'$, where $\chi^R_{\dot{x}\dot{x}}(t)$ is the susceptibility for the velocity $v = \dot{x}$. The first term becomes

$$\int_0^\infty e^{i\omega t}\left(\int_0^t \chi^R_{\dot{x}\dot{x}}(t')\,dt'\right)dt\ \langle \dot{x}(0)\,\dot{x}(0)\rangle\,. \tag{4.32}$$

Focussing on the integral, integrating by parts,

$$\begin{aligned}\int_0^\infty e^{i\omega t}\left(\int_0^t \chi^R_{\dot{x}\dot{x}}(t')\,dt'\right)dt &= \frac{e^{i\omega t}}{i\omega}\int_0^t \chi^R_{\dot{x}\dot{x}}(t')\,dt'\Big|_0^\infty - \int_0^\infty \frac{e^{i\omega t}}{i\omega}\chi^R_{\dot{x}\dot{x}}(t)dt &(4.33)\\ &= \frac{e^{i\omega\infty}}{i\omega}\int_0^\infty \chi^R_{\dot{x}\dot{x}}(t')\,dt' - \frac{1}{i\omega}\chi^R_{\dot{x}\dot{x}}(\omega)\,. &(4.34)\end{aligned}$$

The second term for $\langle \dot{x}(\omega)\,\dot{x}(-\omega)\rangle$ Eq. 4.29 involves time t smaller than 0. Here, we can invoque time reversal symmetry. If we look at the signal for fluctuations, we cannot tell whether time is running backwards or forward. So we simply have to use the advanced susceptibility. Or, equivalently, from time translational invariance and a change of variable we can use the previous result

$$\begin{aligned}\int_{-\infty}^0 e^{i\omega t}\langle \dot{x}(t)\,\dot{x}(0)\rangle\,dt &= \int_{-\infty}^0 e^{i\omega t}\langle \dot{x}(0)\,\dot{x}(-t)\rangle\,dt &(4.35)\\ &= \int_0^\infty e^{-i\omega t}\langle \dot{x}(0)\,\dot{x}(t)\rangle\,dt &(4.36)\\ &= \frac{e^{-i\omega\infty}}{i\omega}\int_0^\infty \chi^R_{\dot{x}\dot{x}}(t')\,dt' + \frac{1}{i\omega}\chi^R_{\dot{x}\dot{x}}(-\omega) &(4.37)\end{aligned}$$

where I have just made the replacement $\omega \to -\omega$ in the preceeding result. Note that because the velocity is a real variable as a function of time, $\chi^R_{\dot{x}\dot{x}}(-\omega) = \chi^{R*}_{\dot{x}\dot{x}}(\omega) = \chi^A_{\dot{x}\dot{x}}(\omega)$. Adding everything up, and using equipartition

$$\langle \dot{x}(0)\,\dot{x}(0)\rangle = \frac{k_B T}{M} \tag{4.38}$$

we have

$$\begin{aligned}\frac{M}{\mathcal{T}}\langle \dot{x}(\omega)\,\dot{x}(-\omega)\rangle &= \left(-\frac{1}{i\omega}\chi^R(\omega) + \frac{1}{i\omega}\chi^A(\omega)\right)M\langle \dot{x}(0)\,\dot{x}(0)\rangle &(4.39)\\ S_{\dot{x}\dot{x}}(\omega) &= \frac{i}{\omega}\left(\chi^R(\omega) - \chi^A(\omega)\right)k_B T = -\frac{2k_B T}{\omega}\chi''_{\dot{x}\dot{x}}(\omega) &(4.40)\end{aligned}$$

The minus sign is definitly wrong Q.E.D.

Remark 30 *We have tacitly assumed the so-called Onsager's regression hypothesis, namely that the fluctuations decay just like the macroscopic motion.*

4.4 *Fluctuations may also be seen as generated from fluctuating internal forces. and sum-rules come out naturally. The Langevin approach

If the fluctuations in x our caused by some spontaneously generated by internal forces that fluctuate, using our definition of the propagator, we can write

$$\begin{aligned} \langle x(\omega) x^*(\omega)\rangle &= \chi^R(\omega)\chi^{R*}(\omega)\left\langle |F_{in}(\omega)|^2\right\rangle & (4.41)\\ &= \frac{(1/m)^2}{\left(\omega^2-\omega_0^2+\omega\gamma''(\omega)\right)^2+\left(\omega\gamma'(\omega)\right)^2}\left\langle |F_{in}(\omega)|^2\right\rangle . & (4.42)\end{aligned}$$

Where $\left\langle |F_{in}(\omega)|^2\right\rangle$ is the spectrum of the internal force that I will find here in the simple case of a constant damping constant. It can also be found in the more general case of a frequency dependent damping constant by comparison with the result found in the previous section.

Remark 31 *The internal force F_{in} here is called a Langevin force. If the equation of motion is written with that force acting on the oscillator, it is known as a stochastic Langevin equation.*

One can use the equipartition theorem to determine the value of $\left\langle |F_{in}(\omega)|^2\right\rangle$. Indeed, in such a case, equipartition tells us that

$$\frac{1}{2}M\left\langle\left(\frac{dx}{dt}\right)^2\right\rangle=\frac{1}{2}k_BT. \tag{4.43}$$

The quantity in brackets is related to an integral over the correlation function. More specifically, taking the integral of the equation (4.29) that relates the correlation function in frequency and in time, we find, integrating by parts,

$$\begin{aligned}\int_{-\infty}^{\infty}\omega^2\langle x(\omega)x^*(\omega)\rangle\frac{d\omega}{2\pi} &= \mathcal{T}\left\langle\left(\frac{dx}{dt}\right)\left(\frac{dx}{dt}\right)\right\rangle\\ &= \mathcal{T}\frac{k_BT}{m} & (4.44)\end{aligned}$$

where again we assumed time-translational invariance, *i.e.* that $\langle x(t)x(t')\rangle$ is a function only of $t-t'$.

I will study only the case where $\gamma'=\gamma$ is a constant, i.e. when $\gamma(\omega)$ is independent of ω. In that case, we can assume that $\left\langle |F_{in}(\omega)|^2\right\rangle$ is independent of frequency. The integral can then be done as follows:

$$\begin{aligned}\int_{-\infty}^{\infty}\omega^2\langle x(\omega)x^*(\omega)\rangle\frac{d\omega}{2\pi} &= \int_{-\infty}^{\infty}\frac{(1/m)^2\omega^2}{\left(\omega^2-\omega_0^2\right)^2+(\omega\gamma)^2}\left\langle |F_{in}|^2\right\rangle\frac{d\omega}{2\pi} & (4.45)\\ &= \int_{-\infty}^{\infty}\frac{\omega^2}{m^2\omega\gamma}\mathrm{Im}\left[\frac{1}{-\omega^2+\omega_0^2-i\omega\gamma}\right]\left\langle |F_{in}|^2\right\rangle\frac{d\omega}{2\pi} & (4.46)\\ &= \int_{-\infty}^{\infty}\frac{\omega^2}{m^2\omega\gamma}\mathrm{Im}\left\{\frac{-1}{\left(\widetilde{\omega}^+-\widetilde{\omega}^-\right)}\left[\frac{1}{\omega-\widetilde{\omega}^+}\right.\right. & (4.47)\\ &\quad \left.\left.-\frac{1}{\omega-\widetilde{\omega}^-}\right]\right\}\left\langle |F_{in}|^2\right\rangle\frac{d\omega}{2\pi} & (4.48)\end{aligned}$$

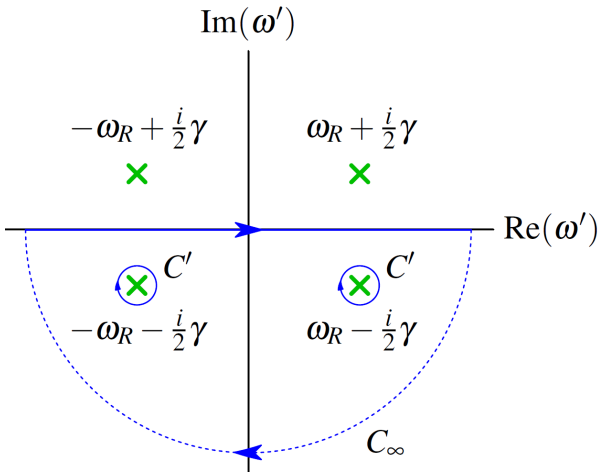


Figure 4-4 Pole structure of the imaginary part of the susceptibility. One can add the contour at infinity to the integral on the real axis. This closed contour can be deformed to the contour $\mathcal{C}'$ which goes around the two poles in the lower half-pane.

In the third line of that equation we have decomposed in partial fractions. The poles of the last integrand are those found in Eq.(2.7), $\widetilde{\omega}^{\pm} = -i\frac{\gamma}{2} \pm \omega_R$. Those of the integrand in the first line above are illustrated in Fig.(4-4).

The integral converges only if the all the terms implicit in taking the imaginary part are included. The original integral converges, so does the sum of all the terms, but not each of the terms individually. This means that if we decide to complete the contour, say, in the lower half-plane, we must do it for all the terms. We cannot complete the contour in the lower half-plane for some of the terms, and in the upper half-plane for others. There is no contribution from a semi-circular contour at infinity $\mathcal{C}_\infty$. Hence, we can choose to close the contour in the lower half-plane, using $\operatorname{Im} X = (1/2i)(X + X^*)$, so that Cauchy's theorem allows us to deform the contour so that it becomes $\mathcal{C}'$ around the two poles of the lower half-plane, giving us

$$\int_{-\infty}^{\infty} \omega^2 \left\langle x(\omega)\, x^*(\omega) \right\rangle \frac{d\omega}{2\pi} = i \frac{1}{m^2\gamma} \frac{1}{2i} \frac{\left(\widetilde{\omega}^+ - \widetilde{\omega}^-\right)}{\left(\widetilde{\omega}^+ - \widetilde{\omega}^-\right)} \left\langle |F_{in}|^2 \right\rangle = \mathcal{T}\, \frac{k_B T}{m} \tag{4.49}$$

from which we find

$$\left\langle |F_{in}|^2 \right\rangle = \mathcal{T}\, 2m\gamma k_B T.$$

$\left\langle |F_{in}(\omega)|^2 \right\rangle$ is independent of frequency for a delta correlated noise, $\langle F_{in}(t)\, F_{in}(t') \rangle = A\delta(t)$.

We can now substitute in the expression (4.42) relating the fluctuations to the force to obtain,

$$\boxed{S_{xx}(\omega) \equiv \tfrac{1}{\mathcal{T}} \left\langle x(\omega)\, x^*(\omega) \right\rangle = \int_{-\infty}^{\infty} e^{i\omega\left(t-t'\right)} \left\langle x(t)\, x(t') \right\rangle d(t-t')} \tag{4.50}$$

$$= \frac{(1/m)^2}{\left(\omega^2 - \omega_0^2\right)^2 + (\omega\gamma)^2} 2m\gamma k_B T$$

$$\boxed{S_{xx}(\omega) = \chi''(\omega)\, \tfrac{2k_B T}{\omega}} \tag{4.51}$$

where in the last line we used our result for the imaginary part of the susceptibility, Eq. (3.29). The last equation is the classical limit of the fluctuation-dissipation

theorem. Note that the last equalities prove that $2k_BT\omega\chi''(\omega) = \omega^2 S_{xx}(\omega)$ where $S_{xx}(\omega)$ is clearly an even function of ω.[3]

The propagator is now expressed in terms of an equilibrium correlation function

$$\boxed{\chi''(\omega) = \frac{\omega}{2k_BT}\int_{-\infty}^{\infty} e^{i\omega(t-t')}\langle x(t)\,x(t')\rangle\, d(t-t')} \tag{4.52}$$

We will see that a representation of the susceptibility in terms of a correlation function can always be found.

Remark 32 *The result for the fluctuation-dissipation theorem in the classical limit Eq.(4.51) is valid even when the damping is frequency dependent. In that case, the spectrum of the fluctuating force is not white since it becomes frequency dependent* $\left\langle |F_{in}(\omega)|^2 \right\rangle = \mathcal{T}\, 2m\gamma'(\omega)\, k_BT$. *This is a sort of detailed-balance condition, which we shall see in more detail later. The fluctuating force in any frequency interval is related to the dissipation in that same frequency range. A proof of the general fluctuation-dissipation theorem Eq.(4.51) using the Caldeira-Leggett [47] representation of* $\gamma(\omega)$*, presented above, may be found in the lecture notes of Devoret [67] on electrical circuits.*

Remark 33 *In the quantum case, the prefactor entering the proportionality between* $\chi''(\omega)$ *and* $S_{xx}(\omega)$ *must be modified, but the dissipation* $\chi''(\omega)$ *remains related to the fluctuations* $S_{xx}(\omega)$ *through a prefactor that depends only on frequency and absolute temperature. This is a truly remarkable result.*

Remark 34 *Especially in the context of electrical circuits, the fluctuation-dissipation theorem is known as Nyquist's theorem, as we mentioned above. The relation between diffusion constant and viscosity discovered by Einstein is another form of the fluctuation-dissipation theorem. Indeed, the viscosity appears in the response to an external force whereas diffusion controls density fluctuations.*

Remark 35 *Given* $S_{xx}(\omega) = \chi''(\omega)\frac{2k_BT}{\omega}$*, the relation*

$$\frac{1}{\mathcal{T}}\int_{-\infty}^{\infty}\langle x(\omega)\,x^*(\omega)\rangle\frac{d\omega}{2\pi} = \int_{-\infty}^{\infty} S_{xx}(\omega)\frac{d\omega}{2\pi} \tag{4.53}$$

$$= \langle x(0)\,x(0)\rangle = \frac{k_BT}{k} = \frac{k_BT}{m\omega_0^2} \tag{4.54}$$

that also follows from the equipartition theorem only in the Caldeira-Leggett example where x *enters quadiatically in the Hamiltonian, translates into*

$$\int_{-\infty}^{\infty} S_{xx}(\omega)\frac{d\omega}{2\pi} = k_BT\int_{-\infty}^{\infty}\frac{\chi''(\omega)}{\omega}\frac{d\omega}{\pi} = \frac{k_BT}{k}. \tag{4.55}$$

This is our first example of a thermodynamic sum rule.

Remark 36 *Eq.(4.44) also implies the sum rule*

$$\int_{-\infty}^{\infty}\omega^2 S_{xx}(\omega)\frac{d\omega}{2\pi} = k_BT\int_{-\infty}^{\infty}\omega\chi''(\omega)\frac{d\omega}{\pi} = \frac{k_BT}{m} \tag{4.56}$$

$$\int_{-\infty}^{\infty}\omega\chi''(\omega)\frac{d\omega}{\pi} = \frac{1}{m}$$

It will be clear in the next chapter that the latter sum-rule follows classically from the equal-time Poisson bracket between momentum and position. This is our first example of an f-sum rule. Note that in the last integral, high frequencies are more important. And in the end, the integral does not depend on dissipation at all! This is quite general. High-frequency response is reactive, not dissipative.

[3] This is valid only in the classical limit. The fluctuations do not have a specific parity in the quantum mechanical case.

5. IRREDUCIBLE SELF-ENERGY AND VIRTUAL PARTICULES IN A (ALMOST) CLASSICAL CONTEXT

You can begin to understand rather easily the concepts of self-energy and virtual particules in the simple context of the classical harmonic oscillator. There are limitations to this analogy, but it is not too bad. I will work with the propagator in Eq.(4.24) that we obtained for an infinite bath. Recall that in this chapter, the propagator and the susceptibility are the same. This is not always the case.

5.1 The concept of self-energy emerges naturally when one does a power series expansion

Suppose I write the propagator $\mathcal{D}^R(\omega)$ in the form more standard for phonons, namely Eq.(3.4). The quantity $\Pi^R(\omega)$ is proportional to the square of the coupling k'' between the original oscillator of frequency ω_0 and the infinite bath, namely it depends on the square of the only non-zero element of V (defined in the matrix form Eq.(4.7)) that describes the coupling of the mass M with the bath of oscillator. Let $\Pi_n^R(\omega)$ be the order n expansion of $\Pi^R(\omega)$ in powers of k''. This means that if I have a perturbation theory that allows me to compute the propagator, to fourth order in V for example, I will obtain

$$\mathcal{D}^R(\omega) \equiv \frac{1/M}{-(\omega+i\eta)^2+\omega_0^2} - \frac{(1/M)^2\left(2\omega_0\Pi_2^R(\omega)+2\omega_0\Pi_4^R(\omega)\right)M}{\left(-(\omega+i\eta)^2+\omega_0^2\right)^2} + \frac{(1/M)^3\left(2\omega_0\Pi_2^{(2)R}(\omega)M\right)^2}{\left(-(\omega+i\eta)^2+\omega_0^2\right)^3} + \dots \tag{5.1}$$

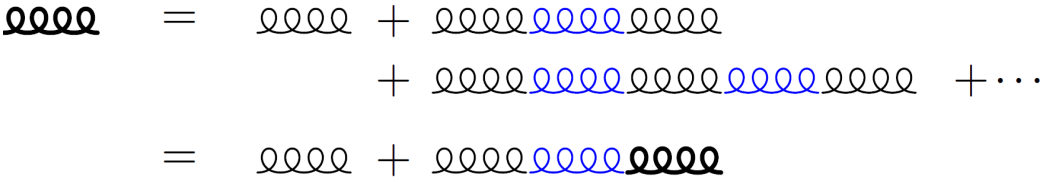


Figure 5-1 Power series expansion for the harmonic oscillator with mass M.The thin black curly line is the bare propagator for that oscillator, the thin blue curly line is the bare propagator for the bath and the thick black curly line is the dressed propagator for the oscillator of mass M. The last line resums the series to infinite order.

I can represent this series diagrammatically as illustrated in Fig.(5-1). The black wavy line represents the unperturbed propagator

$$\mathcal{D}_0^R(\omega) = \frac{1/M}{-(\omega+i\eta)^2+\omega_0^2} \tag{5.2}$$

and the blue wavy line represents the so-called irreducible self-energy calculated to only second order in V,

$$2\omega_0\Pi_2^R(\omega)M. \tag{5.3}$$

You can check that the constant k'' that couples the oscillator ω_0 to the bath in the detailed matrix form Eq.(4.6) also enters the first diagonal matrix element of the bath (and also in ω_0 but we assume we have taken it into account there). Hence, that is why to fourth-order in V,there is an extra term in the power series expansion Eq.(5.1) for the propagator. Since what we are after is the position of the poles of $\mathcal{D}^R(\omega)$ that represent the true eigenmodes of the system, what clearly makes more sense is to compute $\Pi^R(\omega)$ only to second order in V and to put it back in the form of Eq.(3.4), namely

$$\mathcal{D}^R(\omega) \simeq \frac{1/M}{\left(-(\omega+i\eta)^2+\omega_0^2+2\omega_0\Pi_2^R(\omega)\right)}. \tag{5.4}$$

In other words, what makes most sense is to find a power series for the self-energy. This is where we hide our ignorance.

Remark 37 *The expression "irreducible" can have slightly different meanings depending on context. Here we mean that the self-energy is the set of diagrams in Fig. (5-1) that cannot be cut in two by removing a bare propagator line.*

Remark 38 *Self-energy: One encounters the self-energy mostly in the context of interactions. In the present context, one would instead speak of a hybridization function. Nevertheless, the mathematics is well illustrated by the above example.*

Remark 39 *Why resum: Another reason to resum the series expansion Eq.(5.1), is that if we stop at some finite order, we see that $\mathcal{D}^R(\omega)$ has poles of order two, three etc, instead of the simple poles expected from the spectral representation.*

5.2 Virtual particles

The notion of virtual particles is not always clear. Let me try a somewhat clumsy analogy to explain this with the harmonic oscillator. Let me begin with the definition of a "particle" in this special context. When the harmonic oscillator is quantized, its energy takes discrete values separated by $\hbar\omega$. When the energy goes up by $\hbar\omega$, we say that there is one more phonon in the system. A phonon is a "particle" because it is corresponds to a transition between eigenstates of a quadratic Hamiltonian that a) has a well defined quantized energy and that b) can be measured.

Let us then consider the excitations at frequency ω_0 of our original harmonic oscillator example as phonons, and the excitations of the eigenmodes of the bath of oscillators as phonons as well. What happens if we couple the two sets of phonons? We say that they hybridize. But there is another way to look at this

here.[1] Damping of the oscillator at ω_0 corresponds to emitting phonons that dissipate in the bath by creating phonons there. When ω_0 is much less than the lowest eigenenergy of the bath $\omega_a^{\min}$ or much larger than the largest $\omega_a^{\max}$ of the bath, there is no dissipation since $\gamma'(\omega_0) = 0$. Nevertheless, the position of the pole is no-longer ω_0, it takes a renormalized value, say ω_R,because even if the damping constant $\gamma'(\omega_R)$ vanishes,by Kramers-Kronig $\gamma''(\omega_R)$ does not vanish as long as there is absorption at some frequency because $\gamma''(\omega_R)$ depends on absorption at all other frequencies

$$\gamma''(\omega_R) = -\mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\gamma'(\omega')}{\omega' - \omega_R}. \tag{5.5}$$

This moves the position of the poles as seen from Eq.(3.29) (we can take γ' infinitesimal to recover a delta function).[2] The eigenmode at this renormalized frequency now contains virtual particles. We say virtual particles because in this situation, the bath does not emit or absorb energy, i.e. no "real" phonon, or measurable quantum of energy, is involved. The wavy blue lines in Fig.(5-1) can be virtual particles from the point of view of the original oscillator at frequency ω_0.

Remark 40 *A "particle" in general occupies a single-particle state that does not need to be an energy eigenstate. The definition looks somewhat circular. This is rooted deeply into wave-particle duality in quantum mechanics and the notion will become clearer when I introduce second quantization. More generally, many quantized excitations of a system can qualify as "quasiparticles".*

[1] We take all frequencies as positive in the rest of this section.

[2] Note that when $\gamma' = 0$, it is no longer justified to neglect the $i\eta$. The spectral weight becomes then a delta function.

6. EXERCICES FOR PART I

Exercise 6.0.1 *Starting from Eq. (2.38) assume that the Kramers Kronig relations Eqs. (2.31) and (2.32) are true and prove that this implies that the Sokhatsky-Weirstrass formulas (2.36) are true.*

Exercise 6.0.2 *En partant de l'éq. (2.38) supposez que les relations de Kramers Kronig (2.31) et (2.32) sont valides et prouvez que ceci implique la validité de la formule de Sokhatsky-Weirstrass (2.36).*

Exercise 6.0.3 *Spectral representation, high-frequency expansion and moments: Let $\chi(z)$ a function of the complex variable z be defined by*

$$\chi(z) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - z}. \tag{6.1}$$

We have shown that this function becomes equal to $\chi^R(\omega)$ defined in this chapter when $z = \omega + i\eta$.

a) Derive the following high-frequency limit (that assumes that $\chi''(\omega)$ vanishes exactly at high-frequency, which is always the case as we will see)

$$\chi(z) \simeq -\frac{1}{z} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \chi''(\omega') \left(\frac{\omega'}{z}\right)^n. \tag{6.2}$$

One calls the coefficients of the expansion in powers of $1/z$ the "moments" of $\chi''(\omega)$.

b) Show that if χ is the propagator for the position of the harmonic oscillator then

$$k_B T \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^{2n-1} \chi''(\omega) = \left\langle \left(\frac{d^n x(t)}{dt^n} \right)^2 \right\rangle \tag{6.3}$$

while the even moments

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^{2n} \chi''(\omega) \tag{6.4}$$

vanish because of time-reversal symmetry. Equations such as 6.9 are called sum rules. They relate the moments of the function that describes dissipation to equal-time correlation functions.

c) Show that our phenomenological model for the harmonic oscillator Eq.(3.3) gives an infinite result for

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^3 \chi''(\omega) \tag{6.5}$$

when one takes $\gamma(\omega)$ independent of ω. This is in disagreement with the fact that the average of the square of the acceleration, $\left\langle \left(\frac{d^2 x(t)}{dt^2} \right)^2 \right\rangle$, cannot be infinite, which demonstrates that one must absolutely take a frequency-dependent $\gamma(\omega)$. In practice, one often needs to live with the fact that all sum-rules cannot be satisfied exactly. One can however use sum rules to improve phenonenological models. Note that despite that fact that the relation (4.51) between fluctuation and dissipation

was established while assuming $\gamma(\omega)$ independent of frequency, it is valid much more generally as we will see. In other words, the disagreement found here is not because the fluctuation-dissipation theorem is not valid. The response of the harmonic oscillator is always related to an equilibrium correlation function, at least to linear order in the applied external force F.

Exercise 6.0.4 *Approximating the imaginary part of the propopagator by a continuous function and its consequences on analyticity:*
As long as the bath is finite, $\mathcal{D}(z=\omega+i\eta)$ has a finite set of poles, infinitesimally close to the real axis so that $\operatorname{Im}\mathcal{D}(\omega+i\eta)$ is a set of delta functions. By going to the continuum limit, these poles coaless into a branch cut and $\operatorname{Im}\mathcal{D}(\omega+i\eta)$ becomes a continuous function.
a) Show the relation between $\operatorname{Im}\mathcal{D}(\omega+i\eta)$ and the discontinuity of $D(z)$ across the real axis, in otherwords the difference between $D(\omega+i\eta)$ and $D(\omega-i\eta)$
b) Show that when the continuous function $\operatorname{Im}\mathcal{D}(\omega+i\eta)$ is approximated by a Lorentzian, the propagator has a pair of isolated poles in the lower-half plane.

Exercise 6.0.5 *Soit la fonction d'une variable complexe z définie par*

$$\chi(z)=\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'-z}. \tag{6.6}$$

Cette fonction devient égale à $\chi^R(\omega)$ lorsque $z=\omega+i\eta$.

b) Obtenez le développement haute-fréquence suivant (qui suppose que $\chi''(\omega)$ s'annule exactement à haute fréquence, ce qui est toujours vrai comme nous verrons)

$$\chi(z)\simeq-\frac{1}{z}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi''(\omega')\left(\frac{\omega'}{z}\right)^n. \tag{6.7}$$

On appelle les coefficients du développement en puissance de $1/z$ les "moments" de $\chi''(\omega)$.

c) Démontrez la règle de somme dite thermodynamique pour l'oscillateur harmonique,

$$\chi(0)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''(\omega)}{\omega}=\frac{1}{k_BT}\left\langle x(t)^2\right\rangle. \tag{6.8}$$

d) Montrez que

$$k_BT\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^{2n-1}\chi''(\omega)=\left\langle\left(\frac{d^nx(t)}{dt^n}\right)^2\right\rangle \tag{6.9}$$

alors que les autres moments,

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^{2n}\chi''(\omega) \tag{6.10}$$

s'annulent par symétrie sous inversion du temps. Les équations comme 6.9 s'appellent règles de somme. Elles relient les moments de la fonction décrivant la dissipation à des fonctions de corrélation à temps égal.

e) Montrez que notre modèle phénoménologique pour l'oscillateur, Eq.(3.3) donne un résultat infini pour

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^{3}\chi''(\omega) \tag{6.11}$$

lorsqu'on prend $\gamma(\omega)$ indépendant de ω. Ceci est en désaccord avec le fait que la moyenne du carré de l'accélération $\left\langle \left(\frac{d^2x(t)}{dt^2} \right)^2 \right\rangle$ ne peut être infinie, ce qui démontre qu'il faut absolument que $\gamma(\omega)$ dépende de ω. En pratique, il faudra vivre avec le fait que toutes les règles de somme ne pourront pas être satisfaites exactement. On peut cependant utiliser les règles de somme pour améliorer les modèles phénoménologiques. Notez que bien que la relation (4.51) entre fluctuation et dissipation ait été établie en supposant $\gamma(\omega)$ independant de la fréquence, elle est valable beaucoup plus généralement, comme nous allons le voir bientôt. Le désaccord trouvé ci-dessus n'est pas causé par le fait que le théorème de fluctuation-dissipation ne s'applique pas de façon générale, du moins à l'ordre linéaire en F.

6.1 Devoir 2, fonctions de réponse, théorème de Kramers Kronig

Exercise 6.1.1 *Fonction de relaxation de Kubo: Dans la limite classique, le théorème de fluctuation-dissipation devient:*

$$\chi"_{A_iA_j}(\mathbf{r},\mathbf{r}';\omega) = \frac{\beta\omega}{2} S_{A_iA_j}(\mathbf{r},\mathbf{r}';\omega).$$

Définissons une fonction $C_{A_iA_j}$ telle que la relation précédente soit toujours vraie, c'est-à-dire que même pour un système quantique on veut que:

$$i\frac{d}{dt} C_{A_iA_j}(\mathbf{r},\mathbf{r}';t) = \frac{2}{\beta}\chi"_{A_iA_j}(\mathbf{r},\mathbf{r}';t).$$

Montrez que cette dernière relation est satisfaite par la définition suivante de $C_{A_iA_j}$

$$C_{A_iA_j}(\mathbf{r},\mathbf{r}';t-t') = \beta^{-1}\int_0^\beta d\beta' [< A_i(\mathbf{r},t)A_j(\mathbf{r}',t'+i\hbar\beta') > - < A_i >< A_j >].$$

Ceci est une autre fonction de corrélation due a Kubo et qui décrit la relaxation.

Exercise 6.1.2 *Constante diélectrique et Kramers-Kronig. Considérons la constante diélectrique d'un milieu isotrope $\epsilon(t)$ comme une fonction de réponse, sans nous soucier de sa représentation en terme de commutateurs. En utilisant le principe de causalité ($\epsilon(t) = 0$ pour $t < 0$), demontrez que $\epsilon(\omega)$ est analytique dans le plan complexe supérieur. Determinez aussi la parité de ϵ_1 et ϵ_2 ($\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$) sous changement de signe de ω. En utilisant ensuite le théorème de Cauchy sur les intégrales des fonctions analytiques, dérivez deux relations de Kramers-Krönig entre les parties réelles et imaginaires de $\epsilon(\omega)$:*

$$\epsilon_1(\omega) - \epsilon_1(\infty) = \frac{2}{\pi}\mathcal{P}\int_0^\infty d\xi \frac{\xi\epsilon_2(\xi)}{\xi^2-\omega^2} \tag{6.12}$$

$$\epsilon_2(\omega) = -\frac{2}{\pi}\omega\mathcal{P}\int_0^\infty d\xi \frac{\epsilon_1(\xi)-\epsilon_1(\infty)}{\xi^2-\omega^2} \tag{6.13}$$

Part II

Correlation functions, general properties

Here we start to use quantum mechanics. Whenever the N-body problem can be solved exactly in d dimensions, the result is a function of Nd coordinates and of time, $\Psi(x_1, y_1, ..., x_d, y_d, ...; t)$. Variational approaches, such as that used in the description of the fractional Quantum-Hall effect, start from such a wave-function. While all the Physics is in the wave-function, it is sometimes not easy to develop a physical intuition for the result. One case where it is possible is when the wave function has a simple variational form with very few physically motivated parameters. We encounter this in the fractional Quantum Hall effect for example, or in BCS theory. Modern numerical methods such as tensor networks or density matrix renormalization group [43] focus on the wave function. But in the cases where perturbation theory can be applied instead, Feynman diagrams help develop a physical intuition.

Whether perturbation theory is applicable or not, we rarely need all the information contained in the wave-function. A reduced description in terms of only a few variables suffices if it allows us to explain what can be observed by experimental probes. Correlation functions offer us such a description.

As for any physical theory, one must first discuss which quantities are observable, or in other words, what it is that we want to compute. Starting this time from quantum theory, we will see that what is measured by experimental probes can in general be expressed as a correlation function, whether the experiment is a scattering experiment, such as neutron diffraction, or a transport measurement, such as conductivity, as long as we are in the linear response regime. It is quite remarkable that whatever the appropriate microscopic description of the system, or whatever the underlying broken symmetry, the result of any of the above two types of experiments can be expressed as a specific correlation function.

We will need to treat two different aspects of correlation functions.

a) The first aspect consists in general properties, which are independent from the specific manner in which we compute correlation functions. We have already extensively discussed these general properties in the context of the classical harmonic oscillator. The properties I have in mind include, for example

- Symmetries
- Positivity
- Fluctuation-dissipation theorems relating linear response and equilibrium fluctuations
- Kramers-Kronig transformations, which follow from causality
- Kubo relations, such as that relating linear response to a specific correlation function.
- Sum rules
- Goldstone theorem, which follows from Bogoliubov inequalities

b) The second aspect concerns methods we need to compute specific correlation functions. Sometimes, phenomenological considerations suffice, like we saw in the harmonic oscillator case with the phenomenological damping constant. Phenomenology sometimes allows to find, with unknown parameters, the functional dependence of correlations functions on, say, wave-vector and frequency. These phenomenological considerations apply in particular in the hydrodynamic regime, and whenever projection operator techniques are used.

As I mentioned in the introduction to part I, microscopic calculations based on specific Hamiltonians and quantum mechanics will lead us to use another type of correlation functions, namely Green's functions. They will occupy a large fraction

of this book. In fact, Green's function are just one type of correlation function. They will appear very naturally. Furthermore, many of the general properties of correlation functions, which we discuss in the present chapter will transpose directly to these functions. Much of this chapter is inspired from Forster [75] which in turn draws heavlily on work of Kadanoff and Martin. [111]

In this part of the book, I intend to

- Show that scattering experiments are a measure of equilibrium fluctuations
- Linear response to an external perturbation can be expressed as an equilibrium correlation function

And this correlation function can be related to equilibrium fluctuations by the fluctuation-dissipation theorem.

- Then I discuss general properties of correlation functions
- and give a specific example of sum-rule calculation.

7. RELATION BETWEEN CORRELATION FUNCTIONS AND EXPERIMENTS

Physical theories are rooted in experiment, hence, the first question is about measurement and how it is performed. If you want to know something about a macroscopic system, you probe it. The elegance of Condensed Matter Physics stems in part from the plethora of probes that can be used. Neutron scattering, electron scattering, nuclear magnetic resonance, resistivity, thermopower, thermal conductivity, Raman and Infrared scattering, muon resonance, the list is long. What they all have in common is that they are weak probes. Quantum mechanics, tells us that all probes influence what they measure. Nevertheless, by looking at the probe, we can tell something about the state of the system. Even the Green's function is a correlation function that can be measured by photoemission, as we will see later.

In this chapter, I want to first illustrate the fact that scattering experiments with weak probes usually measure various equilibrium correlation functions of a system. This is one of the reasons why we will be so concerned with correlation functions. The other reason will be that they also come out from linear response. What I mean by "weak probes" is simply that Fermi's Golden rule and the Born approximation are all that we need to describe the effect of the system on the external probe, and vice-versa. The correlation functions that are measured by scattering experiments are generally refered to as "fluctuations". They will be related to correlation functions that describe the linear response to external forces, and the associated dissipation, by the fluctuation-dissipation theorem.

As an example, I describe in detail in Section (7.2) the case of inelastic electron scattering but it should be clear that similar considerations apply to a large number of cases: inelastic light scattering, neutron scattering, etc. The first figure, (7-1), in that section illustrates what I have in mind. The plan is simply to use Fermi's Golden Rule to compute the differential cross section. We will obtain

$$\boxed{\frac{d\sigma}{d\epsilon_f d\Omega_f} = \left[\frac{m^2}{(2\pi)^3\hbar^5}\frac{k_f}{k_i}\left|V^c_{-\mathbf{q}}\right|^2\right]\int dt\; e^{i\omega t}\left\langle \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)\right\rangle .} \tag{7.1}$$

Forgetting for the moment all the details, the key point is that the cross section is related to the Fourier transform of the density-density correlation function. The trick, due to Van Hove, to derive this formula from the Golden rule is to use the Dirac representation of the delta function for energy conservation and the Heisenberg representation to express the final result as a correlation function. Since in the Born approximation, incident and final states of the probe are plane waves, everything about the probe is known. The only reference to it will be through explicitly known matrix elements and quantum numbers, such as momentum, energy, spin etc...

7.1 Quite generally, Fermi's golden rule in either scattering or relaxation experiments lead observables that are time-dependent correlation functions

To illustrate the main ideas in a simple but sketchy manner, before entering the nitty gritty details, recall that the Hamiltonian for the combined probe and systems is

$$H = H_p^0 + H_s + H_{ps} \tag{7.2}$$

where H_p^0 is the Hamiltonian that describes the evolution of the probe, H_s the Hamiltonian for the system, and H_{ps} the describes the interaction of the probe with the system. In general H_p^0 is simple. It describes the propagation of a free electron for example. The interaction of the system and the probe will generally take the form

$$H_{ps} = gA_s \otimes A_p \tag{7.3}$$

where g is some coupling constant while A_s and A_p are operators that belong respectively to the system and to the probe. In the case where you shoot an electron, these operators are the charge density of each system.

I assume that the final state of the probe belongs to a continuum. Then we can use Fermi's Golden rule that tells us that the transition rate from an initial state i to a final state f is given by

$$\boxed{P_{i\to f} = \tfrac{2\pi}{\hbar} \left|V_{fi}\right|^2 \delta(E_f - E_i - \hbar\omega)} \tag{7.4}$$

where E_i is the initial energy of the system and E_f the final one. The quantum of energy $\hbar\omega$ is the energy lost by the probe, or gained by the system. In other words, $\hbar\omega = \varepsilon_i - \varepsilon_f$,where ε_i and ε_f refer to the probe, in such a way that there is energy conservation for system plus probe: $E_f + \varepsilon_f = E_i + \epsilon_i$. The transition matrix element V_{fi} is given by

$$\begin{aligned} V_{fi} &= \langle s_f| \otimes \langle p_f| H_{ps} |p_i\rangle \otimes |s_i\rangle = g \langle s_f| \otimes \langle p_f| A_s A_p |p_i\rangle \otimes |s_i\rangle \\ &= g \langle p_f| A_p |p_i\rangle \langle s_f| A_s |s_i\rangle \end{aligned} \tag{7.5}$$

where at the beginning and at the end of the experiment, probe and system do not interact, which means that the state of the system is a direct product of the system $|s_i\rangle$ and probe $|p_i\rangle$ states. Hence, we find

$$P_{i\to f} = \frac{2\pi}{\hbar} \left[g^2 \left|\langle p_f| A_p |p_i\rangle\right|^2 \right] \left|\langle s_f| A_s |s_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega). \tag{7.6}$$

The transition probability has thus factored into a prefactor, in square brackets, that is completely independent of the system that is probed. If we know about free electrons, or free neutrons, or whatever the probe, we can compute the prefactor.

What we are interested in is what the transition probability tells us about the system. The final state of the probe is *measured*. That state can be entangled with many states of the system $\langle s_f|$, that are *not* measured. The correct transition probability for the probe then must be computed by summing over all final states of the system $\langle s_f|$. This is like taking the trace over the unobserved states. In other words, what we need is

$$\sum_{s_f} P_{i\to f} = \left[\frac{g^2}{\hbar^2} \left|\langle p_f| A_p |p_i\rangle\right|^2 \right] 2\pi\hbar \sum_{s_f} \left|\langle s_f| A_s |s_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega). \tag{7.7}$$

The fact that not all final states are allowed is taken into account by selection rules in the matrix element and by the energy conserving delta function. The sum over s_f can be taken as unrestricted.

The next elegant step in the derivation is due to van Hove, as mentioned above. It takes advantage of the fact that there is a as sum over final states that can allow us to take advantage of the completeness relation. Using the integral representation of the delta function, $A_s = A_s^\dagger$, and the Heisenberg representation with H_s the system Hamiltonian, $A(t) = e^{iH_s t/\hbar} A_s e^{-iH_s t/\hbar}$, you see that

$$\begin{aligned} 2\pi\hbar \sum_{s_f} |\langle s_f| A_s |s_i\rangle|^2 \delta(E_f - E_i - \hbar\omega) &= \sum_{s_f} \langle s_i| A_s |s_f\rangle \langle s_f| A_s |s_i\rangle \int dt\, e^{i\omega t} e^{-i(E_f - E_i)t/\hbar} \\ &= \int dt\, e^{i\omega t} \sum_{s_f} \langle s_i| e^{iH_s t/\hbar} A_s e^{-iH_s t/\hbar} |s_f\rangle \langle s_f| A_s |s_i\rangle \\ &= \int dt\, e^{i\omega t} \langle s_i| e^{iH_s t/\hbar} A_s e^{-iH_s t/\hbar} A_s |s_i\rangle \qquad (7.8) \\ &= \int dt\, e^{i\omega t} \langle s_i| A_s(t) A_s |s_i\rangle \qquad (7.9) \end{aligned}$$

where in the last equation I have used the completeness relation. Clearly then, the transition probability of the probe is proportionnal to the time Fourier transform of $\langle s_i| A_s(t) A_s |s_i\rangle$ .This object is what is called a correlation function.

In general, at finite temperature we do not know the initial state. All we know is that the probability of each initial state is given by the canonical or grand-canonical distribution for a system in thermal equilibrium with a reservoir. In this case, to compute the transition probability for the probe we simply need the proper thermal average over the initial states of the system, namely it is the following expectation value that enters the transition probability:

Definition 6 *Definition of average:*

$$\begin{aligned} \frac{\sum_i e^{-\beta E_i} \langle s_i| A_s(t) A_s |s_i\rangle}{\sum_i e^{-\beta E_i}} &= \frac{\mathrm{Tr}\left[e^{-\beta H_s} A_s(t) A_s\right]}{\mathrm{Tr}\left[e^{-\beta H_s}\right]} \qquad (7.10) \\ &\equiv \langle A_s(t) A_s\rangle . \qquad (7.11) \end{aligned}$$

In the above equation, I have given the important definition of what is meant by averages $\langle\rangle$. There is a quantum mechanical expectation value and a thermal average.

Correlation functions will essentially always be computed in thermal equilibrium, as above. There is no need to average over the initial state of the probe which is assumed to be in a pure state.

The density matrix is defined by

$$\varrho = e^{-\beta H_s} / \mathrm{Tr}\left[e^{-\beta H_s}\right] . \qquad (7.12)$$

In the grand canonical ensemble, that we will use essentially all the time, you can think of H_s as containing $-\mu N$, where μ is the chemical potential and N the number of operator. Then, we can write

$$\langle A_s(t) A_s\rangle = \mathrm{Tr}\left[\varrho A_s(t) A_s\right] . \qquad (7.13)$$

Overall then, we have that

$$\frac{\sum_i e^{-\beta E_i} \sum_{s_f} P_{i\to f}}{\sum_i e^{-\beta E_i}} = \left[\frac{g^2}{\hbar^2} |\langle p_f| A_p |p_i\rangle|^2\right] \int dt\, e^{i\omega t} \langle A_s(t) A_s\rangle . \qquad (7.14)$$

Everything about the prefactor representing a weak probe should be known, including the coupling constant g. That quantity is just the electric charge for example in the cas of electron scattering. The information on the system is in the Fourier transform of the fluctuations of the operator A_s.

Clearly, the above is a canevas that can be used for a wide range of probes of materials. With linear response theory, it forms the foundation of measurement theory for us. In the next section, I perform the detailed calculation for electron scattering. You can skip that section on first reading.

Definition 7 *Density matrix: As we mentioned, the quantity*

$$\boxed{\varrho \equiv \frac{e^{-\beta H}}{\mathrm{Tr}\left[e^{-\beta H}\right]}} \tag{7.15}$$

is often called the density matrix. The fact that thermal averages are traces is an important fact that we will often use later. In the grand canonical ensemble, which will be used most of the time, we have instead

$$\boxed{\varrho \equiv \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left[e^{-\beta(H-\mu N)}\right]}} \tag{7.16}$$

Appendix (A.1) gives a more general refresher on the concept of density matrix.

Remark 41 *In atomic physics (quantum information) when a two-level system (a qubit) is in an excited state, this is not a stationnary state of the whole system. It can decay to the ground state because of its coupling to the electromagnetic field. In this case, the "probe" is the atom (qubit) and the "system" is the electromagnetic environment. With a coupling of the form* $\mathbf{j} \cdot \mathbf{A}$*, where* $\mathbf{j}$ *is the current and* $\mathbf{A}$ *the vector potential, we see that the decay rate depends on the correlation function between the vector potential at two different times, in other words, it depends on vacuum fluctuations of the electromagnetic field. More precisely, it is the size of the vacuum fluctuations at the transition frequency of the qubit that determines the transition rate.*

Remark 42 *In the case of a nuclear spin coupled to electron spins on a lattice, the relaxation of the nuclear spin can be considered as a measure of the* ***local*** *electron spin fluctuations at the frequency that corresponds to the Zeeman splitting of the nuclear-spin energy levels.* $(1/T_1) \sim \langle S^s(\omega) S^z(\omega) \rangle$*. That energy is minuscule compared with energy scales in condensed matter. A field of* $1\ T$ *corresponds to a nuclear Zeeman splitting of about* $0,5 \times 10^{-3}\ K$*, which is smaller than typical electronic Zeeman splitting by the ratio of the mass of the electron to the mass of the proton. Since the frequency is so low, we can use the classical fluctuation dissipation theorem, which means that* $(1/T_1) \sim k_B T\, \chi''_{S^z S^z}(\omega)/\omega$*. When the susceptibility is wave-vector dependent, we must sum over all wave vectors to obtain the local spin susceptibility.*

7.2 *Details of the derivation for the specific case of electron scattering

I follow Ref. [75]. Consider the experiment illustrated on figure (7-1). $\mathcal{V}$ is the volume of the system, and Ω a quantization volume.

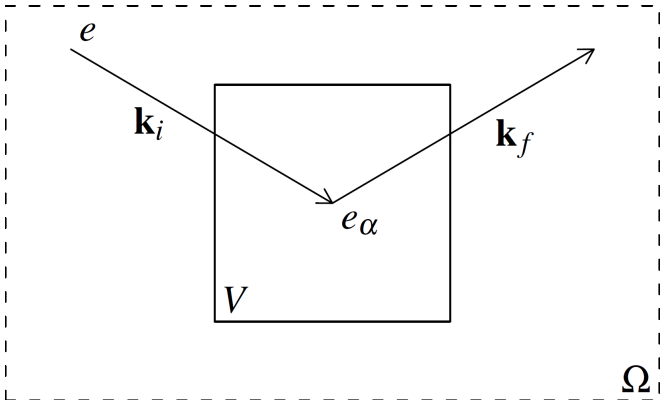


Figure 7-1 Electron scattering experiment. Ω is the quantization volume for the incoming and outgoing plane waves while V is the sample's volume. Each charge inside is labeled by e_α while the probe's charge is e and the incident and outgoing momenta are respectively $\mathbf{k}_i$ and $\mathbf{k}_f$.

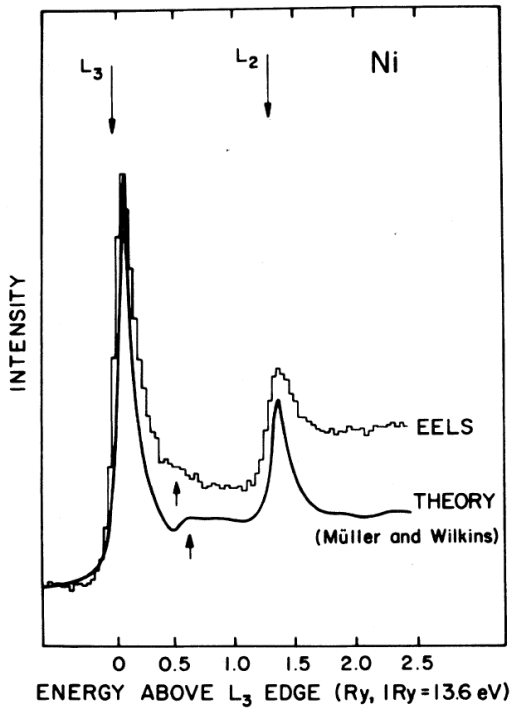


Figure 7-2 Energy loss spectroscopy for scattering from $2p_{1/2}$ and $2p_{3/2}$ states (L_2 and L_2) of Nickel to empty $3d$ electrons that form the valence band, compared with band structure calculations. The calculations are for the Fourier transform of the density-density correlation function, as discussed in this section. That correlation function is evaluated in the dipole approximation, i.e. from the first term in the expansion of $e^{-i\mathbf{q}\cdot\mathbf{r}}$, because this is the leading matrix element for the atomic transition from $2p$ to $3d$. Figure reproduced from R.D. Leapman, L.A. Grunes, and P.L. Fejes, Phys. Rev. B **26**, 614 (1982).

This experiment is also known as EELS, energy loss electron spectroscopy. Comparison between theory and experiment for Ni is shown in Fig.(7-2).

The Hamiltonian of the system is H and the interaction between the probe electron and the system is simply the potential energy $v(\mathbf{R})$ felt by the probe-electron of charge e at position $\mathbf{R}$ due to the N other charged particles inside the system, namely

$$v(\mathbf{R}) = \sum_{\alpha=1}^{N} e_\alpha V^c(\mathbf{R} - \mathbf{r}_\alpha) = \int d^3r \rho(\mathbf{r}) V^c(\mathbf{R} - \mathbf{r}) \tag{7.17}$$

with $V^c(\mathbf{R})$ the Coulomb potential and

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{N} e_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \tag{7.18}$$

the charge density operator for the system being probed. Fermi's Golden rule tells us that the transition rate from an initial state i to a final state f is given by

$$\boxed{P_{i\to f} = \tfrac{2\pi}{\hbar} \left|V_{fi}\right|^2 \delta(E_f - E_i - \hbar\omega)} \tag{7.19}$$

where E_i is the initial energy of the system and E_f the final one. Correspondingly, the initial and final energies and momentum of the probe electron are given by,

$$\begin{aligned} \epsilon_f &= \epsilon_i - \hbar\omega \\ \hbar\mathbf{k}_f &= \hbar\mathbf{k}_i - \hbar\mathbf{q}. \end{aligned} \tag{7.20}$$

We proceed to evaluate the matrix element as far as we can. It should be easy to eliminate explicit reference to the probe electron since it has rather trivial plane-wave initial and final states. It is natural to work in the basis where the system's initial and final eigenstates are energy eigenstates, respectively $|i\rangle$ and $|f\rangle$, while for the probe electron they are $|\mathbf{k}_i\rangle$ and $|\mathbf{k}_f\rangle$. The latter eigenstates in the box of volume Ω are plane waves:

$$\langle \mathbf{R} \left|\mathbf{k}_i\right\rangle = \frac{1}{\Omega^{1/2}} e^{i\mathbf{k}_i\cdot\mathbf{R}}$$

Then, in the Born approximation, we have that

$$V_{fi} = \langle f| \otimes \langle \mathbf{k}_f| \int d^3r \rho(\mathbf{r}) V^c(\mathbf{R} - \mathbf{r}) \ \left|\mathbf{k}_i\right\rangle \otimes |i\rangle \tag{7.21}$$

where the plane-wave matrix element can easily be evaluated

$$\int d^3R \left\langle \mathbf{k}_f\right| R\rangle \ V^c(\mathbf{R} - \mathbf{r}) \ \langle R| \left.\mathbf{k}_i\right\rangle = \Omega^{-1} \int d^3R e^{i(\mathbf{k}_i - \mathbf{k}_f)\cdot\mathbf{R}} V^c(\mathbf{R} - \mathbf{r}) = \frac{V^c_{-\mathbf{q}}}{\Omega} e^{i\mathbf{q}\cdot\mathbf{r}} \tag{7.22}$$

so that substitution in the expression for the matrix element gives,

$$V_{fi} = \frac{V^c_{-\mathbf{q}}}{\Omega} \int d^3r \quad \langle f| \rho(\mathbf{r}) \left|i\right\rangle e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{V^c_{-\mathbf{q}}}{\Omega} \langle f| \rho_{-\mathbf{q}} \left|i\right\rangle . \tag{7.23}$$

Substituting back in Fermi's Golden rule (7.19), we obtain

$$P_{i\to f} = \frac{2\pi}{\hbar} \left|\frac{V^c_{-\mathbf{q}}}{\Omega}\right|^2 \langle i| \rho_{\mathbf{q}} \left|f\right\rangle \langle f| \rho_{-\mathbf{q}} \left|i\right\rangle \delta(E_f - E_i - \hbar\omega). \tag{7.24}$$

Only the momentum and energy of the probe electron appear in this final expression, as we had hoped.

Definition 8 *Note in passing that we use the following definitions for Fourier transforms in the continuum*

$$\boxed{f_{\mathbf{q}} = \int d^3r\ f(\mathbf{r})\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}} \tag{7.25}$$

$$\boxed{f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} f_{\mathbf{q}}\mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}} \tag{7.26}$$

$$\boxed{g_\omega = \int dt\ g(t)e^{i\omega t}} \tag{7.27}$$

$$\boxed{g(t) = \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t}} \tag{7.28}$$

To compute the cross section of that probe electron, one proceeds in the usual manner described in textbooks. We will use a standard approach, but a more satisfactory derivation of cross section based on incident wave packets can be found in Ref.([83]). The total cross section, whose units are those of a surface, is equal to

$$\sigma = \frac{\text{Number of transitions per unit time}}{\text{Number of incident particles per unit time per unit surface}} \tag{7.29}$$

What we want is the differential cross section, in other words we want the cross section per solid angle $d\Omega_f$ and per energy interval $d\epsilon_f$. This is computed as follows. Since we cannot resolve the final electron state to better than $d\epsilon_f d\Omega_f$ all the final states in this interval should be counted. In other words, we should multiply $P_{i\to f}$ by the number of free electron states in this interval, namely

$$\Omega d^3k_f/(2\pi)^3 = \Omega k_f m d\epsilon_f d\Omega_f \hbar^{-2}/(2\pi)^3. \tag{7.30}$$

We should also trace over all final states $|f\rangle$ of the system since those are not measured. These states are constrained by conservation laws as we can see from the fact that energy conservation is insured explicitly by the delta function, while momentum conservation should come out automatically from the matrix element. The initial state of the system is also unknown. On the other hand, we know that the system is in thermal equilibrium, so a canonical average over energy eigenstates should give us the expected result. The differential cross section for scattering in an energy interval $d\epsilon_f$ and solid angle $d\Omega_f$ should then read,

$$\begin{aligned}\frac{d\sigma}{d\epsilon_f d\Omega_f} &= \frac{\text{Number of transitions per unit time in given solid angle and energy interval}}{\text{Number of incident particules per unit time per unit surface}}. \\ &= \left[\frac{\Omega k_f m\hbar^{-2}/(2\pi)^3}{\hbar k_i/(m\Omega)}\right] \frac{\sum_i e^{-\beta E_i}\sum_f P_{i\to f}}{\sum_i e^{-\beta E_i}}\end{aligned} \tag{7.31}$$

where we have used that the number of incident particles per unit time per unit surface is the velocity $\hbar k_i/m$ divided by the volume.

When we substitute the explicit expression for the transition probability in this last equation, it is possible to make the result look like an equilibrium correlation function by using Van Hove's trick to rewrite the matrix elements coming in the transition probability. Using the Heisenberg representation for the time evolution of the operators

$$\mathcal{O}(t) = e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar} \tag{7.32}$$

and taking H as the Hamiltonian for the system excluding probe electron, we have, $H|i\rangle = E_i|i\rangle$ so that

$$2\pi\hbar \langle i|\rho_{\mathbf{q}}|f\rangle \delta(E_f - E_i - \hbar\omega) = \int dt\ e^{i\omega t}\langle i|\rho_{\mathbf{q}}|f\rangle e^{-i(E_f-E_i)t/\hbar} \tag{7.33}$$

$$= \int dt\, e^{i\omega t} \langle i| e^{iHt/\hbar} \rho_{\mathbf{q}} e^{-iHt/\hbar} |f\rangle = \int dt\, e^{i\omega t} \langle i| \rho_{\mathbf{q}}(t) |f\rangle \,. \tag{7.34}$$

Substituting this expression in the equation for the transition probability, (7.24)

$$\sum_f P_{i\to f} = \left| \frac{V^c_{-\mathbf{q}}}{\Omega\hbar} \right|^2 \int dt\, e^{i\omega t} \langle i| \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) |i\rangle \tag{7.35}$$

the cross section is proportional to

$$\frac{\sum_i e^{-\beta E_i} \int dt\, e^{i\omega t} \langle i| \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) |i\rangle}{\sum_i e^{-\beta E_i}} = \frac{\sum_i \int dt\, e^{i\omega t} \langle i| e^{-\beta H} \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) |i\rangle}{\sum_i e^{-\beta E_i}} \tag{7.36}$$

$$= \int dt\, e^{i\omega t} \frac{Tr\left[e^{-\beta H} \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0)\right]}{Tr\left[e^{-\beta H}\right]} = \int dt\, e^{i\omega t} \left\langle \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \right\rangle \,. \tag{7.37}$$

More explicitly, we find Eq.(7.1) quoted at the beginning of the section. We thus have succeeded in expressing the inelastic electron-scattering experiment as a measurement of equilibrium density fluctuations!

8. TIME-DEPENDENT PERTURBATION THEORY

To compute the response of a system to a weak external probe, such as an applied electric field or temperature gradient, as opposed to a scattering probe as above, it seems natural to use perturbation theory. We will be interested in the response to linear order in the external probe. In fact, perturbation theory will be useful in many other contexts in this book, since this is the method that is behind adiabatic continuity. In this chapter we thus first pause to recall the various representations, or pictures, of quantum mechanics, introducing the interaction representation as the framework where perturbation theory is most easily formulated. Then we go on to derive linear response theory in the next chapter. If you already know about perturbation theory, you can skip to the next chapter.

8.1 Schrödinger and Heisenberg pictures.

Whether in classical or quantum mechanics, a basic property of the Hamiltonian is that it is the generator of infinitesimal time translations, Schrödinger's equation for a time-dependent Hamiltonian takes the form,

$$\boxed{i\hbar\frac{\partial|\psi_S(t)\rangle}{\partial t} = \mathcal{H}(t)\,|\psi_S(t)\rangle\,.} \tag{8.1}$$

It may look strange to have a Hamiltonian that depends on time. But when there is a semi-classical external probe, like a large electric field, acting on a system, then the part of the Hamiltonian that contains the external probe will just be a number (not an operator), leading to a time-dependent electric field.

Using the fact that $\mathcal{H}(t)$ is Hermitian, one can easily prove that $\partial\langle\psi_S|\psi_S\rangle/\partial t = 0$, in other words that probability is conserved. Hence, the solution of this equation will be given by

$$|\psi_S(t)\rangle = U(t,t_0)\,|\psi_S(t_0)\rangle \tag{8.2}$$

where $U(t,t_0)$ is a unitary operator, equal to an exponential only when $\mathcal{H}(t)$ is time independent. In general

$$U(t_0,t_0) = 1 \tag{8.3}$$

and

$$\boxed{i\hbar\frac{\partial U(t,t_0)}{\partial t} = \mathcal{H}(t)U(t,t_0).} \tag{8.4}$$

If time-reversal symmetry applies then

$$U(t_0,t)U(t,t_0) = 1. \tag{8.5a}$$

The adjoint is defined as usual

$$\begin{aligned}\langle\psi_S(t)| &= \langle U(t,t_0)\psi_S(t_0)| \\ &= \langle\psi_S(t_0)|\,U(t,t_0)^\dagger\,,\end{aligned} \tag{8.6}$$

where we used the usual definition of the adjoint of an operator $\mathcal{A}$: $\langle k|\ \mathcal{A}l\rangle = \left\langle \mathcal{A}^\dagger k\right|\ l\rangle$. Note that one takes the adjoint, but in the case of interest, that does not mean transposing t and t_0.

Conservation of probability gives

$$U(t,t_0)^\dagger U(t,t_0) = 1 \tag{8.7}$$

so that combining the last result with the definition of the inverse, we have,

$$U(t,t_0)^{-1} = U^\dagger(t,t_0). \tag{8.8}$$

Furthermore, *when we can use time-reversal symmetry,* Eq.(8.5a), (and only in that case) we also have

$$U(t,t_0)^{-1} = U(t_0,t). \tag{8.9}$$

By definition, for all values of t, the expectation value of an operator is the same in either the Schrödinger, or the Heisenberg picture.

$$\boxed{\langle\psi_S(t)|\,\mathcal{O}_S\,|\psi_S(t)\rangle = \langle\psi_H|\,\mathcal{O}_H(t)\,|\psi_H\rangle\,.} \tag{8.10}$$

In the Heisenberg picture the operators are time-dependent while in the Schrödinger picture, only the wave functions are time dependent. Let us choose $t = 0$ to be the time where both representations coincide. The choice of this time is arbitrary, but taking $t = 0$ simplifies greatly the notation. We have then that

$$\mathcal{O}_S(t=0) = \mathcal{O}_H(t=0) \equiv \mathcal{O}_S \tag{8.11}$$

$$\psi_S(t=0) = \psi_H(t=0) \equiv \psi_S \tag{8.12}$$

Using the expression for the time-dependent wave function, and the equality of matrix elements Eq.(8.10), we obtain

$$\mathcal{O}_H(t) = U^\dagger(t,0)\mathcal{O}_S U(t,0). \tag{8.13}$$

One recovers all the usual results for *time-independent* Hamiltonians by noting that in this case, the solution of Schrödinger's equation is,

$$\boxed{U(t,t_0) = e^{-i\mathcal{H}(t-t_0)/\hbar}.} \tag{8.14}$$

Remark 43 *When there is time-reversal invariance, then it is useful to replace the adjoint by the time-reversed operator, so that the connection between Heisenberg and Schrödinger picture Eq.(8.13) becomes*

$$\mathcal{O}_H(t) = U(0,t)\mathcal{O}_S U(t,0). \tag{8.15}$$

Because we do not want to assume for the time being that there is time-reversal invariance, we shall stick here with the usual expression Eq.(8.13) but in much of the later chapters, the above representation will be used. Aharonov and others have been proponents of this time symmetric formulation of quantum mechanics (Physics Today, Novembre 2010).

8.2 Interaction picture and perturbation theory

Perturbation theory is best formulated in the "interaction representation". In this picture, one can think of both operators and wave functions as evolving, as we will see. We take

$$\boxed{\mathcal{H}(t) = H_0 + \delta\mathcal{H}(t)} \tag{8.16}$$

where H_0 is time-independent as above, but the proof can be generalized to time-dependent H_0 simply by replacing $e^{iH_0t/\hbar}$ everywhere below by the appropriate evolution operator. The definition of the evolution operator in the interaction representation $U_I(t,0)$ is given by

$$U(t,0) \equiv e^{-iH_0t/\hbar}U_I(t,0). \tag{8.17}$$

If t is less than zero, then the interaction picture is defined by

$$U(0,t) \equiv U_I(0,t)e^{iH_0t/\hbar}. \tag{8.18}$$

The two definitions coincide at $t = 0$, namely $U_I(0,0) = 1$. This definition is useful because *when we can assume time-reversal symmetry*, the above definitions are consistent with $U(t,0)U(0,t) = I$. In general then, when we have $t_0 < 0$ then the evolution operator is given by

$$\boxed{U(t,t_0) \equiv e^{-iH_0t/\hbar}U_I(t,t_0)e^{iH_0t_0/\hbar}}. \tag{8.19}$$

We have used the fact that $U_I(t,t_0)$ obeys the same general properties of unitarity as an ordinary evolution operator, as can easily be checked. Again the interaction representation will coincide with the other two at $t = t_0 = 0$.

If we write again the equality of matrix elements in the general case, *without assuming time-reversal symmetry*, we obtain

$$\langle\psi_S(t)|\,\mathcal{O}_S\,|\psi_S(t)\rangle = \langle\psi_S|\,U^\dagger(t,0)\mathcal{O}_SU(t,0)\,|\psi_S\rangle \tag{8.20}$$

$$= \langle\psi_S|\,U_I^\dagger(t,0)e^{iH_0t/\hbar}\mathcal{O}_Se^{-iH_0t/\hbar}U_I(t,0)\,|\psi_S\rangle \tag{8.21}$$

$$= \langle\psi_S|\,U_I^\dagger(t,0)\mathcal{O}_I(t)\,U_I(t,0)\,|\psi_S\rangle \tag{8.22}$$

This last result is important. It can be interpreted as saying that the operators in the interaction representation evolve with

$$\boxed{\mathcal{O}_I(t) = e^{iH_0t/\hbar}\mathcal{O}_Se^{-iH_0t/\hbar}} \tag{8.23}$$

while the wave functions obey

$$\boxed{|\psi_I(t)\rangle = U_I(t,0)\,|\psi_S\rangle} \tag{8.24}$$

In other words, in the interaction picture both the operators and the wave function evolve and at $t = 0$ they coincide.

Remark 44 *The justification for the definition of U_I above is that when the external perturbation $\delta\mathcal{H}(t)$ is small, $U_I(t,0)$ is close to unity. The corresponding wave-function in the interaction picture evolves slowly as the last equation shows. It is as if we had gotten rid of the rapid time evolution caused by H_0. This is sometimes referred to as going to the rotating frame, especially in the field of nuclear magnetic resonance or quantum computing.*

We still have to find the equation of motion for $U_I(t,t_0)$. The result will justify why we introduced the interaction representation. Start from Schrödinger's equation, which as we saw above in Eq. (8.4) is equivalent to

$$i\hbar\frac{\partial U(t,t_0)}{\partial t} = \mathcal{H}(t)U(t,t_0) \tag{8.25}$$

then the equation of motion for $U_I(t,0)$, namely

$$H_0e^{-iH_0t/\hbar}U_I(t,0) + e^{-iH_0t/\hbar}i\hbar\frac{\partial}{\partial t}U_I(t,0) = \mathcal{H}(t)e^{-iH_0t/\hbar}U_I(t,0) \tag{8.26}$$

$$i\hbar\frac{\partial}{\partial t}U_I(t,0) = e^{iH_0t/\hbar}\delta\mathcal{H}(t)e^{-iH_0t/\hbar}U_I(t,0). \tag{8.27}$$

so that using the definition of time evolution of an arbitrary operator in the interaction representation as above (8.23), the equation for the time evolution operator $U_I(t,0)$ in the interaction representation may be written,

$$i\hbar\frac{\partial}{\partial t}U_I(t,0) = \delta\mathcal{H}_I(t)U_I(t,0) \tag{8.28}$$

with the initial condition

$$U_I(0,0) = 1. \tag{8.29}$$

As expected, Eq.(8.28) tells us that, if there is no perturbation, U_I is equal to unity for all times and only the operators and not the wave function evolve. The interaction representation then reduces to the Heisenberg representation. Multiplying the equation of motion from the right by $U_I(0,t_0)$, where t_0 is less than 0, we have for an arbitrary initial time

$$\boxed{i\hbar\tfrac{\partial}{\partial t}U_I(t,t_0) = \delta\mathcal{H}_I(t)U_I(t,t_0)} \tag{8.30}$$

We will come back later to a formal solution of this equation. To linear order in the external perturbation, it is an easy equation to solve by iteration using the initial condition as the initial guess. Indeed, integrating on both sides of the equation of motion (8.30) and using the initial condition, $U_I(t_0,t_0) = 1$ we have

$$\boxed{U_I(t,t_0) = 1 - \tfrac{i}{\hbar}\int_{t_0}^{t} dt'\ \delta\mathcal{H}_I(t')U_I(t',t_0)} \tag{8.31}$$

which, iterated to first order, gives,

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \tag{8.32}$$

and correspondingly

$$U_I^\dagger(t,t_0) = 1 + \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \tag{8.33}$$

because Hamiltonians are self adjoint.

Remark 45 *The number* 1 *that appears on the right-hand side of the last two equation operates on the Hilbert space as the identity matrix.*

Remark 46 *Other interpretation of the interaction picture: As we will see later, another possible interpretation of the interaction representation is that one needs to sum over all possible quantum histories, namely, for example, sum over all possible scatterings of electrons between themselves if the perturbation is the interaction between the electrons. This is where the physical picture is dependent on perturbation theory.*

9. LINEAR-RESPONSE THEORY

We are interested in the response of a system to a weak external perturbation. The electrical conductivity is the response to a weak applied field, the thermal conductivity the response to a weak thermal gradient etc. The result will be again an equilibrium correlation function. In fact, we can already guess that if we evolve some operator B in the interaction representation with a U_I on the right and a $U_I^\dagger$ on the left to first order in $\delta\mathcal{H}_I(t')$ as in the last two equations of the previous section, we will simply end up with the thermal average of a commutator. We will be able to relate the latter correlation function to equilibrium correlation functions of the type just calculated at the end of the last section by relying on the general quantum version of the "fluctuation-dissipation theorem" encountered in Part I. The plan to compute the effect of an external perturbation is to add it to the Hamiltonian and then to treat it as a perturbation, taking the full interacting Hamiltonian of the system H as the unperturbed Hamiltonian. Let us move to the details, that are unfortunately a bit messy, but really straightforward.

Let

$$\mathcal{H}(t) = H + \delta\mathcal{H}(t) \tag{9.1}$$

where H is the Hamiltonian of the system under study (that we called H_s in the example of system interacting wih probe above) and $\delta\mathcal{H}(t)$ is the perturbation that does not commmute with H in general. The time-dependent Hamiltonian is defined as

$$\boxed{\delta\mathcal{H}(t) = -\int d^3r A_i(\mathbf{r}) a_i(\mathbf{r},t).} \tag{9.2}$$

In this expression, A_i is some observable of the system (excluding external perturbation) in the Schrödinger representation, while $a_i(\mathbf{r},t)$ is a classical external field. Examples of such couplings to external fields include the coupling to a magnetic field $\mathbf{h}$ through the magnetization $\mathbf{M}$, $(A_i(\mathbf{r}) = M_z(\mathbf{r});\ a_i(\mathbf{r},t) = h_z(\mathbf{r},t))$ or the coupling to an electromagnetic vector potential $\mathbf{A}$ through a current $\mathbf{j}$, $(A_i(\mathbf{r}) = j_x(\mathbf{r})\delta_{i,x};\ a_i(\mathbf{r},t) = A_x(\mathbf{r},t)\delta_{i,x})$ or that of a scalar potential ϕ through the density ρ $(A_i(\mathbf{r}) = \rho(\mathbf{r});\ a_i(\mathbf{r},t) = \phi(\mathbf{r},t))$. In this approach, it is clear that the external perturbation is represented in the *semi-classical approximation*, in other words it is not quantized, by contrast again with the scattering of a probe with a system that we discussed above.

In the case of interest to us the external perturbation in the interaction representation is of the form,

$$\boxed{\delta\mathcal{H}_I(t) = -\int d^3r A_i(\mathbf{r},t) a_i(\mathbf{r},t)} \tag{9.3}$$

where for short we wrote $A_i(\mathbf{r},t)$ to represent a system's observable evolving in the system's Heisenberg representation,

$$A_i(\mathbf{r},t) = e^{iHt/\hbar} A_i(\mathbf{r}) e^{-iHt/\hbar}. \tag{9.4}$$

Suppose we want the expectation value of the observable B in the presence of the external perturbation turned on at time t_0. Then, starting from a thermal equilibrium state $\widehat{\varrho} = e^{-\beta H}/\mathrm{Tr}\left[e^{-\beta H}\right]$ at time t_0, it suffices to evolve the operator $B(\mathbf{r})$ defined in the Schrödinger picture with the full evolution operator, including

the external perturbation [1]

$$\langle B(\mathbf{r},t)_{n.e.}\rangle = \left\langle U^{\dagger}(t,t_0)B(\mathbf{r})U(t,t_0)\right\rangle . \tag{9.5}$$

In this expression, the subscript $n.e.$ on the left reminds us that the time dependence includes that from the external perturbation. Using the interaction representation Eq.(8.19), *with H now playing the role of H_0 in the previous section*, the last equation becomes

$$\langle B(\mathbf{r},t)_{n.e.}\rangle = \left\langle e^{-iHt_0/\hbar}U_I^{\dagger}(t,t_0)e^{iHt/\hbar}B(\mathbf{r})e^{-iHt/\hbar}U_I(t,t_0)e^{iHt_0/\hbar}\right\rangle \tag{9.6}$$

$$\langle B(\mathbf{r},t)_{n.e.}\rangle = \left\langle U_I^{\dagger}(t,t_0)B(\mathbf{r},t)U_I(t,t_0)\right\rangle . \tag{9.7}$$

In this last expression, $B(\mathbf{r},t)$ on the right-hand side is now in the system's Heisenberg representation *without the external perturbation*. In the previous section, this Hamiltonian was called H_0. To cancel the extra $e^{-iHt_0/\hbar}$ and $e^{iHt_0/\hbar}$ appearing in the equation for the evolution operator in Eq.(8.19), we used the facts that the trace has the cyclic property and that the density matrix Eq. (7.12), namely $\widehat{\varrho} = e^{-\beta H}/\mathrm{Tr}\left[e^{-\beta H}\right]$ commutes with $e^{iHt_0/\hbar}$. This expression for the density matrix is justified by the fact that initially the external probe is absent.

Using the explicit expression Eq.(9.3) for the external perturbation in the equation for the evolution operator in the interaction representation (8.32), we have that the term linear in applied field

$$\delta\langle B(\mathbf{r},t)\rangle \equiv \langle B(\mathbf{r},t)_{n.e.}\rangle - \langle B(\mathbf{r},t)\rangle \tag{9.8}$$

is then given by,

$$\delta\langle B(\mathbf{r},t)\rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt' \int d^3r' \,\langle [B(\mathbf{r},t), A_i(\mathbf{r}',t')]\rangle \, a_i(\mathbf{r}',t'). \tag{9.9}$$

It is customary to take $t_0 = -\infty$, assuming that the perturbation is turned-on adiabatically slowly. One then defines a "retarded" response function, or susceptibility χ^R, by

$$\boxed{\delta\langle B(\mathbf{r},t)\rangle = \textstyle\int_{-\infty}^{\infty} dt' \int d^3r' \,\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')a_i(\mathbf{r}',t')} \tag{9.10}$$

with,

$$\boxed{\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t') = \tfrac{i}{\hbar}\,\langle [B(\mathbf{r},t), A_i(\mathbf{r}',t')]\rangle}. \tag{9.11}$$

Following our previous definition with the harmonic oscillator Eq. (3.14), this is also written in the form

$$\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t') = 2i\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t')\theta(t-t'), \tag{9.12}$$

where you can read off the definition of $\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t')$ by comparing the last two equations. This response function $\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')$ is called "retarded" because the response always comes after the perturbation, as expected in a causal system. The function $\theta(t-t')$ ensures this causality. One can also define anti-causal response functions. We come back to this later. We notice that the linear response is given by an equilibrium correlation function where everything is determined by the Hamiltonian H without the external probe.

This completes our derivation of the different types of correlation functions measured by the two great types of weak probes: scattering probes and semiclassical probes. We move on to discuss properties of these correlation functions and relations between them.

[1] We let the density matrix take its initial equilibrium value. This is physically appealing. But we could have as well started from a representation where it is the density matrix that evolves in time and the operators that are constant.

Remark 47 *Translationally invariant case: Since we compute equilibrium averages, the susceptibility* $\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')$ *can depend only on the time difference. In the translationally invariant case, the susceptibility is also a function of only* $\mathbf{r}-\mathbf{r}'$ *so that Fourier transforming the expression for the linear response (9.10), we obtain from the convolution theorem in this case,*

$$\boxed{\delta\langle B(\mathbf{q},\omega)\rangle = \chi^R_{BA_i}(\mathbf{q},\omega)a_i(\mathbf{q},\omega).} \tag{9.13}$$

Remark 48 *Frequency of the response: The response is at the same frequency as the external field, a feature which does not survive in non-linear response.*

Remark 49 *Onsager reciprocity relations: Given the expression for the response function in terms of a commutator of Hermitian operators, it is clear that the response of the operator* B *to an external perturbation that couples to* A *is simply related to the response of* A *to a perturbation that couples to* B*, in other words where the operators have reversed roles. These are "Onsager's reciprocity relations". A classic example occurs in the context of thermopower. In that case, there is a relation the case where a thermal gradient causes a voltage difference and the case where a voltage difference causes a thermal gradient. In the first case, we refer to the Seebeck effect and the other case the Peltier effect.*

Remark 50 *Validity of linear response and heating: Finally, we can ask whether it is really justified to linearize the response. Not always since the external perturbation can be large. But certain arguments suggest that it is basically never correct in practice to linearize the response. Indeed, assume we apply an external electric field* E*. As long as the energy gained by the action of the field is smaller than* k_BT*, the linearization should be correct. In other words, linear response theory should be valid for a time*

$$t < \frac{k_BT}{eEv}. \tag{9.14}$$

This is unfortunately a ridiculously small time. Taking $v \approx \sqrt{k_BT/m}$ *the condition becomes* $t < \sqrt{mk_BT}/eE$ *with* $E = 1V/cm$*,* $\sqrt{mk_BT}/eE \approx \sqrt{10^{-30}10^{-23}10^{2}}/10^{-19} \approx 10^{-6}s$*. If we take the Fermi velocity for* v*, the time is even smaller. One finds that unless there is a temperature gradient, or an explicit interaction with a system in equilibrium (such as phonons), the second order term in perturbation theory is secular, i.e. it grows linearly with time. This is nothing more than the phenomenon of Joule heating.[233] We are then forced to conclude that linear response theory applies, only as long as the system is maintained in equilibrium by some means: for example by explicitly including interactions with phonons which are by force taken to be in thermal equilibrium, or by allowing for a thermal gradient in the system that carries heat to the boundaries. From the point of view of the Boltzmann equation, one can see explicitly that if the second-order term in* E *is kept small by collisions with a system in thermal equilibrium, then the linear term is basically equal to what we would have obtained by never going to second-order in the first place.[233][234][237]*

Remark 51 *Reversibility and linear response: Other arguments against linear response theory center on the fact that a correlation function where operators all evolve reversibly cannot describe irreversible processes. [240] We have seen in Part I and will see explicitly again later that it is possible to compute irreversible absorption with this approach. Irreversibility appears in the infinite-volume limit.*

Remark 52 *At the operator level, causality comes automatically from the equations of motion for the evolution operator Eq. (8.32). In other words, the value of*

the evolution operator at time t, or of the wave function, depends only on what happened at previous times. But we know that in the measurement process of a single event, the results can only be predicted with a certain probability. That probability can be calculated from the wave function, but there is a fundamental randomness in quantum mechanics that makes certain events appear without precise cause. Here I will always compute expectation values, so we have strict causality and we are never directly confronted with this problem.

10. GENERAL PROPERTIES OF CORRELATION FUNCTIONS

There are unfortunately very few things that one can know exactly about a piece of condensed matter. Turning this around, it is in fact remarkable that we know at least a few things. So it is useful to become familiar with such exact results. We begin with analytic properties that do not depend on the microscopic model considered. This has at least two advantages: a) to check whether approximation schemes satisfy these exact relations b) to formulate phenomenological relations which are consistent. We will see that approximate calculations usually cannot satisfy all known exact relations for correlation functions, but it will be obvious that violating certain relations is more harmful than violating others. Many of the general properties which we will discuss in the present context have trivial generalizations for Green's function. Working on these general properties now will make them look more natural later when we introduce the curious Green's function beast!

10.1 Notations and definition of χ''

To start with, recall the definition

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') = \frac{i}{\hbar}\left\langle [B(\mathbf{r},t),A(\mathbf{r}',t')]\right\rangle \theta(t-t'). \tag{10.1}$$

I define one more correlation function which will, in most cases of physical interest, play the role of the quantity that describes absorption. Welcome χ''

$$\boxed{\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \tfrac{1}{2\hbar}\left\langle [B(\mathbf{r},t),A(\mathbf{r}',t')]\right\rangle .} \tag{10.2}$$

Why do I do this? With this definition, we have

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') = 2i\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t')\theta(t-t'). \tag{10.3}$$

Look at back at our harmonic oscillator and see how retarded functions look when transformed back to time by staring at Eq. (3.14). The η can be seen as ensuring that the Fourier transform back to frequency exists and has the right properties. A much more detailed discussion appears in Remark (65).

The definition now looks natural. The factor of two in the denominator of the definition looks strange, but it will allow χ'' to generally satisfy the Kramers-Kronig relations in their standard form. The quantity χ''_{BA} has symmetry properties, discussed below, that suffice to find those of the retarded response. It also contains all the physics, except causality that is represented by the θ function.

To shorten the notation, we will also use the short hand

$$\boxed{\chi^R_{A_iA_j}(t-t') = \tfrac{i}{\hbar}\left\langle [A_i(t),A_j(t')]\right\rangle \theta(t-t').} \tag{10.4}$$

where we include in the indices i and j the positions as well as any other label of the operator such as vector or spin component. In this notation, we have

not assumed translational invariance. We did however assume time-translation invariance. Since we are working with equilibrium averages above, this is always true.

Corresponding to the short-hand notation, we have

$$\boxed{\chi''_{A_iA_j}(t-t') \equiv \tfrac{1}{2\hbar}\left\langle [A_i(t), A_j(t')]\right\rangle}. \tag{10.5}$$

$$\boxed{\chi^R_{A_iA_j}(t-t') = 2i\chi''_{A_iA_j}(t-t')\theta(t-t').} \tag{10.6}$$

Remark 53 *All the physics will be in $\chi''_{A_iA_j}(t-t')$ clearly. And, following our discussion of the response of the classical harmonic oscillator, the Fourier transform of the retarded susceptibilities $\chi^R_{A_iA_j}(t-t')$ will obey Kramers-Kronig relations and have a spectral representation.*

Remark 54 *If A and B are Hermitian, then $\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t')$ must be real, which means that $\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t')$ is purely imaginary, as we expect from the commutator of any pair of Hermitian operators, such as $[x,p]=i\hbar$. This phase difference of $\pi/2$ will be responsible with the fact that $\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t')$ will often be related to dissipation. We saw an example of that in Section (3.3).*

Remark 55 *Classical limit: In the classical limit, commutators divided by $i\hbar$ become Poisson brackets. Sum rules arise from evaluating commutators at equal-time ($t=t'$), as will become clear shortly. Similarly then, in the classical limit, one can obtain sum rules from the evaluation of Poisson brackets at equal time. Sum rules also exist in classical mechanics, as we saw from our example of the simple harmonic oscillator. The relation between Poisson brackets and commutators gives us a deeper reason to understand why sum rules exist in both the quantum and classical realm.*

10.2 Symmetry properties of H and symmetry of the response functions

The quantity $\chi''_{A_iA_j}(t-t')$ contains all the non-trivial information on the response. Indeed, the causal response is simply obtained by multiplying by a trivial $\theta(t-t')$ function. Certain symmetries of this response function depend on the particular symmetry of the Hamiltonian, others are quite general. We begin with properties that depend on the symmetry of H. [75]

Let S be a symmetry of the Hamiltonian. By this we mean that the operator S representing the symmetry commutes with the Hamiltonian

$$[H,S]=0 \tag{10.7}$$

To be more precise, in the context of statistical mechanics we say that S is a symmetry of the system when it commutes with the density matrix

$$[\varrho,S]=0 \tag{10.8}$$

In other words,

$$S\varrho S^{-1}=\varrho \tag{10.9}$$

thus the spectrum of the density matrix is unaffected by the symmetry operation. The operator S is in general unitary or antiunitary as we will see below.

To extract non-trivial consequences of the existence of a symmetry, note that the cyclic property of the trace allows us to act on the operators instead of on the basis functions. In other words, we have

$$\begin{aligned}\langle\mathcal{O}\rangle &= \mathrm{Tr}[\rho\mathcal{O}] = \mathrm{Tr}[S\varrho S^{-1}\mathcal{O}] \\ &= \mathrm{Tr}[\varrho S^{-1}\mathcal{O}S]\end{aligned}$$

$$\boxed{\left\langle S^{-1}\mathcal{O}S\right\rangle = \langle\mathcal{O}\rangle} \tag{10.10}$$

It is because S and $\mathcal{O}$ in general do not commute that the above equation leads to non-trivial consequences. When two different operators are involved in the expectation value, as will be the case below for χ'', note that

$$\left\langle S^{-1}\mathcal{O}_1\mathcal{O}_2S\right\rangle = \left\langle\left(S^{-1}\mathcal{O}_1S\right)\left(S^{-1}\mathcal{O}_2S\right)\right\rangle \tag{10.11}$$

which is valid even if $\mathcal{O}_1$ and $\mathcal{O}_2$ are not at the same time since by hypothesis S commutes with H and hence with the time-evolution operator.

Let us look in turn at the consequences of translational invariance and of invariance under a parity transformation $\mathbf{r}_\alpha \to -\mathbf{r}_\alpha$.

10.2.1 Translational invariance

When there is translational invariance, it means that if all operators are translated by $\mathbf{R}$, the thermal averages are unchanged. In other words,

$$\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA}(\mathbf{r}+\mathbf{R},t;\mathbf{r}'+\mathbf{R},t') \tag{10.12}$$

so that χ''_{BA} is a function of $\mathbf{r}-\mathbf{r}'$ only. Since we already know that χ''_{BA} is a function only of $t-t'$, in such cases we write

$$\boxed{\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA}(\mathbf{r}-\mathbf{r}';t-t')} \tag{10.13}$$

In the general case, to go to Fourier space one needs two wave vectors, corresponding respectively to $\mathbf{r}$ and $\mathbf{r}'$ but in the translationally invariant case, only one wave vector suffices. (You can prove this by changing integration variables in the Fourier transform to the center of mass and difference variables).

10.2.2 *Parity

Under a parity transformation, operators transform as follows

$$P^{-1}\mathcal{O}(\mathbf{r})P = \varepsilon^P\mathcal{O}(-\mathbf{r}) \tag{10.14}$$

where $\varepsilon^P = \pm 1$. This number is known as the "signature" under parity transformation. That $\varepsilon^P = \pm 1$ is the only possibility for simple operators like density and momentum follows from the fact that applying the parity operation twice is the same as doing nothing. In other words, $P^2 = 1$. To be more specific, $\varepsilon^P_\rho = 1$ for density since performing the symmetry operation $\mathbf{r}_\alpha \to -\mathbf{r}_\alpha$ for every particle coordinate appearing in the density operator in first quantization

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{N} e_\alpha\delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{10.15}$$

we find

$$P^{-1}\rho(\mathbf{r})P = \sum_{\alpha=1}^{N} e_\alpha \delta(\mathbf{r}+\mathbf{r}_\alpha) = \sum_{\alpha=1}^{N} e_\alpha \delta(-\mathbf{r}-\mathbf{r}_\alpha) = \rho(-\mathbf{r}). \tag{10.16}$$

For the momentum operator, $\varepsilon_p^P = -1$, as we can show by the following manipulations

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^{N} \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{10.17}$$

$$P^{-1}\mathbf{p}(\mathbf{r})P = \sum_{\alpha=1}^{N} -\frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r}+\mathbf{r}_\alpha) = -\sum_{\alpha=1}^{N} \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(-\mathbf{r}-\mathbf{r}_\alpha) = -\mathbf{p}(-\mathbf{r}).$$

In general then, this implies that

$$\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{r},t;-\mathbf{r}',t') \tag{10.18}$$

When we also have translational invariance, the last result means that $\chi''_{BA}(\mathbf{r}-\mathbf{r}';t-t')$ is even or odd in $\mathbf{r}-\mathbf{r}'$ depending on whether the operators have the same or opposite signatures under parity. Correspondingly, the Fourier transform in the translationally invariant case is odd or even, as can easily be proven by a change of integration variables in the Fourier transform

$$\boxed{\chi''_{BA}(\mathbf{q};t-t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{q};t-t')} \tag{10.19}$$

Remark 56 *To clarify the meaning of the operators above, recall that for example to obtain the charge density of a two-particle wave function, you need to compute*

$$\begin{aligned} \langle\psi|\,\rho(\mathbf{r})\,|\psi\rangle &= e\int d^3\mathbf{r}_1 \int d\mathbf{r}_2 \psi^*(\mathbf{r}_1,\mathbf{r}_2)\,\rho(\mathbf{r})\,\psi(\mathbf{r}_1,\mathbf{r}_2) \\ &= e\int d^3\mathbf{r}_2 \psi^*(\mathbf{r},\mathbf{r}_2)\,\psi(\mathbf{r},\mathbf{r}_2) + e\int d^3\mathbf{r}_1 \psi^*(\mathbf{r}_1,\mathbf{r})\,\psi(\mathbf{r}_1,\mathbf{r}) \end{aligned} \tag{10.20}$$

which gives the contributions to the charge density at point $\mathbf{r}$ *from all the particles.*

10.2.3 Time-reversal symmetry in the absence of spin is represented by complex conjugation for the wave function and by the transpose for operators

What happens to operators under time reversal we can easily guess by knowing the classical limit. To take simple cases, position does not change but velocity and momentum change sign. To achieve the latter result with the momentum density operator

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^{N} \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{10.21}$$

it appears that complex conjugation suffices. It works because $\mathbf{p}(\mathbf{r})$ is hermitian so that complex conjugation suffices as I will show belos. Does this mean that for the wave function, the operation of time reversal is simply complex conjugation? The answer is yes, except that in the most general case, there can be an additional unitary operation. We will encounter the latter in the case of spin in the following subsection. What we cannot guess from the classical limit is what happens to the wave function under time reversal. But inspired by the case of momentum, it is

natural to suggest that in the simplest case, time reversal corresponds to complex conjugation. Inverting time again would mean taking the complex conjugate again and hence returning to the original state. That is reassuring. If we accept that time reversing an operator is taking its complex conjugate, then H^* should correspond to time inversion of H.

We can give another plausibility argument. Consider the solution of the Schrödinger equation *for a time-independent Hamiltonian:*

$$\psi_S(t) = e^{-iHt/\hbar}\psi_S(0). \tag{10.22}$$

Suppose that H involves the square of momentum and some space dependent potential so that it is clearly invariant under time reversal. Then, evolving some state backwards from an initial state $\widetilde{\psi}_S(0)$ means that

$$\widetilde{\psi}_S(-t) = e^{iHt/\hbar}\widetilde{\psi}_S(0). \tag{10.23}$$

But by taking the complex conjugate of the Schrödinger equation and noting that the Hamiltonian we have in mind has the property $H = H^*$, we find that

$$\psi_S^*(t) = e^{iHt/\hbar}\widetilde{\psi}_S^*(0). \tag{10.24}$$

It thus looks as if the complex conjugate just evolves backward in time.

We can see the full time-inversion invariance in an alternate manner by doing the quantum mechanical analog of the following classical calculation for equations of motion that are time-reversal invariant. Evolve a system for a time t_0, stop and invert all velocities and evolve again for a time t_0. If we change the sign of all velocities again we should have recovered the initial state. The quantum mechanical analog is as follows. a) Start from $\psi_S(0)$ .b) Evolve it until time t_0.We then have the state $\psi_S(t_0) = e^{-iHt_0/\hbar}\psi_S(0)$ .c) Take time inversion on that state. This is the equivalent in classical mechanics of inverting all velocities. Quantum mechanically, the new state is $\psi_S^*(t_0) = e^{iH^*t_0/\hbar}\psi_S^*(0)$. d) Evolve that state for a time t, again using the usual time evolution operator for the usual Shcrödinger equation, not its complex conjugate i.e. $\psi_S^*(t_0+t) = e^{-iHt/\hbar}\left(e^{iH^*t_0/\hbar}\psi_S^*(0)\right)$. If we follow our classical analogy, when $t = t_0$, we should have returned to our initial state if H is time-reversal invariant, except that the velocities have changed sign. In quantum mechanics, time reversal invariant means $H = H^*$. When this is the case, what we find for the quantum mechanical state is $\psi_S^*(t_0+t_0) = \psi_S^*(0)$ .The equivalent of changing the velocities again in the classical case is that we take complex conjugation. That returns us indeed to the original state $\psi_S(0)$. That is all there is in the simplest scalar case. Time inversion means taking complex conjugate.

A system in equilibrium obeys time-inversion symmetry, unless an external magnetic field is applied. This means that equilibrium averages evaluated with time-reversed states are equal to equilibrium averages evaluated with the original bases. In fact time-inversion symmetry is a very subtle subject. A very complete discussion may be found in Gottfried [83] and Sakurai [206]. We present an over-simplified discussion. Let us call T_t the operator that time-reverses a state. This is the operation of complex conjugation that we will call K. The first thing to notice it that it is unlike any other operator in quantum mechanics. In particular, the Dirac notation must be used with extreme care. Indeed, for standard operators, say X, we have the associative axiom

$$\langle\alpha| X |\beta\rangle = \langle\alpha| \quad (X|\beta\rangle) = (\langle\alpha| X) \quad |\beta\rangle \tag{10.25}$$

This is clearly incorrect if X is the complex conjugation operator. Hence, we must absolutely specify if it acts on the right or on the left. Hence, we will write $\underrightarrow{K}$ when we want to take the complex conjugate of a ket, and $\underleftarrow{K}$ to take the complex conjugate of a bra.

Proposition 9 ***Remark 57*** *Antiunitary operators: Time reversal is an antiunitary operation. The key property that differentiates an anti-unitary operator from a unitary one is its action on a linear combination*

$$T_t\left(a_1\left|\psi_1\right\rangle + a_2\left|\psi_2\right\rangle\right) = a_1^* T_t\left|\psi_1\right\rangle + a_2^* T_t\left|\psi_2\right\rangle \tag{10.26}$$

In general such an operator is called antilinear. Antiunitarity comes in when we restrict ourselves to antilinear operators that preserve the norm. The time reversal operator is such an operator. Under time reversal, an arbitrary matrix element preserves its norm, but not its phase. This is easy to see from the fact that for an arbitrary matrix element $\langle\psi_1|\underleftarrow{K}\underrightarrow{K}|\psi_2\rangle = \langle\psi_2|\psi_1\rangle \neq \langle\psi_1|\psi_2\rangle$ *the phase changes sign under complex conjugation while the square modulus* $\langle\psi_2|\psi_1\rangle\langle\psi_1|\psi_2\rangle$ *is invariant. Gottfried[83] shows that only discrete transformations (not continuous ones) can be described by anti-unitary operators. This reference also discusses the theorem by Wigner that states that if we declare that two descriptions of quantum mechanics are equivalent if* $|\langle\psi_2|\psi_1\rangle| = \left|\left\langle\psi_2'\middle|\psi_1'\right\rangle\right|$ *(equality of "rays") then both unitary and anti-unitary transformations are allowed.*

- **Remark 58** *The adjoint is not the inverse. Note that* $T_t^\dagger T_t = \underleftarrow{K}\underrightarrow{K}$*, so this last quantity is not the identity because the rightmost complex conjugation operator acts to the right, and the leftmost one to the left. Again, it is not convenient to talk about time-reversal in the usual Dirac notation.*

Returning to the action of the time reversal operation on a Schrödinger operator, we see that the expectation value of an arbitrary operator between time reversed states is

$$\langle i|\underleftarrow{K}\mathcal{O}\underrightarrow{K}|j\rangle = \left(\langle i|\underleftarrow{K}\right)\left(\underrightarrow{K}\mathcal{O}^*|j\rangle\right) = \left(\langle i|\underleftarrow{K}\underrightarrow{K}|\mathcal{O}^* j\rangle\right) = \langle j|\mathcal{O}^{\dagger *}|i\rangle\,. \tag{10.27}$$

In the above expression, we used one of the properties of the hermitian product, namely $\langle k|l\rangle^* = \langle l|k\rangle$, as well as the definition of the adjoint of an operator $\mathcal{A}$: $\langle k|\mathcal{A}l\rangle = \left\langle\mathcal{A}^\dagger k\middle| l\right\rangle$ which implies, that $\langle k|\mathcal{A}|l\rangle^* = \langle l|\mathcal{A}^\dagger|k\rangle$. Applying this expression Eq.(10.27) for diagonal expectation values, and recalling that the density matrix is real and hermitian, we find for equilibrium averages,

$$\boxed{\left\langle\underleftarrow{K}\mathcal{O}\underrightarrow{K}\right\rangle = \left\langle\mathcal{O}^{\dagger *}\right\rangle = \varepsilon^t\left\langle\mathcal{O}^\dagger\right\rangle}\,. \tag{10.28}$$

The last equality defines the signature of the time-reversal operation for operators. One easily finds that $\epsilon^t = +1$ for position while $\epsilon^t = -1$ for velocity or momentum, etc... Note that $\mathcal{O}^{\dagger *}$ is the transpose of the operator. The signature under complex conjugation can only be ± 1, since applying complex conjugation twice is equivalent to the identity.

We can use this last result to find the effect of the time-reversal invariance on general correlation functions. The action of time reversal Eq.(10.28) gives, when A and B are *self-adjoint* operators, and in addition the Hamiltonian is real ($\underrightarrow{K}H = H\underrightarrow{K}$)

$$\begin{aligned}\left\langle\underleftarrow{K}A(t)B\underrightarrow{K}\right\rangle &= \left\langle B^* e^{-iHt/\hbar}A^* e^{iHt/\hbar}\right\rangle \\ &= \epsilon_A^t\epsilon_B^t\left\langle BA(-t)\right\rangle\end{aligned} \tag{10.29}$$

In addition to the signature, the order of operators is changed as well as the sign of time. For $\chi''_{A_iA_j}(t-t')$ this immediately leads to

$$\chi''_{A_iA_j}(t-t') = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(-t'-(-t)) \tag{10.30}$$

and for the corresponding Fourier transform in frequency,

$$\boxed{\chi''_{A_iA_j}(\omega) = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(\omega)}. \tag{10.31}$$

Seeing $\chi''_{A_iA_j}(\omega)$ as a matrix in A_iA_j, helps to remember this result a stating that time reversal transposes this matrix and multiplies it by the signature of each of its operators.

- **Remark 59** *In the case of an equilibrium average where both the density matrix and the Hamiltonian commute with the time-reversal operation, we have, as in Eq.(10.10),*

$$\left\langle T_t^{-1}\mathcal{O}T_t\right\rangle = \langle\mathcal{O}\rangle\,. \tag{10.32}$$

Hence as expected, Eqs.(10.28) and (10.32) together imply that Hermitian operators that have an odd signature with respect to time reversal symmetry have a vanishing expectation value in equilibrium.

10.2.4 *Time-reversal symmetry in the presence of spin necessitates a matrix representation

Spin should transform under time reversal like angular momentum $\mathbf{r}\times\mathbf{p}$, in other words it should change sign since $\mathbf{r}$ does not while $\mathbf{p}$ does. Complex conjugation has this property for $\mathbf{r}\times\mathbf{p}$ but not for spin represented by Pauli matrices. We should really wait for the section where we treat fermions to discuss this problem but we can start to address it here. To come out from the problem that complex conjugation does not suffice anymore, it suffices to notice that in general the time reversal operator has to be represented by a unitary operator times complex conjugation. The resulting operator is still anti-unitary, as can easily be proven. Let us thus write

$$T_t = \underrightarrow{K}U \tag{10.33}$$

where $\underrightarrow{K}$ is complex conjugation again and U is a unitary operator $U^\dagger U = 1$ in spin space that we need to find. Note that the action on a bra is given by

$$U^\dagger\underleftarrow{K} \tag{10.34}$$

Let us first repeat the steps of calculating expectation values in time-reversed states, as in Eq.(10.27), but for the more general case

$$\langle i|\,U^\dagger\underleftarrow{K}\mathcal{O}\underrightarrow{K}U\,|j\rangle = \left(\langle i|\,U^\dagger\underleftarrow{K}\right)\left(\underrightarrow{K}\mathcal{O}^*U\,|j\rangle\right) = \left(\langle Ui|\,\underleftarrow{K}\underrightarrow{K}\,|\mathcal{O}^*Uj\rangle\right) = \langle j|\,U^\dagger\mathcal{O}^{\dagger *}U\,|i\rangle \tag{10.35}$$

Computing the equilibrium trace with $U^\dagger\mathcal{O}^{\dagger *}U$ is thus equivalent to computing the equilibrium trace in time-reversed states but with $\mathcal{O}$. If we take for $\mathcal{O}$ the spin $\boldsymbol{\sigma}$, the net effect of the time-reversal operation should be to change the direction of the spin, in other words, we want

$$U^\dagger\boldsymbol{\sigma}^{\dagger *}U = -\boldsymbol{\sigma} \tag{10.36}$$

The expression for U will depend on the basis states for spin. Using the Pauli matrix basis

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad ; \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad ; \quad \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{10.37}$$

we have $\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$, and $\sigma_x^* = \sigma_x$, $\sigma_y^* = -\sigma_y$, $\sigma_z^* = \sigma_z$ so that Eq.(10.36) for time reversal gives us the following set of equations for the unitary operator U

$$U^\dagger \sigma_x U = -\sigma_x \tag{10.38}$$

$$U^\dagger \sigma_y U = \sigma_y \tag{10.39}$$

$$U^\dagger \sigma_z U = -\sigma_z \tag{10.40}$$

Given the fundamental properties of Pauli matrices

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 0 \quad \text{for } i \neq j$$

$$\sigma_i^2 = 1 \tag{10.41}$$

$$\sigma_i \sigma_j = i\sigma_k \tag{10.42}$$

where i, j, k are cyclic permutations of x, y, z, the solution to the set of equations for U is

$$U = e^{i\delta}\sigma_y \tag{10.43}$$

where δ is an arbitrary real phase. This is like a π rotation along the y axis so that already we can expect that up will be transformed into down as we were hoping intuitively. In summary, the time reversal operator in the presence of spin multiplies the spin part by $e^{i\delta}\sigma_y$ and takes the complex conjugate.

$$T_t = \underrightarrow{K} e^{i\delta}\sigma_y \tag{10.44}$$

Note the action of this operator on real spinors quantized along the z direction

$$T_t \left|\uparrow\right\rangle = -ie^{-i\delta} \left|\downarrow\right\rangle \tag{10.45}$$

$$T_t \left|\downarrow\right\rangle = ie^{-i\delta} \left|\uparrow\right\rangle \tag{10.46}$$

The time reversal operator thus transforms up into down and vice versa but with a phase. Even if we can choose $e^{i\delta} = i$ to make the phase real, the prefactor cannot be $+1$ for both of the above equations. In particular, note that $T_t T_t \left|\uparrow\right\rangle = -\left|\uparrow\right\rangle$, another strange property of spinors. The application of two time reversal operations on spinors is like a 2π rotation around y so that it changes the phase of the spinor. It can be proven that this result is independent of the choice of quantization axis, as we can expect.[83] As far as the main topic of the present section is concerned, observables such as angular momentum will have a simple signature under time reversal (they are always two spinors that come in for each observable A_i) so that the results of the previous section are basically unmodified.

When $\chi''_{A_i A_j}(\omega)$ is real, the properties of being a commutator (10.48) and of Hermiticity (10.50) allow us to further show that $\chi''_{A_i A_i}(\omega)$ is also an odd function of frequency, an important result that we show in the following section.

10.3 Properties that follow from the definition and proof that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$

In this section, several exact results are shown, but the one I will use most often is $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$. Let us thus write down the general symmetry properties of $\chi''_{A_i A_j}(t - t')$ that simply follow from its definition (10.5). These properties are independent of the specific form of the Hamiltonian. It only needs to be Hermitian.

- *Commutator:* Since it is a commutator, we have

$$\chi''_{A_iA_j}(t-t') = -\chi''_{A_jA_i}(t'-t) \tag{10.47}$$

which when we move to frequency space with $\int dt\, e^{i\omega t}$ reads,

$$\boxed{\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)}. \tag{10.48}$$

- *Hermiticity:* Taking the observables as Hermitian, as is the case most of the time (superconductivity leads to an exception), one can use the cyclic property of the trace and the Hermiticity of the density matrix to show that

$$\chi''_{A_iA_j}(t-t') = \left[\chi''_{A_jA_i}(t'-t)\right]^*. \tag{10.49}$$

(Proof for Hermitian operators: $\langle [A_i, A_j]\rangle^* = Tr\left\{\rho A_iA_j - \rho A_jA_i\right\}^*$
$= Tr\left\{A_jA_i\rho - A_iA_j\rho\right\} = Tr\left\{\rho\left[A_j, A_i\right]\right\}$ with ρ the density matrix.)

In Fourier space, this becomes,

$$\boxed{\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^*}. \tag{10.50}$$

In other words, seen as a matrix in the indices A_i, A_j, the matrix $\chi''_{A_iA_j}(\omega)$ is hermitian at all frequencies.

Remark 60 *Non-hermitian operators: It is important to note that the operators A_i may be non-Hermitian, as is the case for superconductivity. In such cases, one should remember that the above property may not be satisfied.*

As an example of the use of the last equation, consider $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega)$ for density response. We obtain the equality $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^*$. Taking Fourier transforms in space, this implies that this response function, measurable through energy-loss electron spectroscopy, is real:

$$\boxed{\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^*}. \tag{10.51}$$

Quite generally, using the commutator property Eq.(10.48) and time-reversal symmetry Eq.(10.31) to interchange the two operators, we see that *for operators that have the same signature under time reversal*

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_iA_j}(-\omega), \tag{10.52}$$

in other words, that function, $\chi''_{A_iA_j}(\omega)$, that we will call the spectral function below, is odd (and continuous it turns out so that it vanishes at $\omega = 0$), a property we will use for thermodynamic sum rules below.

Most useful property: The most important consequence of this section that I will often use is that correlation functions such as $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ are not only real but also odd in frequency as follows directly from the last equation,

$$\boxed{\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega).} \tag{10.53}$$

Remark 61 *Here is a less general way of deriving* $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$ *that rests on invariance under parity. We first use Hermiticity Eq.(10.50) in the form*

$$\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* \tag{10.54}$$

to show that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ *is real*

$$\begin{aligned}
\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) &= \int d^3\mathbf{r} \int d^3\mathbf{r}' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) && (10.55)\\
&= \left[\int d^3\mathbf{r} \int d^3\mathbf{r}' e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* && (10.56)\\
&= \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^* && (10.57)
\end{aligned}$$

The commutator property Eq.(10.48), $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega)$ *and symmetry under parity transformation Eq.(10.19),* $\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega) = \chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$ *then suffice to show that* $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ *is also odd in frequency* $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$.

10.4 Kramers-Kronig relations follow from causality

You are familiar with optical conductivity for example, or with frequency dependent impedance. Generally one can measure the real and imaginary parts of frequency-dependent response functions, namely the dissipative and reactive parts of the response. Those are not independent. In reality, all the information on the system is in $\chi''_{A_iA_j}(\omega)$. That is the single function containing the physics. We have already encountered the Kramers-Kronig relations in the introduction with the simple harmonic oscillator. So this section is repetitive.

Since the physics is in a single function, there are relations between real and imaginary parts of response functions. These are the Kramers-Kronig relation. These are by far the best known and most useful properties for response functions. The Kramers-Kronig relation follows simply from causality. Causality is insured by the presence of the θ function in the expression for the response functions Eq.(10.6). Causality simply states that the response to an applied field at time t' occurs only at time t later. This is satisfied in general in our formalism, as can be seen by looking back at the formula for the linear response Eq.(9.10). Kramers-Kronig relations are the same causality statement as above, seen from the perspective of Fourier transforms.

Let us recall what was done before. The fact that there is a Heaviside $\theta(t-t')$ function implies that the Fourier transform of $\chi^R_{A_iA_j}(t-t')$ cannot have any pole in the complex upper half-plane of frequency because of the exponential. Conversely, analyticity of $\chi^R_{A_iA_j}(\omega)$ implies that in time there is a $\theta(t-t')$ function. Analyticity of the response $\chi^R_{A_iA_j}(\omega)$ in the upper half-plane and the contour shown in Fig. (2-2) that avoids the singularity on the real axis implies that if we define $\chi^R_{A_iA_j}(\omega) = \mathrm{Re}\,\chi^R_{A_iA_j}(\omega) + i\,\mathrm{Im}\,\chi^R_{A_iA_j}(\omega)$ then the Kramers-Kronig relation follow:

$$\boxed{\mathrm{Re}\,\chi^R_{A_iA_j}(\omega) = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\,\chi^R_{A_iA_j}(\omega)}{\omega'-\omega}} \tag{10.58}$$

$$\boxed{\mathrm{Im}\,\chi^R_{A_iA_j}(\omega) = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\,\chi^R_{A_iA_j}(\omega)}{\omega'-\omega}.} \tag{10.59}$$

This is completely general.

Remark 62 *The above Kramers-Kronig relations assume that $\chi^R_{A_iA_j}(\omega)$ falls off at least as a small power of ω at infinity. If there is a term that does not decay, it needs to be subtracted off before we can apply the Hilbert transforms.*

Remark 63 *Kramers-Kronig and time reversal: The Kramers Krönig relations do not depend on subtleties of signatures under time-reversal. Everything about the system is in $\chi''_{A_iA_j}(\omega)$. The following special cases are the most often encountered: When A_i and A_j are hermitian, we have seen in Eq. (10.50) that $\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^*$. This implies that $\chi''_{A_jA_i}(\omega)$ is real when either $A_i = A_j$ or when there is time-reversal symmetry Eq. (10.31) with A_i and A_j that have the same signature under time reversal. Correspondingly, $\chi'_{A_iA_j}(\omega)$ is real, as implied by the Kramers Kronig relation. So, if we write $\chi^R_{A_iA_j}(\omega) = \chi'_{A_iA_j}(\omega) + i\chi''_{A_iA_j}(\omega)$ then $\chi'_{A_iA_j}(\omega)$ is the real part of $\chi^R_{A_iA_j}(\omega)$ and $\chi''_{A_iA_j}(\omega)$ the imaginary part.*

$$\boxed{\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = \chi''_{A_iA_j}(\omega)} \tag{10.60}$$

Remark 64 *For two hermitian operators A_i, A_j with opposite signatures under time reversal, Eqs.(10.31) and hermiticity (10.50) imply that $\chi''_{A_iA_j}(\omega')$ is purely imaginary. In this case,*

$$\boxed{\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = i\chi''_{A_iA_j}(\omega)}. \tag{10.61}$$

10.5 Spectral representation and Kramers-Kronig relations

It is instructive to perform a derivation of Kramers-Kronig relations that starts from our explicit expression for the susceptibility in terms of χ''. Inspired by what we found for the harmonic oscillator in Chapter (3.2) I recall that in real time, our response looks similar to what we had in Eq. (3.14), namely

$$\chi^R_{A_iA_j}(t-t')e^{-\eta(t-t')} = 2i\chi''_{A_iA_j}(t-t')\theta(t-t')e^{-\eta(t-t')}. \tag{10.62}$$

If

$$\chi^R_{A_iA_j}(\omega) = \int \frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega + i\eta)}, \tag{10.63}$$

then Fourier transforming this equation will give us the previous one in time, as we saw for the harmonic oscillator, without the need of any assumption about whether $\chi''_{A_iA_j}(\omega')$ is real or imaginary.

If we start from $\chi^R_{A_iA_j}(t-t')$, we proceed just as in Chapter (3.2). The steps will not be repeated.[1] As long as η is finite, we can go back and forth between the time and the frequency representation. And whether we are interested in $\chi^R_{A_iA_j}(t-t')$ or in $\chi^R_{A_iA_j}(\omega)$, the physical response is always obtained by taking the $\eta \to 0$ limit at the end.

[1] Here it is not generally true that $\mathrm{Im}\,\chi^R_{A_iA_j}(\omega) = \chi''_{A_iA_j}(\omega)$.The special case $A_i = A_j$ gives an example where the previous equality is correct. This was the case for our harmonic oscillator example.

Remark 65 *Another explanation of η : We want to know $\delta\langle B(\mathbf{r},t)\rangle$. To insure a steady state when we integrate differential equations forward in time, we want to damp out residual effects of the initial conditions at $t\to\infty$. This is like for the solution in time of the harmonic oscillator that we did in the introductory chapters, but in the limit of infinitesimal damping. To this end, it suffices to multiply $\delta\langle B(\mathbf{r},t)\rangle$ by $e^{-\eta t}$ where η is infinitesimal.The equation for the response in time (10.6) is then simply multiplied by $e^{-\eta t}=e^{-\eta\left(t-t'\right)}e^{-\eta t'}$, so that $\chi^R_{A_iA_j}(t-t')$ still depends only on the time difference and the analogous factor, $e^{-\eta t'}$, multiplies the external field. When we take Fourier transforms, $\int_{-\infty}^{\infty}d(t-t')e^{i\omega(t-t')}$, everything proceeds as before, except that we can use the extra convergence factor $e^{-\eta(t-t')}$, to make sense out of the Fourier transform of the Heaviside theta function if the convolution theorem is used.*

Remark 66 *It is important to note that the external field is also multiplied by $e^{-\eta t'}$ so that its Fourier transform will also show $\omega+i\eta$.*

This function is called the "retarded response" to distinguish it from what we would have obtained with $\theta(t'-t)$ instead of $\theta(t-t')$. The retarded response is causal, in other words, the response occurs only after the perturbation. In the anti-causal case ("advanced response") the response all occurs *before* the perturbation is applied. In the latter case, the convergence factor is $e^{-\eta(t'-t)}$ instead of $e^{\eta(t'-t)}$. Introducing a new function defined in the whole complex plane z,

$$\boxed{\chi_{A_iA_j}(z)=\int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-z}} \tag{10.64}$$

we can write for the retarded response,

$$\boxed{\chi^R_{A_iA_j}(\omega)=\lim_{\eta\to0}\chi_{A_iA_j}(z)|_{z=\omega+i\eta}} \tag{10.65}$$

and for the advanced one, which we hereby define,

$$\boxed{\chi^A_{A_iA_j}(\omega)=\lim_{\eta\to0}\chi_{A_iA_j}(z)|_{z=\omega-i\eta}.} \tag{10.66}$$

Using the above results, it is easy to see that $\chi^R_{A_iA_j}(\omega)$ is analytic in the upper-half plane, while $\chi^A_{A_iA_j}(\omega)$ is analytic in the lower-half plane. The advanced function is useful mathematically but it is acausal, in other words the response occurs before the perturbation. In the time representation it involves $\theta\left(t'-t\right)$ instead of $\theta\left(t-t'\right)$.

$\chi_{A_iA_j}(z)$ is a function which is equal to $\chi^R_{A_iA_j}(\omega)$ for z infinitesimally above the real axis, and to $\chi^A_{A_iA_j}(\omega)$ for z infinitesimally below the real axis. On the real axis of the complex z plane $\chi_{A_iA_j}(z)$ has a cut whenever $\chi''_{A_iA_j}(\omega)\neq0$ since, using the Sokhatsky Weirstrass formula Eq. (2.36)

$$\left[\chi_{A_iA_j}(\omega+i\eta)-\chi_{A_iA_j}(\omega-i\eta)\right] = 2i\chi''_{A_iA_j}(\omega) \tag{10.67}$$

$$\chi^R_{A_iA_j}(\omega)-\chi^A_{A_iA_j}(\omega) = 2i\chi''_{A_iA_j}(\omega) \tag{10.68}$$

Remark 67 *The last result does not rely on $\chi''_{A_iA_j}(\omega)$ being real, so it is an important general result.*

Definition 10 *Equations such as (10.64) are called spectral representations.*

So much for taking the Fourier transform of a response which is so simple looking in its ordinary time version Eq.(10.6).

10.6 *Positivity of $\omega\chi''(\omega)$ and dissipation

The proof of this section essentially follows the steps used for the simple harmonic oscillator in Chapter (3.3).

We want to show that the key function of the previous discussion, namely $\chi''_{A_iA_j}(\omega)$, contains all the information on the dissipation. Since stability of a thermodynamic system implies that an external applied field of any frequency must do work the dissipation must be positive, which in turns means, as we now demonstrate, that $\omega\chi''_{A_iA_j}(\omega)$ is a positive-definite matrix.

Since the change in the energy of the system due to the external perturbation is given by the perturbation Hamiltonian Eq.(9.2), this means that the power dissipated by the external world is

$$\frac{dW}{dt} = \frac{d\delta\mathcal{H}(t)}{dt} = -\int d^3r A_i(\mathbf{r})\frac{da_i(\mathbf{r},t)}{dt} = -A_i\frac{da_i(t)}{dt}. \tag{10.69}$$

In the last equality, we have used our short-hand notation and included position in the index i. The integral over $\mathbf{r}$ then becomes a sum over i which is not written explicitly since **we take the convention that repeated indices are summed over.** Taking the expectation value in the presence of the external perturbation, we find

$$\frac{dW}{dt} = -\left[\langle A_i\rangle + \langle\delta A_i\rangle\right]\frac{da_i(t)}{dt} \tag{10.70}$$

where $\langle A_i\rangle$ is the equilibrium expectation value, and $\langle\delta A_i\rangle$ the linear response. Taking the total energy absorbed over some long period of time T, the condition for the dissipated energy to be positive is,

$$\overline{W} = -\int_{-T/2}^{T/2} dt \quad \langle\delta A_i(t)\rangle\frac{da_i(t)}{dt} > 0. \tag{10.71}$$

For $\langle\delta A_i\rangle$ we have written explicitly all the time dependence in the operator instead. Taking $T\to\infty$ and getting help from Parseval's theorem, the last result may be written,

$$-\int\frac{d\omega}{2\pi}\langle\delta A_i(\omega)\rangle\, i\omega a_i(-\omega) > 0. \tag{10.72}$$

Finally, linear response theory gives

$$-\int\frac{d\omega}{2\pi}a_i(-\omega)\chi^R_{A_iA_j}(\omega)i\omega a_j(\omega) > 0 \tag{10.73}$$

Changing dummy indices as follows, $\omega\to-\omega$, $i\to j$, $j\to i$ and adding the new expression to the old one, we obtain the requirement,

$$\overline{W} = -\frac{1}{2}\int\frac{d\omega}{2\pi}a_i(-\omega)\left[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\right]i\omega a_j(\omega) > 0. \tag{10.74}$$

Calling the spectral representation (10.65) to the rescue, we can write

$$\left[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\right] = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega + i\eta)} - \int\frac{d\omega'}{\pi}\frac{\chi''_{A_jA_i}(\omega')}{\omega' - (-\omega + i\eta)}. \tag{10.75}$$

We know from the fact that $\chi''_{A_iA_j}$ is a commutator that (10.48) $\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)$. Using this identity and the change of variables $\omega'\to-\omega'$ in the last integral, we immediately have that

$$\left[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\right] = \int\frac{d\omega'}{\pi}\chi''_{A_iA_j}(\omega')\left[\frac{1}{\omega' - \omega - i\eta} + \frac{1}{-\omega' + \omega - i\eta}\right] \tag{10.76}$$

$$= 2i\chi''_{A_iA_j}(\omega). \tag{10.77}$$

Substituting all this back into the last equation for the dissipated energy, and using the fact that since the applied field is real, then $a_i(-\omega) = a_i^*(\omega)$, we get

$$\int \frac{d\omega}{2\pi} a_i^*(\omega) \left[\chi''_{A_iA_j}(\omega)\omega\right] a_j(\omega) > 0. \tag{10.78}$$

This is true whatever the time-reversal signature of the operators A_i, A_j. Furthermore, since we can apply the external field at any frequency, we must have

$$\boxed{a_i^*(\omega) \left[\chi''_{A_iA_j}(\omega)\omega\right] a_j(\omega) > 0} \tag{10.79}$$

for all frequencies. For hermitian operators we have seen in Eq. (10.50) that $\chi''_{A_iA_j}(\omega)$ behaves as a Hermitian matrix. So its eigenvalues are real. Going to the basis where $\chi''_{A_iA_j}$ is diagonal, we see that the previous equation implies that all the eigenvalues are positive. This is the definition of a positive-definite matrix. Also, when there is only one kind of external perturbation applied,

$$\boxed{\chi''_{A_iA_i}(\omega)\omega > 0.} \tag{10.80}$$

We have seen that for Hermitian operators with the same signature under time reversal, $\chi''_{A_iA_i}(\omega)$ is a real and odd function of frequency so the above equation is satisfied.

One can check explicitely that $\chi''_{A_iA_i}(\omega)$ contains spectral information about excited states by doing backwards the steps that lead us from Fermi's golden rule to correlation functions.

Remark 68 *For Hermitian operators A_i, A_j, the matrix $\chi''_{A_iA_i}(\omega)$ is Hermitian, hence its eigenvalues are real, even if off-diagonal matrix elements between operators that do not have the same signature under time reversal are purely imaginary.*

10.7 A short summary of basic symmetry properties and constraints on χ''

We summarize the results of the last few sections that concern χ''. In the first row, we explicitly write the $\mathbf{r}, \mathbf{r}'$ dependence, in the second rwo we take the space fourier transform and in the rest the spatial indices are hidden in the indicies i and j appearing with A_i. $\epsilon^t_{A_i}$ is the signature under time reversal of the operator A_i, while $\epsilon^P_{A_i}$ is the signature under parity of the operator A_i.

Basic property	**Implies for χ''**
H is invariant under translation	$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} - \mathbf{r}'; t - t')$
H is invariant under parity	$\chi''_{BA}(\mathbf{q}; \omega) = \varepsilon^P_B \varepsilon^P_A \chi''_{BA}(-\mathbf{q}; \omega)$
H is invariant under time reversal	$\chi''_{A_iA_j}(\omega) = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(\omega)$
χ'' is a commutator	$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)$.
χ'' contains hermitian operators only	$\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^*$.
Positivity of dissipation	$\chi''_{A_iA_j}(\omega)\omega$ is a positive definite matrix

Remark 69 *The result concerning time reversal invariance can be remembered from the fact that apart from the signatures, it looks like transposition, which is basically what time reversal does for the thermal average of an operator. Similarly if we look at A_i and A_j as indices, the relation coming from hermiticity looks like hermiticity of the $\chi''_{A_iA_j}(\omega)$ matrix.*

A result we will use later that is a consequence of hermiticity and time-reversal symmetry is that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ is real and an odd function of frequency $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$.

10.8 *Fluctuation-dissipation theorem

In this section, I generalize the fluctuation-dissipation theorem that seemed very special with the constant-damping approximation I considered for the simple harmonic oscillator. That theorem is very important and much more general. This very useful theorem relates linear response to equilibrium fluctuations measured in scattering experiments. Here I give the derivation in the general quantum case. It takes the form,

$$\boxed{S_{A_iA_j}(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega) = 2\hbar(1+n_B(\omega))\chi''_{A_iA_j}(\omega)} \tag{10.81}$$

where $n_B(\omega) = 1/\left(e^{\beta\hbar\omega}-1\right)$ is the Bose factor while the "structure factor" or correlation function is defined by,

$$S_{A_iA_j}(t) \equiv \langle A_i(t)A_j\rangle - \langle A_i\rangle\langle A_j\rangle = \langle (A_i(t)-\langle A_i\rangle)(A_j(0)-\langle A_j\rangle)\rangle \tag{10.82}$$

$$\equiv \langle \delta A_i(t)\delta A_j\rangle\,. \tag{10.83}$$

(Note that $\langle A_i(t)\rangle = \langle A_i(0)\rangle = \langle A_i\rangle$) This is also known as the Callen-Welton [48] a more general version of the Nyquist-Johnson theorem [178].We have already encountered the charge structure factor in the context of inelastic neutron scattering. Clearly, the left-hand side of the fluctuation-dissipation theorem Eq.(G.13) is a correlation function for fluctuations while the right-hand side contains the dissipation function χ'' just discussed. This is a key theorem of statistical physics.

Remark 70 *We recover the classical fluctuation-dissipation theorem in the usual classical limit where $\hbar\omega \ll k_BT$. Indeed, in that case the Bose function becomes $n_B(\omega) = 1/\left(e^{\beta\hbar\omega}-1\right) \simeq 1/\beta\hbar\omega = k_BT/\hbar\omega$ which is much larger than unity so that the fluctuation-dissipation theorem Eq.(G.13) becomes $S_{A_iA_j}(\omega) = (2k_BT/\omega)\chi''_{A_iA_j}(\omega)$ as we had found in Eq.(4.51). Returning to the derivation of our cross-sections in Sec.(7) with the golden rule ($A_i = A_j$), you see that $\hbar\omega$ is the energy given to the system by the probe. Negative ω means that the system gives energy to the probe. We thus expect that $S_{A_iA_j}(\omega) = 0$ at $T = 0$ when ω is negative since a system in its ground state cannot give energy. On the other hand, at positive ω, the system absorbs energy, which it can always do. That is what the above formula predicts, as can be checked in the quantum limit, namely $|\beta\hbar\omega| \to \infty$. Indeed, in that case $2\hbar/\left(1-e^{-\beta\hbar\omega}\right) \to 2\hbar$ for positive ω, and $2\hbar/\left(1-e^{-\beta\hbar\omega}\right) \to 0$ for negative ω. Fluctuations do not vanish in a quantum system at $T = 0$. Classical mechanics, by contrast, would predict that all fluctuations disappear. We pointed out at the end of Chapter (7) that the transition rate between an excited atomic level and the ground state is proportional to the fluctuations of the electromagnetic field at the transition frequency. This implies that the electromagnetic field is also quantized, otherwise excited states of atoms would not decay.*

To prove the theorem, it suffices to trivially relate the definitions,

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\langle[A_i(t),A_j]\rangle = \frac{1}{2\hbar}\langle[\delta A_i(t),\delta A_j]\rangle \quad (10.84)$$

$$= \frac{1}{2\hbar}\langle\delta A_i(t)\delta A_j - \delta A_j\delta A_i(t)\rangle \quad (10.85)$$

$$= \frac{1}{2\hbar}\left(S_{A_iA_j}(t) - S_{A_jA_i}(-t)\right) \quad (10.86)$$

then to use the key following identity that we set to prove,

$$\boxed{S_{A_jA_i}(-t) = S_{A_iA_j}(t - i\hbar\beta)}. \quad (10.87)$$

This kind of periodicity of equilibrium correlation functions will be used over and over in the context of Green's functions. It will allow to define Fourier expansions in terms of so-called Matsubara frequencies.

The proof of the identity simply uses the definition of the time evolution operator and the cyclic property of the trace. More specifically using the cyclic property of the trace, we start with,

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}\delta A_j\delta A_i(t)\right] = Z^{-1}Tr\left[\delta A_i(t)e^{-\beta H}\delta A_j\right]. \quad (10.88)$$

Using $e^{-\beta H}e^{\beta H} = 1$ to recover the density matrix on the left, simple manipulations and Heisenberg's representation for the time-evolution of the operators gives,

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}e^{\beta H}\delta A_i(t)e^{-\beta H}\delta A_j\right] \quad (10.89)$$

$$= Z^{-1}Tr\left[e^{-\beta H}\delta A_i(t - i\hbar\beta)\delta A_j\right] = S_{A_iA_j}(t - i\hbar\beta). \quad (10.90)$$

This is precisely what we wanted to prove. The rest is an exercise in Fourier transforms,

$$\int dt e^{i\omega t}S_{A_iA_j}(t - i\hbar\beta) = \int dt e^{i\omega(t+i\hbar\beta)}S_{A_iA_j}(t) = e^{-\beta\hbar\omega}S_{A_iA_j}(\omega). \quad (10.91)$$

To prove the last result, we had to move the integration contour from t to $t + i\hbar\beta$, in other words in the imaginary time direction. Because of the convergence factor $e^{-\beta H}$ in the traces, expectations of any number of operators of the type $e^{iHt}Ae^{-iHt}$ are analytic in the imaginary time direction for $-i\hbar\beta < t < i\hbar\beta$, hence it is permissible to displace the integration contour as we did. Fourier transforming the relation between $\chi''_{A_iA_j}(t)$ and susceptibility Eq.(10.84), one then recovers the fluctuation-dissipation theorem (G.13).

A few remarks before concluding.

Remark 71 *Alternate derivation: Formally, the Fourier transform gives the same result as what we found above if we use the exponential representation of the Taylor series,*

$$S_{A_iA_j}(t - i\hbar\beta) = e^{-i\hbar\beta\frac{\partial}{\partial t}}S_{A_iA_j}(t).$$

Remark 72 *Relation to detailed balance: The Fourier-space version of the periodicity condition (10.87) is a statement of detailed balance:*

$$\boxed{S_{A_jA_i}(-\omega) = e^{-\beta\hbar\omega}S_{A_iA_j}(\omega)}. \quad (10.92)$$

Indeed, in one case the energy $\hbar\omega$ is absorbed in the process, while in the other case it has the opposite sign (is emitted). In Raman spectroscopy, when the photon

comes out with less energy than it had, we have Stokes scattering. In the reverse process, with a frequency transfer ω of opposite sign, it comes out with more energy. This is called anti-Stokes scattering. The cross section for Stokes scattering say, will be proportional to $S_{A_iA_j}(\omega)$ as we saw with our golden rule calculation. The ratio of the anti-Stokes and the Stokes cross sections will be given by the Boltzmann factor $e^{-\beta\hbar\omega}$, which is a statement of detailed balance. This is one way of seeing the basic physical reason for the existence of the fluctuation-dissipation theorem: Even though the response apparently had two different orders for the operators, the order of the operators in thermal equilibrium can be reversed using the cyclic property of the trace, or equivalently the principle of detailed balance.

Remark 73 *Physical explanation of fluctuation-dissipation theorem: Physically, the fluctuation-dissipation theorem is a statement that the return to equilibrium is governed by the same laws, whether the perturbation was created by an external field or by a spontaneous fluctuation. This is the Onsager regression hypothesis that we discussed in the context of the simple harmonic oscillator in the introduction.*

10.9 Lehmann representation and spectral representation

Definition 11 *The function that contains the information on the physics, $\chi''_{A_iA_j}(\omega')$ is called the spectral function.*

The reason for this name is that, as we discussed in section (10.6), $\chi''_{A_iA_j}(\omega')$ contains information on dissipation or, alternatively, on the spectrum of excitations. Hence, in that kind of equations, the response is expressed in terms of the spectrum of excitations. We will also have spectral representations for Green's functions.

In this section, I introduce the Lehmann representation. It is extremely useful to prove exact properties of the spectral function and to obtain relations between different kinds of correlation function. For example, here I will show again the fluctuation-dissipation theorem. Later, the relation between retarded functions and their expression in Matsubara frequencies will also be easy to see from the Lehmann representation. That representation also allows us to see the connection with the spectrum of excitations and develop physical intuition, since it express $\chi''_{A_iA_j}(\omega')$ in terms of matrix elements and excitation energies.

I begin with the definition and use the Heisenberg equations of motion and insert a complete set of energy eigenstates so that we find

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\mathrm{Tr}\left[\varrho\left(A_i(t)A_j(0) - A_j(0)A_i(t)\right)\right] \tag{10.93}$$

$$= \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\Big[\langle n|e^{iE_nt/\hbar}A_ie^{-iE_mt/\hbar}|m\rangle\langle m|A_j|n\rangle - \langle n|A_j|m\rangle\langle m|e^{iE_mt/\hbar}A_ie^{-iE_nt/\hbar}|n\rangle\Big] \tag{10.94}$$

Changing dummy summation indices m and n in the last term, we have

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle e^{i(E_n-E_m)t/\hbar} \tag{10.95}$$

so that the Fourier transform is

$$\chi''_{A_iA_j}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \langle n| A_i |m\rangle \langle m| A_j |n\rangle \ \pi \, \delta\left(\hbar\omega - (E_m - E_n)\right) \tag{10.96}$$

$$\chi''_{A_iA_j}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \langle n| A_i |m\rangle \langle m| A_j |n\rangle \ \pi \, \delta\left(\hbar\omega - (E_m - E_n)\right) \left(1 - e^{-\beta\hbar\omega}\right). \tag{10.97}$$

Substituting in the spectral representation Eq.(10.64), we find

$$\boxed{\chi_{A_iA_j}(z) = \textstyle\sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \frac{\langle n|A_i|m\rangle\langle m|A_j|n\rangle}{(E_m - E_n) - \hbar z}} \tag{10.98}$$

From this, one trivially deduces, by letting $z \to \omega + i\eta$, the so-called Lehmann representation for the retarded response function. The poles are indeed simple poles in the lower-half frequency plane, as we wanted to prove. They are just below the real axis, a distance η along the imaginary direction. The position of the poles carries information on the excitation energies of the system. The residue at a given pole will depend on the value of $\chi''_{A_iA_j}$ at the corresponding value of the real coordinate of the pole. The residues tell us how strongly the external probe and system connect the two states. The Lehmann representation reminds us of low order perturbation theory in the external probe.

Note that doing the replacement $\omega \to -\omega$ is equivalent to exchanging the indices m and n and A_i for A_j so that

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega) \tag{10.99}$$

which we found above in Eq. (10.48) as a consequence of the commutator property. You can do something similar for other properties.

Remark 74 *The poles of the reponse function for the simple harmonic oscillator were near the resonance frequency ω_0. For the quantum version, ω_0 should be obtained from the difference in energy between two eigenstates, divided by $\hbar$. The above result for the poles of the response functions are not surprising in this context.*

Remark 75 *Bohr's correspondence principle: Consider the diagonal case, $A_i = A_j$. We have seen in Sec.(10.6) that $\chi''_{A_iA_i}(\omega)$ is related to absorption. From the explicit form for that quantity, Eq.(10.96), we see the the absorption will occur at energies $\hbar\omega$ that correspond to the difference in energy between eigenstates, $E_m - E_n$, in accord with Bohr's correspondence principle.*

Remark 76 *From the form Eq. (10.97) of the spectral representation, the fluctuation-dissipation theorem Eq. (G.13) follows immediately.*

To refine our physical understanding of $\chi''_{A_iA_j}(\omega)$ let us go back to the original form we found in the time domain, Eq.(10.94), before we changed dummy indices. Taking Fourier transforms directly on this function, we find

$$\begin{aligned}\chi''_{A_iA_j}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} &[\langle n| A_i |m\rangle \langle m| A_j |n\rangle \ \pi \, \delta\left(\hbar\omega - (E_m - E_n)\right) \\ &- \langle n| A_j |m\rangle \langle m| A_i |n\rangle \ \pi \, \delta\left(\hbar\omega - (E_n - E_m)\right)]. \end{aligned} \tag{10.100}$$

If we take the zero temperature limit, $\beta \to \infty$, we are left with $Z = e^{-\beta E_0}$ where E_0 is the ground state energy and the above formula reduces to

$$\begin{aligned}\lim_{\beta\to\infty} \chi''_{A_iA_j}(\omega) = \sum_{m} &[\langle 0| A_i |m\rangle \langle m| A_j |0\rangle \ \pi \, \delta\left(\hbar\omega - (E_m - E_0)\right) \\ &- \langle 0| A_j |m\rangle \langle m| A_i |0\rangle \ \pi \, \delta\left(\hbar\omega - (E_0 - E_m)\right)] \end{aligned} \tag{10.101}$$

For $m = 0$, $\chi''_{A_i A_j}(\omega)$ vanishes. Then, only excited states contribute and $E_m - E_0 > 0$. For positive frequencies only the first term contributes and it contributes only if $\hbar\omega$ is equal to the energy of an excitation in the system, namely $E_m - E_0$, and if the external probe through A_j, and the measured operator A_i, have a non-vanishing matrix element that connects the excited and ground state. Clearly then, $\chi''_{A_i A_j}(\omega)$ is related to absorption. The second term contributes only for negative frequencies. External probes that are in $\cos(\omega t) = \left(e^{i\omega t} + e^{-i\omega t}\right)/2$ couple to both positive and negative frequencies. It is not surprising that both positive and negative frequencies enter $\chi''_{A_i A_j}(\omega)$. At finite temperature, contributions to positive frequencies can also come from the second term and contributions to negative frequencies can also come from the first term.

Remark 77 *Clearly, the spectral representation is valid, whether $\chi''_{A_i A_j}(\omega)$ is real or not, odd or not.*

Remark 78 *In an infinite system, if $\chi''_{A_i A_j}(\omega')$ is a continuous function and then the poles of $\chi_{A_i A_j}(z)$ are below the real axis, but not ncessarily close to it if we make an approximation for $\chi''_{A_i A_j}(\omega')$. The passage from a series of poles to a continuous function is what introduces irreversibility in many-body systems, as we have seen with the simple harmonic oscillator in Chapter (4). This is also discussed in problem (6.0.4).*

Remark 79 *Since $\langle n| A |m\rangle \langle m| A |n\rangle$ is equal to $|\langle m| A |n\rangle|^2$ for a Hermitian operator A, it is clear that the spectral weight $\chi''_{A_i A_j}(\omega)$ is positive when $A_i = A_j$. This will be the case when we compute conductivity for example, but this is not the case for thermopower, for example, where the measured quantity A_i is electrical current and the perturbation is a temperature gradient that couples to the energy density A_j.*

10.10 Sum rules

All the many-body Physics of the response or scattering experiments is in the calculation of unequal-time commutators. These commutators in general involve the time evolution of the systems and thus they are non-trivial to evaluate. However, equal-time commutators are easy to evaluate in general using the usual commutation relations. Equal-time corresponds to integral over frequency as seen from Fourier space. Hence the name sum rules. We will not in general be able to satisfy all possible sum-rules since this would mean basically an exact solution to the problem, or computing infinite-order high-frequency expansion. In brief, sum-rules are useful to

- Relate different experiments to each other.
- Establish high frequency limits of correlation functions.
- Provide constraints on phenomenological parameters or on approximate theories.

10.10.1 Thermodynamic sum-rules

In this section, I show that our formalism is consistent with well known facts in elementary quantum statistical mechanics. Recall that in the grand canonical ensemble, the average number of particles is given by,

$$\langle N \rangle = \mathrm{Tr}\left[e^{-\beta(H-\mu N)} N \right] / Z. \tag{10.102}$$

Since total particle number is conserved, N commutes with the Hamiltonian, and we have the classical result

$$\langle NN \rangle - \langle N \rangle^2 = \frac{1}{\beta} \left(\frac{\partial N}{\partial \mu} \right)_{T,V}. \tag{10.103}$$

The $\langle N \rangle^2$ comes from th derivative of Z with respect to μ. In a way, this is a relation between fluctuations on the left-hand side, and response on the right-hand side. Let us see if this can be derived from the relation we found between fluctuations and response, namely the fluctuation-dissipation theorem.

By definition,

$$\langle NN \rangle - \langle N \rangle^2 = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega) \tag{10.104}$$

Because $n_{\mathbf{q}}$ for $\mathbf{q} = \mathbf{0}$ is simply the total number of particles N and hence is conserved, $\langle n_{\mathbf{q}=\mathbf{0}}(t)\, n_{\mathbf{q}=\mathbf{0}} \rangle$ is time independent. In frequency space then, this correlation function is a delta function in frequency. This can be confirmed from the Lehmann representation. For such a conserved quantity, we expect that the long-wavelength response, namely at small $\mathbf{q}$, all the weight will be near zero frequency so for $\mathbf{q}$ sufficiently small, the fluctuation-dissipation theorem Eq.(G.13) becomes

$$\lim_{\mathbf{q}\to\mathbf{0}} S_{nn}(\mathbf{q},\omega) = \lim_{\mathbf{q}\to\mathbf{0}} \frac{2\hbar}{1-e^{-\beta\hbar\omega}} \chi''_{nn}(\mathbf{q},\omega) = \lim_{\mathbf{q}\to\mathbf{0}} \frac{2}{\beta\omega} \chi''_{nn}(\mathbf{q},\omega) \tag{10.105}$$

from which we obtain

$$\langle NN \rangle - \langle N \rangle^2 = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega) \tag{10.106}$$

$$= \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\beta\omega} = \frac{1}{\beta} \left(\frac{\partial N}{\partial \mu} \right)_{T,V} \equiv \frac{1}{\beta} \chi_{nn}. \tag{10.107}$$

where χ_{nn} is a "susceptibility". Another way to write this is

$$\boxed{k_B T \chi_{nn} = S_{nn}.} \tag{10.108}$$

In this form, the density fluctuations are related to the response $(\partial N/\partial\mu)_{T,V}$ (itself related to the compressibility) and we have what is known as the thermodynamic sum rule

$$\lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} = \left(\frac{\partial N}{\partial \mu} \right)_{T,V} = \chi_{nn}, \tag{10.109}$$

which in this case is known as the compressibility sum rule.

Thermodynamic sum rules can be seen from another point of view. Suppose we compute the linear response to a time-independent perturbation. In addition to

the previous example where we looked at the response of the the density to a chemical potential shift, another example would be the response of the magnetization to a time-independent magnetic field. This should be the magnetic susceptibility. To remain general, I look at the response of operator A_i to the external field a_j coupled to A_j. However, I have to assume that A_i and A_j are conserved quantities so that the above assumptions about the limit $\mathbf{q} \to \mathbf{0}$ apply.

Naturally, we have to leave the adiabatic switching-on, i.e. the infinitesimal η. Returning to the notation where $\mathbf{q}$ is explicitly written, we have

$$\delta \langle A_i(\mathbf{q},\omega=0)\rangle = \chi^R_{A_iA_j}(\mathbf{q},\omega=0)a_j(\mathbf{q},\omega=0) \tag{10.110}$$

Recalling that the thermodynamic derivatives are in general for uniform ($\mathbf{q}=0$) applied probes, the above formula becomes,

$$\boxed{\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{A_iA_j}(\mathbf{q},\omega=0) = \frac{\partial A_i}{\partial a_j} \equiv \chi_{A_iA_j}.} \tag{10.111}$$

where $\chi_{A_iA_j}$ is a thermodynamic susceptibility. But the spectral representation (10.64) gives us

$$\chi^R_{A_iA_j}(\mathbf{q},\omega=0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega - i\eta}. \tag{10.112}$$

Assuming that A_i and A_j have the same signature under time reversal, the usual Sokhatsky-Weirstrass relation Eq. (2.36) tells us that

$$\chi^R_{A_iA_j}(\mathbf{q},\omega=0) = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega} + \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \chi''_{A_iA_j}(\mathbf{q},\omega) i\pi\delta(\omega). \tag{10.113}$$

so that $\chi^R_{A_iA_j}(\mathbf{q},\omega=0)$ does not have an imaginary part because $\chi''_{A_iA_j}(\mathbf{q},0)$ vanishes since $\chi''_{A_iA_j}(\mathbf{q},\omega)$ is odd and continuous at $\omega=0$. Physically, there is no contribution from the imaginary part on the grounds that there can be no zero-frequency dissipation in a stable system. But we know from our use of the fluctuation-disssipation theorem above that $\lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega}$ converges. So the principal part in the above equation is then superfluous as expected from the fact that $\chi''_{A_iA_j}(\mathbf{q},\omega)$ vanishes linearly in ω for small ω when it is odd. This can be confirmed from the Lehmann representation. The limit $\eta \to 0$ that is usually taken after the integral is done can be taken before since there is no singularity. We thus obtain the following general expression relating susceptibility $\chi_{A_iA_j}$ to $\chi''_{A_iA_j}$ through a sum rule

$$\boxed{\chi_{A_iA_j} = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega}}. \tag{10.114}$$

$$\chi_{A_iA_j} = \lim_{\mathbf{q}\to\mathbf{0}} \lim_{\omega\to 0} \chi^R_{A_iA_j}(\mathbf{q},\omega). \tag{10.115}$$

For thermodynamic quantities, the $\omega \to 0$ limit is always taken before the $\mathbf{q} \to \mathbf{0}$ limit. It will be the other way around for transport coefficients.

Remark 80 *To be completly general, one can keep the principal part. But if you do, the $\eta \to 0$ limit must be taken before the $\mathbf{q} \to \mathbf{0}$ limit. The above is the general form of thermodynamic sum rules.*

Remark 81 *Thermodynamic sum-rule and moments: Thermodynamic sum-rules are in a sense the inverse first moment over frequency of $\chi''_{A_iA_j}(\mathbf{q},\omega)$ (the latter being analogous to the weight). Other sum-rules are over positive moments, as we now demonstrate.*

Remark 82 *Another way to see that we can neglect the η is that the perturbation can be time independent for this kind of response, so we do not need to worry about causality. There is no dissipation, so the response is completely time symmetric. This is the famous quasistatic limit in thermodynamics.*

10.10.2 The order of limits when ω or $\mathbf{q}$ tends to zero is important for χ

It is extremely important to note that for thermodynamic sum rules, the $\omega \to 0$ limit is taken first, before the $\mathbf{q} \to 0$ limit as stated in one of the last remarks. The other limit describes transport properties as we shall see. Take as an example of a $\mathbf{q} = \mathbf{0}$ quantity the total number of particles. Then

$$\chi''_{NN}(t) = \frac{1}{2\hbar}\langle [N(t), N] \rangle = 0 \tag{10.116}$$

This quantity vanishes for all times because N being a conserved quantity it is independent of time, and it commutes with itself. Taking Fourier transforms, $\chi''_{NN}(\omega)$ vanishes for all frequencies. This implies that for conserved quantities

$$\boxed{\chi^R_{A_i A_j}(\mathbf{q} = \mathbf{0}, \omega) = 0.} \tag{10.117}$$

Hence, we must take the $\mathbf{q} \to \mathbf{0}$ limit after the $\omega \to 0$ limit to obtain thermodynamic sum rules.

Another important question is that of the principal part integral. If we take the $\mathbf{q} \to \mathbf{0}$ limit at the end, as suggested above, we do not run into problems. *As follows from a problem,14.0.1* where we have a diffusion. In the long wave length limit one finds

$$\chi''_{nn}(\mathbf{q}, \omega) = \frac{2Dq^2\omega}{\omega^2 + (Dq^2)^2}\chi_{nn} \tag{10.118}$$

where D is the diffusion constant. One can check explicitly, with that expression, that at any finite q, it does not matter whether we take or not the principal part integral. We did not take it in Eq.(10.109). If we take the limit $\mathbf{q} \to \mathbf{0}$ before doing the integral however, $\lim_{\mathbf{q}\to\mathbf{0}} \chi''_{nn}(\mathbf{q}, \omega)$ is proportionnal to $\chi_{nn}\omega\delta(\omega)$ so it is important NOT to take the principal part integral to get the correct result.

Remark 83 *Order of limits for the termodynamic sum rules: The last result can be stated as follows. Under the integral sign the $\eta \to 0$ limit of the spectral representation Eq. (10.113) must be taken before the $\mathbf{q} \to \mathbf{0}$ limit. We also see this as follows. If we return to the original form $\lim_{\eta\to 0} 1/(\omega - i\eta) = \lim_{\eta\to 0} \omega/(\omega^2 + \eta^2) + i\eta/(\omega^2 + \eta^2)$, and then do the integral of the first term (real part), we can check that we have to take the $\eta \to 0$ limit under the integral sign before the $\mathbf{q} \to \mathbf{0}$ limit to recover the result obtained by doing the integral at finite $\mathbf{q}$ and then taking the $\mathbf{q} \to \mathbf{0}$ limit (the latter is unambiguous and does not depend on the presence of the principal part in the integral). Physically, this means that the adiabatic turning-on time must be longer than the diffusion time to allow the conserved quantity to relax. This is summarized by the following set of equations*

$$\lim_{\mathbf{q}\to\mathbf{0}} \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi}\frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} \tag{10.119}$$

$$\neq \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q}\to\mathbf{0}} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} \tag{10.120}$$

Remark 84 *Extracting the diffusion constant from a limit: The phenomenological hydrodynamic limit Eq.(10.118) shows that the diffusion constant can be obtained from*

$$2D\chi_{nn} = \lim_{\omega\to 0}\lim_{\mathbf{q}\to\mathbf{0}} \frac{\omega}{q^2}\chi''_{nn}(\mathbf{q},\omega).$$

The order of limits is crucial. This has been extensively discussed by Kadanoff and Martin.[111] For quantities related to transport, it is $\lim_{\mathbf{q}\to\mathbf{0}}$ *that comes first, contrary to the thermodynamic sum-rule case.*

Remark 85 *The fact that the* $\mathbf{q}\to\mathbf{0}$ *and* $\omega\to 0$ *limits cannot be inverted is intimaterlyt related to the in finite size limit that we are considering. Dissipation in the* $\omega\to 0$ *limit is an emergent phenomenon that can be observed in the infinite size limit, namely when* $\mathbf{q}\to\mathbf{0}$ *first.*

10.10.3 Moments, sum rules, and their relation to high-frequency expansions.

The n'th moment of a probability distribution is defined as the average of the random variable to the power n. By analogy, we define the n'th moment of the spectral function by $\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega)$. For operators with the same signature under time reversal, even moments vanish while odd moments of $\chi''_{A_iA_j}$ are related to equal-time commutators that are easy to compute, at least formally:

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega) = \left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left(i\frac{\partial}{\partial t}\right)^n e^{-i\omega t}2\chi''_{A_iA_j}(\omega)\right]_{t=0} \tag{10.121}$$

$$= \frac{1}{\hbar}\left\langle\left[\left(i\frac{\partial}{\partial t}\right)^n A_i(t),A_j(0)\right]\right\rangle_{t=0} = \frac{1}{\hbar}\left\langle\left[\left[\left[A_i(t),\frac{H}{\hbar}\right],\frac{H}{\hbar}\right]...,A_j(0)\right]\right\rangle_{t=0}. \tag{10.122}$$

This may all easily be computed through n equal-time commutations with the Hamiltonian.

These moments determine the high frequency behavior of response functions. One does expect that high frequencies are related to short times, and if time is short enough it is natural that commutators be involved. Let us see this. Suppose the spectrum of excitations is bounded, as usually happens when the input momentum $\mathbf{q}$ is finite. Then, $\chi''_{A_iA_j}(\omega') = 0$ for $\omega' > \Lambda$ where Λ is some large frequency. Then, for $\omega > \Lambda$, we can expand the denominator since the condition $\omega'/\omega \ll 1$ will always be satisfied within the integration range. This gives us a high-frequency expansion,

$$\boxed{\chi^R_{A_iA_j}(\mathbf{q},\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'-\omega-i\eta}} \tag{10.123}$$

$$\boxed{\approx \sum_{n=1}^{\infty}\frac{-1}{\omega^{2n}}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}(\omega')^{2n-1}\chi''_{A_iA_j}(\mathbf{q},\omega')} \tag{10.124}$$

where we have assumed that we are in a situation where $\chi''_{A_iA_j}$ is odd, which implies that only odd moments of $\chi''_{A_iA_j}$ do not vanish. Clearly, in the $\omega\to\infty$ limit, the susceptibilities in general scale as $1/\omega^2$, a property we will use later in the context of analytic continuations.

Remark 86 *Classical limit: Note that there are as many* $1/\hbar$ *as there are commutators in the expression for the moments Eq. (10.122).This means that there is a classical limit since commutators divided by* $\hbar$ *turn into Poisson brackets in the classical limit.*

10.10.4 The f-sum rule as an example

The f-sum rule is one of the most widely used moment of a correlation function, particularly in the context of optical conductivity experiments. It is quite remarkable that this sum rule does not depend on interactions, so it should be valid independently of many details of the system. If we return to our high-frequency expansion in terms of moments, Eq.(10.124), we will find that

$$\chi^R_{nn}(\mathbf{q},\omega) \approx \frac{-1}{\omega^2}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\omega'\chi''_{nn}(\mathbf{q},\omega') + \ldots = -\frac{n\mathbf{q}^2}{m\omega^2} + \ldots . \tag{10.125}$$

This is equivalent to saying that at very high frequency the system reacts as if it was composed of free particles. It is the inertia that determines the response, like for a harmonic oscilator well above the resonance frequency.You can return to Eq.(3.3) for the simple oscillator to verify this result from our introductory example.

Let us derive that sum rule, which is basically a consequence of particle conservation. When the potential-energy part of the Hamiltonian commutes with the density operator, while the kinetic-energy part is that of free electrons (not true for tight-binding electrons) we find that

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{n\mathbf{q}^2}{m}.} \tag{10.126}$$

This is the f sum-rule. It is valid for an arbitrary value of the wave vector $\mathbf{q}$. It is a direct consequence of the commutation-relation between momentum and position, and has been first discussed in the context of electronic transitions in atoms.

Just a bit of notation before I begin the proof. Using translational invariance one can write,

$$\int d\left(\mathbf{r}-\mathbf{r}'\right)e^{-i\mathbf{q}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}f(\mathbf{r}-\mathbf{r}') = \frac{1}{\mathcal{V}}\int d\mathbf{r}e^{-i\mathbf{q}\cdot r}\int d\mathbf{r}'e^{-i\mathbf{q}\cdot r'}f(\mathbf{r}-\mathbf{r}') \tag{10.127}$$

where $\mathcal{V}$ is the integration volume. This follows by changing coordinates to center of mass and relative coordinates in the integration. The integral over center of mass gives the factor of volume.

The proof of the $f-$sum rule is as follows. From the above results for moments

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{i}{\hbar\mathcal{V}}\left\langle\left[\frac{\partial n_{\mathbf{q}}(t)}{\partial t}, n_{-\mathbf{q}}(t)\right]\right\rangle \tag{10.128}$$

$$= -\frac{1}{\hbar^2\mathcal{V}}\left\langle\left[\left[H, n_{\mathbf{q}}(t)\right], n_{-\mathbf{q}}(t)\right]\right\rangle . \tag{10.129}$$

The interaction term commutes with the density, so only the kinetic-energy part of H contributes. The computation of the equal-time commutator is self-explanatory.

$$n_{\mathbf{q}} = \int d\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\sum_{\alpha}\delta(\mathbf{r}-\mathbf{r}_\alpha) = \sum_{\alpha}e^{-i\mathbf{q}\cdot\mathbf{r}_\alpha} \tag{10.130}$$

$$\left[p^x_\beta, n_{\mathbf{q}}\right] = \frac{\hbar}{i}\left[\frac{\partial}{\partial x_\beta}, \sum_{\alpha}e^{-i\mathbf{q}\cdot\mathbf{r}_\alpha}\right] = -\hbar q^x e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}. \tag{10.131}$$

where p^x_β is the momentum in the direction x of particle β and $\mathbf{r}_\alpha$, $\mathbf{r}_\beta$ are position operators. Since $[\mathbf{p}\cdot\mathbf{p}, n] = \mathbf{p}\left[\mathbf{p}, n\right] + \left[\mathbf{p}, n\right]\mathbf{p}$ we have

$$\left[H, n_{\mathbf{q}}(t)\right] = \sum_{\beta}\left[\frac{p^2_\beta}{2m}, n_{\mathbf{q}}\right] = \frac{1}{2m}\sum_{\beta}\left(\mathbf{p}_\beta\cdot\left(-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}\right) + \left(-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}\right)\cdot\mathbf{p}_\beta\right) \tag{10.132}$$

$$[[H, n_{\mathbf{q}}(t)], n_{-\mathbf{q}}(t)] = -\frac{1}{m}\sum_{\beta=1}^{N}\hbar^2\mathbf{q}^2 e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}e^{i\mathbf{q}\cdot\mathbf{r}_\beta} = -\frac{\hbar^2\mathbf{q}^2 N}{m} \tag{10.133}$$

which proves the result (G.12) when substituted in the expression in terms of commutator (10.129) with $n \equiv N/\mathcal{V}$. The result of the commutators is a number not an operator, so the thermodynamic average is trivial in this case! (Things will be different with tight-binding models.)

Remark 87 *High order moments: For higher-order moments, there are generally averages of operators to evaluate.*

11. KUBO FORMULAE FOR THE CONDUCTIVITY

A very useful formula in practice is Kubo's formula for the conductivity. The general formula applies to frequency and momentum dependent probes so that it is of more general applicability than only DC conductivity. In fact there are many versions of that formula, that also have analogs for other transport properties. These formula are used in practice to make predictions about light scattering experiments as well as microwave measurements. At the end of this section we will see that conductivity is simply related to dielectric constant by macroscopic electrodynamics. This explains the wide applicability of the Kubo formula. We will see that the $f-$sum rule can be used to obtain a corresponding sum rule on the conductivity that is widely used in practice, for example in infrared light scattering experiments on solids. On a more formal basis, the general properties of the Kubo formula will allow us, following Kohn, to better define what is meant by a superconductor, an insulator and a metal.

After a general discussion of the coupling of light to matter, I discuss in turn longitudinal and transverse response, exposing the consequences of gauge invariance. Follows a brief application to the definition of superconductors, metals and insulators, where I make the connection between conductivity and dielectric constant. I finish with a most interesting application of sum rules that allows us to extract the penetration depth of a superconductor from an optical conductivity measurement.

Remark 88 *We adopt the Système International (SI) units for electromagnetic fields.*

11.1 Coupling between electromagnetic fields and matter, and gauge invariance

Electric field and the magnetic induction are related to vector and scalar potentials by, respectively,

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\nabla}\phi \tag{11.1}$$

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}. \tag{11.2}$$

The gauge transformation

$$\mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla}\Lambda \tag{11.3}$$

$$\phi \to \phi - \frac{\partial \Lambda}{\partial t} \tag{11.4}$$

leaves the electric and magnetic fields invariant. This representation by vector and scalar potentials ensures that the magnetic induction is divergence free, $\nabla \cdot \mathbf{B} = 0$, and that Faraday's law is obeyed, $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial \mathbf{t}$. We say that the theory is gauge invariant. In other words, there are many equivalent ways of representing

the same physics. As emphasized by Wen,[252] this is not a symmetry in the usual sense, it is just a statement about equivalent descriptions.

I will give a more detailed derivation in the next subsection, but you only need to know the so-called minimal-coupling prescription to couple matter and electromagnetic field,[24] one of the most elegant results in physics

$$\mathbf{p}_\alpha = \frac{\hbar}{i}\nabla_\alpha \to \frac{\hbar}{i}\nabla_\alpha - e\mathbf{A}(\mathbf{r}_\alpha, t). \tag{11.5}$$

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\phi(\mathbf{r}_\alpha, t).. \tag{11.6}$$

In this expression e is the charge of the particle, not the elementary charge. The derivatives to the right are called covariant.

Remark 89 *Note that the quantity that has canonical commutation relations with the position operator in all gauges is the conjugate moment operator* $\mathbf{p}_\alpha = \frac{\hbar}{i}\nabla_\alpha$. *Note also that while the following equation* $\left[\mathbf{r}_\beta, \frac{\hbar}{i}\nabla_\alpha + f(\mathbf{r})\right] = i\hbar\delta_{\alpha,\beta}$, *where f is an arbitrary function, could suggest some ambiguity in the definition of the conjugate moment operator, the simple requirement that it should be translationally invariant implies that* $f(\mathbf{r})$ *vanishes.*

Given this, Schrödinger's equation in the presence of an electromagnetic field should read

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi(\mathbf{r}_\alpha, t)\right)\psi = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_\alpha - e\mathbf{A}(\mathbf{r}_\alpha, t)\right)^2\psi + V\psi \tag{11.7}$$

where V is some potential energy. Suppose we write the equation in a different gauge

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi(\mathbf{r}_\alpha, t) + e\frac{\partial\Lambda(\mathbf{r}_\alpha, t)}{\partial t}\right)\psi' = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_\alpha - e\mathbf{A}(\mathbf{r}_\alpha, t) - e\boldsymbol{\nabla}\Lambda(\mathbf{r}_\alpha, t)\right)^2\psi' + V\psi'.$$

The solution ψ' is different since it is not the same equation. There should be such a ψ' since gauge invariance implies that all physical observables should be independent of the gauge, the eigenenergies in particular. Assume that ψ and ψ' correspond to an eigenstate with the same value of the eigenenergy. Then, the solution ψ' that we find is related to ψ with the same eigenvalue in the following way

$$\boxed{\psi'(\mathbf{r}_\alpha, t) = e^{ie\Lambda(\mathbf{r}_\alpha, t)/\hbar}\psi(\mathbf{r}_\alpha, t)}. \tag{11.8}$$

That is easy to check since if we substitute in the equation for ψ', then we recover the previous equation for ψ. This result applies to all eigenstates, hence it is completely general.

Observables should be gauge invariant. That is clearly the case for the potential,

$$\int d^3\mathbf{r}\psi^* V\psi = \int d^3\mathbf{r}\psi'^* V\psi' \tag{11.9}$$

since the phases cancel. The conjugate momentum operator however is not gauge invariant

$$\int d^3\mathbf{r}\psi^*\frac{\hbar}{i}\boldsymbol{\nabla}\psi \neq \int d^3\mathbf{r}\psi'^*\frac{\hbar}{i}\boldsymbol{\nabla}\psi' \tag{11.10}$$

since $\boldsymbol{\nabla}\Lambda \neq 0$. On the other hand, the following quantity $\left(\frac{\hbar}{i}\boldsymbol{\nabla} - e\mathbf{A}(\mathbf{r}_\alpha, t)\right)$ is gauge invariant since

$$\int d^3\mathbf{r}\psi^*\left(\frac{\hbar}{i}\boldsymbol{\nabla} - e\mathbf{A}(\mathbf{r}_\alpha, t)\right)\psi = \int d^3\mathbf{r}\psi'^*\left(\frac{\hbar}{i}\boldsymbol{\nabla} - e\mathbf{A}(\mathbf{r}_\alpha, t) - e\boldsymbol{\nabla}\Lambda\right)\psi'. \tag{11.11}$$

That quantity is the expectation of the mass times the velocity and is thus an observable. This expression is necessary to establish the correct expression for the current.

Remark 90 *Conjugate moment and current are clearly different operators. Current is observable. More on this to come.*

11.1.1 *Invariant action, Lagrangian and coupling of matter and electromagnetic field

[214]

This section is not necessary to understand any other section. It is just useful to recall the fundamental ideas about coupling electromagnetic fields and matter.

Take a single particle of charge e in classical mechanics. The action that couples that particle, or piece of charged matter, to the electromagnetic field should be invariant under a Lorentz transformation and a gauge transformation. The simplest candidate that satisfies this requirement is

$$S_{e-m} = e \int A_\mu dr^\mu \tag{11.12}$$

where we used the summation convention as usual and the four-vectors with r^μ the contravariant four-vector for position

$$A_\mu = (-\phi/c, A_a) \; ; \; r^\mu = \begin{pmatrix} ct \\ r_a \end{pmatrix} \tag{11.13}$$

and the following flat-space metric tensor

$$\eta^{\mu\nu} = \eta_{\mu\nu} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{11.14}$$

The action is clearly Lorentz invariant. It is also gauge invariant since, with

$$\partial_\mu = \left(\frac{1}{c\partial t}, \boldsymbol{\nabla} \right),$$

the gauge transformation

$$S_{e-m} \to e \int (A_\mu + \partial_\mu \Lambda) \, dr^\mu \tag{11.15}$$

only adds a total time derivative to the Lagrangian

$$e \int (\partial_\mu \Lambda) \, dr^\mu = e \int (\partial_\mu \Lambda) \frac{dr^\mu}{dt} dt = e \int \frac{d\Lambda}{dt} dt \tag{11.16}$$

and in the variational principle the Lagrangian does not vary at the limits of time integration.

Remark 91 *In the action, the coordinates of the particle are parametrized by time, in other words,* $\mathbf{r}(t)$ *is what is integrated in the action.*

Speaking of the Lagrangian for light-matter interaction, it can be deduced from

$$S_{e-m} = e\int A_\mu \frac{dr^\mu}{dt}dt = \int \left(-e\phi + e\mathbf{A}\cdot\frac{d\mathbf{r}}{dt}\right)dt = \int L_{e-m}dt \tag{11.17}$$

The coupling of light to matter appears at two places in the equations of motion obtained from the Euler-Lagrange equations. It appears in the Euler-Lagrange equations for matter that involve particle coordinates, and in the Euler-Lagrange equations for the electromagnetic field that involve electromagnetic potentials playing the role of coordinates. The former give Newton's equations with the Lorentz force and the latter Maxwell's equations.

The part of the Lagrangian that involve particle coordinates, neglecting potential energy terms that do not play any role in this derivation, is given by $L = m\mathbf{v}^2/2 + L_{e-m}$, namely

$$\boxed{L = \tfrac{1}{2}m\mathbf{v}^2 - e\left(\phi - \mathbf{A}\cdot\tfrac{d\mathbf{r}}{dt}\right)} \tag{11.18}$$

$$\boxed{L = \tfrac{1}{2}m\mathbf{v}^2 - e\left(\phi - \mathbf{A}\cdot\mathbf{v}\right)} \tag{11.19}$$

It can be verified that the Euler-Lagrange equations with position as the dynamical variable give Newton's equation with the Lorentz force

$$m\frac{d\mathbf{v}}{dt} = e\mathbf{E} + \mathbf{v}\times\mathbf{B}. \tag{11.20}$$

The conjugate moment is

$$\boxed{p_a = \left(\tfrac{\partial L}{\partial v_a}\right)_{\mathbf{r},\mathbf{A}} = mv_a + eA_a \rightarrow \tfrac{\hbar}{i}\tfrac{\partial}{\partial r_a}.} \tag{11.21}$$

It is the conjugate moment $\mathbf{p}$ that obeys commutation relations with position in quantum mechanics, in other words it is $\mathbf{p}_\alpha$ that becomes $\frac{\hbar}{i}\boldsymbol{\nabla}$. I do not add any function of position on that gradient, even though it would give the same commutation relation for two reasons. That function of position is arbitrary, so I can choose it to vanish, but more importantly, as an operator I want $\mathbf{p}_\alpha$ to be translationally invariant.

To find the Hamiltonian, recall also that, with Einstein's summation convention,

$$\begin{aligned} H &= p_a v_a - L = (mv_a + eA_a)\,v_a - \frac{1}{2}mv_a v_a + e\,(\phi - A_a v_a) \\ &= \frac{1}{2}mv_a v_a + e\phi = \frac{1}{2m}\left(p_a - eA_a\right)^2 + e\phi. \end{aligned} \tag{11.22}$$

In the last equation we used the relation between velocity and momentum Eq.(11.21).

The action of the electromagnetic field by itself is written in terms of the Faraday tensor. What is important for our discussion is that the current that appears in Maxwell's equation for $\nabla\times\mathbf{B}$ is generated by the following term

$$\boxed{j_a = ev_a = \left(\tfrac{\partial L_{e-m}}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} = \tfrac{e}{m}\left(p_a - eA_a\right)} \tag{11.23}$$

where in the last equation we have used the equation that relates the conjugate moment to the velocity and vector potential Eq.(11.21). Physically this makes a lot of sense. The current is simply charge times velocity.

In condensed matter physics, we do not generally write down the part of the Hamiltonian that involves only the pure electromagnetic field. But we are interested in coupling matter to the electromagnetic field and we would like to have the

expression for the current that follows from the Hamiltonian where the minimal-coupling prescription has been used. It is indeed possible to satisfy this wish and to obtain the current from the Hamiltonian. It proceeds as follows. Taking for L the full Lagrangian, except for the part that contains only the electromagnetic field, we obtain

$$\left(\frac{\partial L}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} = \left(\frac{\partial \left(p_b v_b - H\right)}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} \tag{11.24}$$

where $\mathbf{p}\left(\mathbf{r},\mathbf{v},\mathbf{A}\right)$ is written in terms of $\mathbf{r},\mathbf{v}$ and $\mathbf{A}$ using the equation for the conjugate moment Eq.(11.23). With the chain rule, we thus find (components of p that are not differentiated are also kept constant)

$$\left(\frac{\partial \left(p_b v_b - H\right)}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} = \left(\frac{\partial p_b}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} v_b - \left(\frac{\partial H}{\partial p_b}\right)_{\mathbf{r},\mathbf{A}} \left(\frac{\partial p_b}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} - \left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{r}}. \tag{11.25}$$

Since Hamilton's equations give $\left(\frac{\partial H}{\partial p_b}\right)_{\mathbf{r},\mathbf{A}} = v_b$, we are left with

$$\boxed{j_a = e v_a = \left(\frac{\partial L}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} = -\left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{r}}.} \tag{11.26}$$

This result comes out because, as usual in a Legendre transform, the first derivative with respect to the conjugate variable $\mathbf{p}$ vanishes. The above expression for the current in terms of a derivative of the Hamiltonian is often used in practice. In this expression, H does not contain the part that involves only electromagnetic potentials.

Remark 92 *In the four-vector notation of the present section, the prescription for minimal coupling, is*

$$\boxed{\partial_\mu \rightarrow \partial_\mu - ieA_\mu/\hbar.} \tag{11.27}$$

Remark 93 *Eq. (11.26) is a special case of a very general property of Legendre transforms. For*

Remark 94 *In thermodynamics pressure is obtained from a derivative of the energy with respect to volume $p = -\left(\partial E/\partial V\right)_S$ if it is the entropy that is kept constant since $dE = TdS - pdV$. But if it is the temperature $p = -\left(\partial F/\partial V\right)_T$ that is kept constant, one performs a Legendre transform between S and T and it is the Helmholtz free energy that must be differentiated with respect to volume to obtain pressure since $dF = -SdT - pdV$. If you recall this result, it may help understand why Eq.(11.26) makes sense.*

11.1.2 *Lagrangian for the electromagnetic field

With our convention for $\eta^{\mu\nu}$, we have

$$\partial^\mu = \left(-\frac{1}{c\partial t}, \boldsymbol{\nabla}\right), \tag{11.28}$$

which allows to write the Faraday tensor as

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu. \tag{11.29}$$

This means, for example that $F^{01} = \partial^0 A^1 - \partial^1 A^0 = E^1/c$, $F^{31} = \partial^3 A^1 - \partial^1 A^3 = B^2$. The electromagnetic Lagrangian density then reads

$$L_e = -\frac{1}{4\mu_0} F^{\mu\nu} F_{\mu\nu} = \frac{\varepsilon_0}{2}\mathbf{E}\cdot\mathbf{E} - \frac{1}{2\mu_o}\mathbf{B}\cdot\mathbf{B} = \frac{\varepsilon_0}{2}\mathbf{E}\cdot\mathbf{E} - \frac{\mu_0}{2}\mathbf{H}\cdot\mathbf{H}, \tag{11.30}$$

with $\mathbf{B}$ the magnetic induction, $\mathbf{H}$ the magnetic intensity, $\varepsilon_0 = 8.85 \times 10^{-12}$ farad/meter is the permittivity of vacuum and $\mu_0 = 4\pi \times 10^{-7}$ henry/meter its permeability. I have used the usual result, $\varepsilon_0 \mu_0 = 1/c^2$.

If we include all pieces of the Lagrangian that contain the electromagnetic scalar and vector poentials, including the one for the interaction with matter Eq.(11.17), we have

$$L = -\frac{1}{4\mu_0} F^{\mu\nu} F_{\mu\nu} + e A_\mu \frac{dr^\mu}{dt}, \tag{11.31}$$

which give Maxwell's equations Eqs.(13) in S.I. units when A_μ is taken as a dynamical variable. The Lorentz force is obtained when we also add the Lagrangian for matter alone.

Remark 95 *In the 2019 version of S.I. units*[1]*, the electric charge and the speed of light are defined. If one can measure one of* ε_0 *or* μ_0*, the other is known since* $\varepsilon_0 c^2 = 4\pi/\mu_0 \sim 10^7$.

11.2 Response of the current to external vector and scalar potentials

We need to find the terms $\delta\mathcal{H}(t) = \delta\mathcal{H}(t)_\phi + \delta\mathcal{H}(t)_{\mathbf{A}}$ added to the Hamiltonian by the presence of the electromagnetic field. Let us begin by the term $\delta\mathcal{H}(t)_{\mathbf{A}}$ coming from the vector potential. Under the minimal coupling prescription, we find (recall that the gradient will also act on the wave function that will multiply the operator)

$$-\frac{\hbar^2}{2m}\nabla_\alpha^2 \to -\frac{\hbar^2}{2m}\nabla_\alpha^2 - \frac{e\hbar}{2mi}\left(\mathbf{A}(\mathbf{r}_\alpha,t)\cdot\nabla_\alpha + \nabla_\alpha\cdot\mathbf{A}(\mathbf{r}_\alpha,t)\right) + \frac{e^2}{2m}\mathbf{A}^2(\mathbf{r}_\alpha,t). \tag{11.32}$$

This means that to linear order in the vector potential, the change in the Hamiltonian is

$$\delta\mathcal{H}(t)_{\mathbf{A}} = -\sum_\alpha \frac{e\hbar}{2mi}\left(\mathbf{A}(\mathbf{r}_\alpha,t)\cdot\nabla_\alpha + \nabla_\alpha\cdot\mathbf{A}(\mathbf{r}_\alpha,t)\right) = -\int d\mathbf{r}\mathbf{A}(\mathbf{r},t)\cdot\mathbf{j}(\mathbf{r}). \tag{11.33}$$

where, continuing with our first-quantization point of view, we defined the *paramagnetic current* for particles of charge e

$$\mathbf{j}(\mathbf{r}) = \frac{e}{2m}\sum_\alpha \left(\delta(\mathbf{r}-\mathbf{r}_\alpha)\mathbf{p}_\alpha + \mathbf{p}_\alpha\delta(\mathbf{r}-\mathbf{r}_\alpha)\right). \tag{11.34}$$

It is important to note that $\mathbf{A}(\mathbf{r},t)$ here plays the role of the external vector potential. It is just a number that commutes with all operators. It is only $\mathbf{A}(\mathbf{r}_\alpha,t)$ that does not commute with momentum $\mathbf{p}_\alpha$ because of the argument of the vector potential. Given the fact that $[\mathbf{r}_\beta,\mathbf{p}_\alpha] = i\hbar\delta_{\alpha,\beta}$ there is an ambiguity in

[1] https ://physicstoday.scitation.org/do/10.1063/PT.6.2.20181116a/full/

the position of the δ function with respect to the momentum operator: We can have $\mathbf{p}_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha)$ or $\delta(\mathbf{r}-\mathbf{r}_\alpha)\mathbf{p}_\alpha$. We see that the symmetrized form comes out naturally from the coupling to the electromagnetic field. We have allowed the semi-classical external field to depend on time.

The paramagnetic current that we found above is the same as that which is found from Schrödinger's equation in the absence of electromagnetic field by requiring that probability density $\psi^*\psi$ be conserved. Unless the system is neutral, it is not observable since it is not gauge invariant. There are two ways to find the observable current. I start with the minimal coupling prescription, Eq.(11.5) and the considerations of Sec.11.1 on gauge invariance of observables. The observable current operator $\mathbf{j}^A(\mathbf{r})$ is obtained from applying the minimal coupling prescription to the paramagnetic current operator Eq.(11.34)

$$\mathbf{j}^A(\mathbf{r}) = \mathbf{j}(\mathbf{r}) - \frac{e^2}{m}\sum_\alpha \mathbf{A}(\mathbf{r}_\alpha)\delta(\mathbf{r}-\mathbf{r}_\alpha) = \mathbf{j}(\mathbf{r}) - \frac{e}{m}\mathbf{A}(\mathbf{r})\rho(\mathbf{r}) \tag{11.35}$$

where I have defined the charge density as before

$$\rho(\mathbf{r}) = en(\mathbf{r}) = e\sum_\alpha \delta\left(\mathbf{r}-\mathbf{r}_\alpha\right). \tag{11.36}$$

The last term in the equation for the current is called the *diamagnetic current.* This is the second time we applied the minimal coupling prediction.

Remark 96 *Other approach: The current* $\mathbf{j}^A(\mathbf{r})$ *can also be obtained from* $-\left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{A}}$, *as explained in the previous section. The last term in the expression for the current Eq. (11.35) comes from the term of order* $\mathbf{A}^2$ *in the Hamiltonian.*

Remark 97 *Our definition of the current-density operator Eq.(11.34) automatically takes care of the relative position of the vector potential and of the gradients in the above equation.*

It is easier to add an ordinary scalar potential. From Schrödinger's equation in the presence of an electromagnetic field Eq.(11.7), the presence of a scalar potential introduces a term

$$\delta\mathcal{H}(t)_\phi = \int d\mathbf{r}\phi(\mathbf{r},t)\rho(\mathbf{r}) \tag{11.37}$$

in the Hamiltonian.

Using the explicit expression for the current Eq.(11.35) and our linear-response formulae in Chapter 9, we finally come to the general expression for the response of the current in direction a to the vector potential,

$$\boxed{\delta\left\langle j_a^A(\mathbf{q},\omega)\right\rangle = \left[\chi^R_{j_a j_b}(\mathbf{q},\omega) - \tfrac{ne^2}{m}\delta_{ab}\right] A_b(\mathbf{q},\omega) - \chi^R_{j_a\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega).} \tag{11.38}$$

There is a sum over the repeated spatial indices b as usual. The term proportional to $-\frac{ne^2}{m}\delta_{ab}$ in this expression, called the diamagnetic term,**??** comes from the last term in the expression for the gauge invariant current Eq.(11.35). Since the density operator there is already multiplied by the vector potential, its average can be taken for the equilibrium ensemble where the average density is independent of position.

The above expression is not gauge invariant in an obvious way. The response is not given in terms of gauge invariant fields. We will show below, using current conservation, that there is indeed gauge invariance. We begin with the case of the transverse response, which is easier.

Remark 98 *Important, what are the perturbations: The vector and scalar potential above are the ones induced by external charges. There is also in general a self-consistent response that I will discuss later.*

11.3 Kubo formula for the transverse conductivity

The above relation between current and electromagnetic potential still does not give us the conductivity. The conductivity relates current to electric field, not to potential. Roughly, for the conductivity σ we have $j = \sigma E$. We thus need to go back to the fields. In addition, the first thing to realize is that the conductivity is a tensor since it relates current in one direction to field applied in any other direction. Moreover, the electromagnetic fields can be transverse or longitudinal, i.e. perpendicular or transverse to the direction of propagation. More generally, the divergence of the transverse part vanishes and the curl of the longitudinal part vanishes. But I will stick with the simpler case of translationally invariant system where wave vectors suffice. Let us begin by discussing this point.

When we study the response to applied fields whose direction is perpendicular to the direction of the wave vector $\mathbf{q}$, we say that we are studying the transverse (or selenoidal) response**.** In this case, $\mathbf{q} \cdot \mathbf{E}(\mathbf{q}, \omega)$=0. The scalar potential contributes only to the longitudinal component of the field (along with the longitudinal contribution from the vector potential) since the gradient is always along $\mathbf{q}$. We can thus disregard for the moment the contribution from the scalar potential and leave it for our study of the longitudinal response, where we will study in detail the question of gauge invariance. The magnetic induction is always transverse since $\nabla \cdot \mathbf{B} = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \times \mathbf{A}$ =0. Let us decompose the vector potential into a transverse and a longitudinal part. This is easily done by using the unit vector $\widehat{\mathbf{q}} = \mathbf{q}/\left|\mathbf{q}\right|$

$$\mathbf{A}^L \equiv \widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \mathbf{A} \equiv \widehat{\mathbf{q}} \left(\widehat{\mathbf{q}} \cdot \mathbf{A}\right) \tag{11.39}$$

$$\mathbf{A}^T \equiv \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \cdot \mathbf{A}. \tag{11.40}$$

In the last expression $\widehat{\mathbf{q}}\widehat{\mathbf{q}}$ is a so-called "dyadic product" representation of the matrix $(\widehat{\mathbf{q}}\widehat{\mathbf{q}})_{ab} = \widehat{q}_a \widehat{q}_b$. The first $\widehat{\mathbf{q}}$ acts on the left and the second one to the right. In the last equation, $\overleftrightarrow{\mathbf{I}}$ is the vector notation for δ_{ab}. We introduced the following notation for the multiplication of tensors with vectors,

$$\left(\overleftrightarrow{\sigma} \cdot \mathbf{A}\right)_a = \sum_b \sigma_{ab} A_b. \tag{11.41}$$

The transverse and longitudinal parts of the conductivity tensor for a homogeneous isotropic system are obtained as follows,

$$\overleftrightarrow{\sigma^T}(\mathbf{q}, \omega) = \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \tag{11.42}$$

$$\overleftrightarrow{\sigma^L}(\mathbf{q}, \omega) = \widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \widehat{\mathbf{q}}\widehat{\mathbf{q}} \tag{11.43}$$

Remark 99 *In a homogeneous system in the absence of a magnetic field, the above gives us all the components of the conductivity,* $\overleftrightarrow{\sigma}(\mathbf{q}, \omega) = \overleftrightarrow{\sigma^T}(\mathbf{q}, \omega) + \overleftrightarrow{\sigma^L}(\mathbf{q}, \omega)$ *because the off-diagonal components vanish, namely* $\widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) = 0$. *There are exceptions however. Topological materials, such as topological insulators and Weyl semimetals have a so-called anomalous Hall effect, in other words a non-vanishing* $\widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right)$ *that occurs in the absence of an applied magnetic field. This will be discussed later. In both of these cases, we are dealing with materials that have at least two bands.*

To simplify the notation, we take the current and applied electric field in the y direction, and the spatial dependence in the x direction. This is what happens

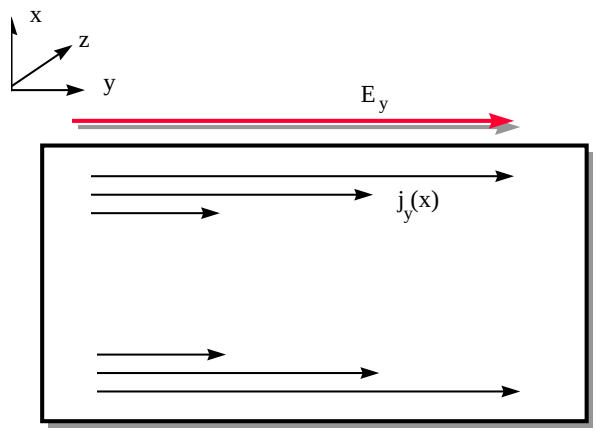


Figure 11-1 Application of a transverse electric field: skin effect.

usually in a wire made of homogeneous and isotropic material in the presence of the skin effect. This is illustrated in Fig.(11-1).

Then the transverse conductivity defined by

$$\delta \left\langle j_y^A(q_x,\omega) \right\rangle \equiv \sigma_{yy}(q_x,\omega) E_y(q_x,\omega) \tag{11.44}$$

for such a homogeneous system follows from the relation between current and vector potential Eq.(11.38) and from the relation between electric field and vector potential $\mathbf{E} = -\partial \mathbf{A}/\partial t$:

$$E_y(q_x,\omega) = i(\omega + i\eta) A_y(q_x,\omega) \tag{11.45}$$

which gives for the transverse conductivity

$$\boxed{\sigma_{yy}(q_x,\omega) = \frac{1}{i(\omega+i\eta)} \left[\chi^R_{j_y j_y}(q_x,\omega) - \frac{ne^2}{m} \right]} \tag{11.46}$$

Remark 100 *The first term in the above equation is usually called the paramagnetic current, and the last term the diamagnetic current.*

Remark 101 *A trick for Fourier transforms: The results that involve Fourier transforms are easier to derive if we think of a single Fourier component, such that* $A_y(\mathbf{r},t) = e^{i\mathbf{q}\cdot\mathbf{r} - i(\omega+i\eta)t} \; A_y(\mathbf{q},\omega)$.

Remark 102 *Causality and time Fourier transforms: We used the trick explained in the context of Kramers-Kronig relations which amounts to using* $\omega + i\eta$ *because the field is adiabatically switched on.*

Remark 103 *Definitions of transverse conductivity: In the presence of a magnetic field, off-diagonal pieces of the conductivity tensor do not vanish, in other words,* $\sigma_{xy}(0,\omega)$ *for example, can be different from zero. One often calls this the transverse conductivity. This is most often called the Hall conductivity. The definition of transverse and longitudinal above is related to the relative direction of the current and its spatial dependence.*

11.4 Kubo formula for the longitudinal conductivity and *f*-sum rule

When $\mathbf{q}$ is in the direction of the electric field, we say that we are considering the longitudinal (or potential) response. Using the consequences of charge conservation on the response functions χ'', it is possible to rewrite the expression which involves both scalar and vector potential Eq.(11.38) in a way that makes the response look explicitly invariant under gauge transformations. This is the plan for this section.

11.4.1 A gauge invariant expression for the longitudinal conductivity that follows from current conservation

As usual current conservation and gauge invariance are intimately related. We know, roughly, that the scalar potential couples to density while the vector potential couples to current. Since gauge invariance implies that the same (longitudinal) electric field can represented by either a scalar or a vector potential, it is clear that there is a consequence for the relation between charge and current. This consequence is current conservation. In more technical terms, Noether's theorem states that to each continuous transformation that leaves the action invariant, corresponds a conserved quantity. Using this theorem, gauge invariance leads to current conservation, namely

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = -\nabla \cdot \mathbf{j}(\mathbf{r},t) \tag{11.47}$$

$$\frac{\partial \rho(\mathbf{q},t)}{\partial t} = -i\mathbf{q} \cdot \mathbf{j}(\mathbf{q},t). \tag{11.48}$$

We can use current conservation to replace the charge-density operator in the term describing the response of the scalar potential by a current density, which will make the response Eq.(11.38) look more gauge invariant. Take $\mathbf{q}$ in the x direction to be specific. Some gymnastics on the time-dependent susceptibility in terms of commutator and Heaviside function gives,

$$\frac{\partial \chi^R_{j_x\rho}(q_x,t)}{\partial t} = \delta(t)\frac{i}{\hbar\mathcal{V}}\left\langle [j_x(q_x,0),\rho(-q_x,0)]\right\rangle + \theta(t)\frac{i}{\hbar\mathcal{V}}(-iq_x)\left\langle [j_x(q_x,0),j_x(-q_x,-t)]\right\rangle . \tag{11.49}$$

In the last term above, I have transferred the time dependence on the charge-density operator using time-translation invariance, and then used $\frac{\partial\rho(-q_x,-t)}{\partial t} = -iq_x j_x(-q_x,-t)$. Many minus signs are involved. The equal-time commutator is calculated from the f sum rule. First use the definition of $\chi''_{j_x\rho}(q_x,\omega)$

$$\frac{i}{\hbar\mathcal{V}}\left\langle [j_x(q_x,0),\rho(-q_x,0)]\right\rangle = i\int \frac{d\omega}{\pi}\chi''_{j_x\rho}(q_x,\omega) \tag{11.50}$$

then current conservation

$$= i\int \frac{d\omega}{\pi}\frac{\omega}{q_x}\chi''_{\rho\rho}(q_x,\omega) \tag{11.51}$$

and finally the f sum rule Eq.(G.12) to rewrite the last expression as

$$= iq_x\frac{ne^2}{m} \tag{11.52}$$

Substituting back in the expression for the time derivative of the current-charge susceptibility Eq.(11.49) and Fourier transforming in frequency, we have

$$\boxed{-i(\omega+i\eta)\chi^R_{j_x\rho}(q_x,\omega) = iq_x\frac{ne^2}{m} - iq_x\chi^R_{j_xj_x}(q_x,\omega).} \tag{11.53}$$

Using this in the general formula for the response of the current Eq.(11.38) the longitudinal linear response function can be written in terms of the gauge invariant electric field in two different ways:

$$\delta\left\langle j^A_x(q_x,\omega)\right\rangle = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right](i(\omega+i\eta)A_x(q_x,\omega) - iq_x\phi(q_x,\omega)) \tag{11.54}$$

$$= \left[\frac{1}{iq_x}\chi^R_{j_x\rho}(q_x,\omega)\right](i(\omega+i\eta)A_x(q_x,\omega) - iq_x\phi(q_x,\omega))\,. \tag{11.55}$$

Hence, replacing the gauge-invariant combination of potentials by the field,

$$E_x(q_x,\omega) = i(\omega+i\eta)A_x(q_x,\omega) - iq_x\phi(q_x,\omega) \tag{11.56}$$

we find the following Kubo formulae for the longitudinal conductivity $\delta\left\langle j^A_x(q_x,\omega\right\rangle \equiv \sigma_{xx}(q_x,\omega)E_x(q_x,\omega)$

$$\boxed{\sigma_{xx}(q_x,\omega) = \tfrac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega) - \tfrac{ne^2}{m}\right] = \left[\tfrac{1}{iq_x}\chi^R_{j_x\rho}(q_x,\omega)\right].} \tag{11.57}$$

Using gauge invariance and the $f-$sum rule, the above result for the longitudinal response will soon be rewritten in an even more convenient manner in Eq. (11.74).

11.4.2 Further consequences of gauge invariance and relation to f sum-rule.

The electric and magnetic fields, as well as all observable quantities are invariant under gauge transformations,

$$\mathbf{A} \to \mathbf{A} + \nabla\Lambda \tag{11.58}$$

$$\phi \to \phi - \frac{\partial\Lambda}{\partial t} \tag{11.59}$$

Let $\phi = 0$. Then

$$\delta\left\langle j^A_x(q_x,\omega)\right\rangle = \left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right]A_x(q_x,\omega) \tag{11.60}$$

Doing a gauge transformation with $\Lambda(x,0)$ independent of time ($\omega = 0$) does not induce a new scalar potential ($\phi = 0$). The response to this pure gauge field through the vector potential $\boldsymbol{\nabla}\Lambda$ should be zero since it corresponds to zero electric field. This will be the case if

$$\boxed{\left[\chi^R_{j_xj_x}(q_x,0) - \tfrac{ne^2}{m}\right] = 0}. \tag{11.61}$$

This can be proven explicitly by using the spectral representation and $\chi''_{j_xj_x}(q_x,0) = 0$,

$$\chi^R_{j_xj_x}(q_x,0) = \int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')}{\omega'} \tag{11.62}$$

as well as the conservation of charge,

$$= \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'} = \int \frac{d\omega'}{\pi} \frac{\omega' \chi''_{\rho\rho}(q_x,\omega')}{q_x^2} \tag{11.63}$$

and the f-sum rule (G.12)

$$= \frac{1}{q_x^2} \int \frac{d\omega'}{\pi} \omega' \chi''_{\rho\rho}(q_x,\omega') = \frac{ne^2}{m} = \chi^R_{j_x j_x}(q_x,0). \tag{11.64}$$

The form

$$\boxed{\int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'} = \frac{ne^2}{m}} \tag{11.65}$$

of the above result, obtained by combining Eqs.(11.61) and (11.62) will be used quite often below.

Remark 104 *Order of limits: An* ***important*** *consequence of the above result Eq. (11.61) is that to obtain the longitudinal DC conductivity (i.e. $\omega = 0$) the $q_x = 0$ limit must be taken first. We obtain zero if we take the $\omega = 0$ limit first. Taking the $\omega = 0$ limit first corresponds to looking at a thermodynamic quantity. We will do that for the transverse response of a superconductor to a magnetic field.*

Another possibility is to let $\mathbf{A}$ =0. Then, the general Kubo formula (11.38) gives

$$\delta \langle j_x(\mathbf{q},\omega) \rangle = -\chi^R_{j_x \rho}(\mathbf{q},\omega) \phi(\mathbf{q},\omega). \tag{11.66}$$

If we let $\Lambda(0,t)$ be independent of x, ($\mathbf{q}$ =0) then the vector potential remains zero ($\mathbf{A}$ =0). Again, the response to this pure gauge field through the scalar potential $-\partial\Lambda/\partial t$ must be zero, hence

$$\boxed{\chi^R_{j_x \rho}(0,\omega) = 0}. \tag{11.67}$$

That this is true, again follows from current conservation since

$$\chi^R_{j_x \rho}(0,\omega) = \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x \rho}(0,\omega')}{\omega' - \omega - i\eta} \tag{11.68}$$

and

$$\chi''_{j_x \rho}(0,\omega') = \int dt e^{i\omega' t} \frac{1}{2\hbar \mathcal{V}} \left\langle \left[\int d\mathbf{r} j_\mu(\mathbf{r},t), \int d\mathbf{r}' \rho(\mathbf{r}') \right] \right\rangle = 0 \tag{11.69}$$

where the last equality follows from the fact that the total charge $\int d\mathbf{r}' \rho(\mathbf{r}') = eN$ is a conserved quantity. In other words it commutes with the density matrix, which allows, using the cyclic property of the trace, to show that the commutator of eN with any operator that conserves the number of particles, vanishes.

Remark 105 *Both results Eq.(11.61) and Eq.(11.67) are consistent with the general relation found between both types of correlation functions Eq.(11.53). It suffices to take the $\mathbf{q} \to 0$ limit assuming that $\chi^R_{j_x j_x}(q_x,\omega)$ is finite or diverges less slowly than $1/q_x$ to prove Eq.(11.67) and to take $\omega \to 0$ assuming that $\chi^R_{j_\mu \rho}(q_x,\omega)$ is finite or diverges less slowly than $1/\omega$ to prove Eq.(11.61).*

11.4.3 Longitudinal conductivity sum-rule and a useful expression for the longitudinal conductivity.

The expression for the longitudinal conductivity

$$\sigma_{xx}(q_x,\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_x j_x}(q_x,\omega) - \frac{ne^2}{m}\right] \tag{11.70}$$

can be written in an even more convenient manner by using our previous results Eq.(11.65) obtained from the $f-$sum rule and the spectral representation for the current-current correlation function

$$\sigma_{xx}(q_x,\omega) = \frac{1}{i(\omega+i\eta)}\left[\int \frac{d\omega'}{\pi}\frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'-\omega-i\eta} - \int \frac{d\omega'}{\pi}\frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'}\right] \tag{11.71}$$

$$= \frac{1}{i(\omega+i\eta)}\left[\int \frac{d\omega'}{\pi}\frac{\chi''_{j_x j_x}(q_x,\omega')(\omega+i\eta)}{\omega'\,(\omega'-\omega-i\eta)}\right] \tag{11.72}$$

$$\boxed{\sigma_{xx}(q_x,\omega) = \frac{1}{i}\left[\int \frac{d\omega'}{\pi}\frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'(\omega'-\omega-i\eta)}\right]} \tag{11.73}$$

From this formula, we easily obtain with the usual identity for principal parts, Eq.(**??**)

$$\boxed{\mathrm{Re}\,\sigma_{xx}(q_x,\omega) = \frac{\chi''_{j_x j_x}(q_x,\omega)}{\omega}} \tag{11.74}$$

from which we obtain the conductivity sum rule valid for arbitrary q_x

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{Re}\left[\sigma_{xx}(q_x,\omega)\right] = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\chi''_{j_x j_x}(q_x,\omega)}{\omega} = \frac{ne^2}{2m} = \frac{\varepsilon_0\omega_p^2}{2}} \tag{11.75}$$

directly from the $f-$sum rule Eq.(11.65). In the above expression, ε_0 is the permittivity of the vacuum and ω_p^2 is the plasma frequency, which we will discuss later. Using the fact that the real part of the conductivity is an even function of ω, as follows from the fact that $\chi''_{j_x j_x}(q_x,\omega)$ is odd, the above formula is often written in the form of an integral from 0 to ∞. The case $q_x = 0$ needs a separate discussion, presented in the following section.

Remark 106 *Common expression for the f-sum rule applied to the optical conductivity: This last expression for the optical conductivity sum rule is often written in the form*

$$\int_0^{\infty} d\omega\,\mathrm{Re}\left[\sigma_{xx}(q_x,\omega)\right] = \frac{\pi ne^2}{2m} = \frac{\omega^2_{p,cgs}}{8} = \frac{4\pi\varepsilon_0\omega_p^2}{8} \tag{11.76}$$

Here we have used the fact that the real part of the conductivity is even in frequency, as follows from the fact that $\chi''_{j_x j_x}(q_x,\omega)$ is odd. Also, if we take the cgs units, the plasma frequency is $\omega^2_{p,cgs} = 4\pi ne^2/m$, so that the right-hand side is then $\omega^2_{p,cgs}/8$. In S.I., we have $\omega_p^2 = ne^2/(\varepsilon_0 m)$. So the ratio $\omega^2_{p,cgs}/\omega_p^2$ is given by $4\pi\varepsilon_0$, which just converts e^2 in cgs to $e^2/4\pi\varepsilon_0$ in S.I.

Remark 107 *Alternate expression: There is no principal part in the integrals appearing in the last expression. An equivalent but more cumbersome expression for the longitudinal conductivity, namely,*

$$\boxed{\sigma_{xx}(q_x,\omega) = \mathcal{P}\frac{1}{i\omega}\left[\chi^R_{j_x j_x}(q_x,\omega) - \frac{ne^2}{m}\right] - \pi\delta(\omega)\left[\chi^R_{j_x j_x}(q_x,\omega) - \frac{ne^2}{m}\right]} \tag{11.77}$$

is obtained from Eq.(11.70) by using the expression for principal parts. It is also possible to prove the optical-conductivity sum-rule from this starting point. Indeed, taking the real part and integrating both sides,

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{Re}\left[\sigma_{xx}(q_x,\omega)\right] &= \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\chi''_{j_xj_x}(q_x,\omega)}{\omega}-\frac{\mathrm{Re}\,\chi^R_{j_xj_x}(q_x,0)}{2}+\frac{ne^2}{2m}\\ &= \frac{ne^2}{2m}.\end{aligned}$$

Note that since the conductivity sum rule is satisfied for abitrary q_x, it is also satisfied at $q_x = 0$, a limit we will need when computing the conductivity in the next section.

Remark 108 *Practical use of sum rule: The n that appears in the conductivity sum rule is the full electronic density. In pratical calculations for experiment, one stops integrating at a finite frequency, which is smaller than the binding energy of core electrons. These electrons are then frozen, and the appropriate plasma frequency is calculated with the free electronic density in the conduction band.*

Remark 109 *The case of interactions in lattice models: The $f-$sum rule is particularly useful because it gives a result that is independent of interactions. We will see later that for models on a lattice, this is not quite true anymore.*

Remark 110 *If we need to consider the $q_x \longrightarrow 0$ limit, it is clearly taken last since we integrate over all frequencies, including $\omega = 0$, first. In addition, we are looking at the longitudinal response, hence we need a small non-zero q_x at least to decide that we are looking at the longitudinal response.*

Remark 111 *Thermal and thermoelectric effects: Thermal conductivity and thermoelectric coefficients are longitudinal responses that can be treated in a manner very similar to what was done in this section. There are analogs of the f sum-rule as well.[217]*

12. DRUDE WEIGHT, METALS, INSULATORS AND SUPERCONDUCTORS

All the above considerations about conductivity, correlation functions and sum rules may seem rather formal, and even useless. Let us put what we learned to work. In the present Chapter, we will find some powerful and unexpected results. For example, one can measure the penetration depth, i.e. the distance over which a static magnetic field is expelled by a superconductor, by doing instead a finite frequency conductivity measurement.

If we begin to talk about a superconductor, the first thing that comes to mind is the DC conductivity. Even if in the end we will see that zero resistance or infinite conductivity is not what characterizes a superconductor, this is a legitimate starting point. Suppose we are interested in the DC conductivity. We then need the response for a uniform, or very long wavelength field, i.e. the limit $q_x \to 0$ of our earlier formulae. It is important to notice that this is the proper way to compute the *DC* conductivity: Take the $\mathbf{q} \to 0$ limit, before the $\omega \to 0$ limit. In the opposite limit the response vanishes as we saw from gauge invariance (11.61). Physically, transport probes dynamical quantities. A DC measurement can be seen as the zero frequency limit of a microwave experiment for example. By taking the $\mathbf{q} \to \mathbf{0}$ limit first, we ensure that we are looking at an infinite volume, where energy levels can be arbitrarely close in energy. Then only can we take the zero frequency limit and still get absorption when the state is metallic. Otherwise the discrete nature of the energy states would not allow absorption in the zero frequency limit.

By asking questions about the DC conductivity, we are clearly beginning to ask what is the difference between a perfect metal, a superconductor, and an insulator. This is the question we will focus on in this chapter. Many of the answers were given by Kohn [117]. The first step is to define the Drude weight.

12.1 The Drude weight

In the correct limit $q_x = 0$ first to obtain the uniform *DC* conductivity, the above formulae (11.74) and (11.77) for conductivity give us either the simple formula,

$$\mathrm{Re}\left[\sigma_{xx}(0,\omega)\right] = \frac{\chi''_{j_x j_x}(0,\omega)}{\omega} \tag{12.1}$$

or the more complicated-looking formula

$$\mathrm{Re}\left[\sigma_{xx}(0,\omega)\right] = \mathcal{P}\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} - \pi\delta(\omega)\left[\mathrm{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right] - \frac{ne^2}{m}\right] \tag{12.2}$$

The coefficient of the delta function at zero frequency $\delta(\omega)$ is called the Drude weight D:

$$\boxed{D = \pi \lim_{\omega\to 0}\left[\frac{ne^2}{m} - \mathrm{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right]\right]}. \tag{12.3}$$

The reason for this definition will become clear in the next section when we talk about metals.

Remark 112 *In practice, the delta function in optical experiments is broadened by impurity scattering or scattering due to finite temperature. Whenever there is a peak in the conductivity centered at zero frequency, one refers to it as a Drude peak. The integral under that peak is the Drude weight. One observes narrowing of the Drude weight as the temperature is decreased, but a delta function is never observed in practice in a real metal. Residual scattering from impurities does not allow that to happen.*

Remark 113 *Alternate form: While the Drude weight is the strength of the delta function response in the real part of the conductivity, one can see immediately from the general expression for the longitudinal conductivity, Eq.(11.70), that it can also be extracted from the imaginary part,*

$$D = \pi \lim_{\omega \to 0} \omega \, \mathrm{Im} \left[\sigma_{xx}(0, \omega) \right] . \tag{12.4}$$

This is discussed further in Sec. 12.6.

Remark 114 *Alternate derivation: To be reassured that the Drude weight would also come out from the first expression for the conductivity Eq.(12.1), it suffices to show that both expressions are equal, namely that*

$$\frac{\chi''_{j_x j_x}(0, \omega)}{\omega} - \mathcal{P} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} = -\pi \delta(\omega) \left[\mathrm{Re} \left[\chi^R_{j_x j_x}(0, \omega) \right] - \frac{ne^2}{m} \right] \tag{12.5}$$

To show this, one first notes that given the definition of principal part, the difference on the left-hand side can only be proportional to a delta function. To prove the equality of the coefficients of the delta functions on both sides, it then suffices to integrate over frequency. One obtains

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} - \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} \tag{12.6}$$

$$= \lim_{\omega \to 0} \lim_{q_x \to 0} \left[\frac{ne^2}{m} - \mathrm{Re} \left[\chi^R_{j_x j_x}(q_x, \omega) \right] \right] \tag{12.7}$$

an expression that is clearly correct, as can be shown by using the $f-$sum rule Eq.(11.65) for the first term on the left-hand side and the spectral representation (or Kramers-Kronig representation) of the current-current correlation function for the second term on the left-hand side.

Remark 115 *Contrary to what happened for conserved quantities in thermodynamic sum rules, principal parts here are very relevant.*

12.2 What is a metal

To understand what is a metal, let us first begin by asking what is the Drude weight for free electrons. The answer is that for free electrons, the $q_x \to 0$ conductivity is a delta function at zero-frequency whose Drude weight is $D = \pi ne^2/m$.

Proof: Let the current be $ne\mathbf{v}$. Then, using Newton's equation of motion in an electric field we find ,

$$\frac{\partial \mathbf{j}\left(\mathbf{q}=\mathbf{0},t\right)}{\partial t}=\frac{ne^{2}}{m}\mathbf{E}\left(\mathbf{q}=\mathbf{0},t\right) \tag{12.8}$$

or with a single applied frequency,

$$\mathbf{j}\left(\mathbf{q}=\mathbf{0},\omega\right)=-\frac{1}{i\left(\omega+i\eta\right)}\frac{ne^{2}}{m}\mathbf{E}\left(\mathbf{q}=\mathbf{0},\omega\right). \tag{12.9}$$

From this we see that the conductivity has only a Drude contribution (free acceleration).

$$\operatorname{Re}\frac{\mathbf{j}\left(\mathbf{q}=\mathbf{0},\omega\right)}{\mathbf{E}\left(\mathbf{q}=\mathbf{0},\omega\right)}=\operatorname{Re}\sigma\left(\mathbf{q}=\mathbf{0},\omega\right)=\pi\frac{ne^{2}}{m}\delta\left(\omega\right) \tag{12.10}$$

For interacting electrons, the current of a single particle is no longer a conserved quantity and there is a contribution from $\pi\lim_{\omega\rightarrow0}\operatorname{Re}\left[\chi_{j_{x}j_{x}}^{R}\left(0,\omega\right)\right]$. The rest of the weight is at finite frequency. Hence, the criterion given by Kohn [117] for a system to be a *metal* is that it has a non-zero Drude weight Eq.(12.3) at zero temperature, in other words infinite conductivity or zero resistance even in the presence of interactions. In the presence of elastic scattering, by impurities for example, the zero-temperature Drude weight is broadened. At finite temperature or when there is inelastic scattering with some other system, like the phonons, the delta function is also broadened. The conductivity is not infinite at zero frequency, but it has a weight that can be close to the ideal Drude weight if there is not too much broadening.

Remark 116 *There is no damping in this problem. However, by analogy with the simple case of the harmonic oscillator that we studied in the introductory chapters, and as used erlier, we need to multiply* $\mathbf{j}\left(\mathbf{q}=\mathbf{0},t\right)$ *by an infinitesimal damping* $e^{-\eta t}$ *to reach a steady state when differential equations are propagated forward in time, like we assume here. The* $+i\eta$ *in* $\frac{1}{i(\omega+i\eta)}$ *comes from this procedure applied to Eq.(12.8): All Fourier transforms in time behave as if* $\omega\rightarrow\omega+i\eta$ *in the usual definition when we consider causal processes.*

Remark 117 *Metals and emergence: Metallic behavior is an emergent property that appears in the infinite size limit, like dissipation. It is not a property of the individual atoms. It is not surprising then that the* $q_{x}\rightarrow0$ *and the* $\omega\rightarrow0$ *limits cannot be interchanged.*

Remark 118 *When there is more than a single band involved, a special kind of metal can occur, Weyl semimetals, topological materials that can have an Anomalous Hall effect and curious metallic states. More on this later.*

12.3 What is an insulator

Kohn's criterion [117] for a material to be an *insulator* is that it has a vanishing DC conductivity (or equivalently $D=0$). Remember that the $q_{x}\rightarrow0$ limit must be taken first to obtain the DC conductivity. The DC conductivity then vanishes whenever

$$\lim_{\omega\rightarrow0}\operatorname{Re}\left[\chi_{j_{x}j_{x}}^{R}\left(0,\omega\right)\right]=\lim_{\omega\rightarrow0}\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\chi_{j_{x}j_{x}}''\left(0,\omega'\right)}{\omega'-\omega}=\frac{ne^{2}}{m}. \tag{12.11}$$

Recalling the result obtained from the $f-$sum rule (or equivalently from gauge invariance), (11.65)

$$\chi^R_{j_x j_x}(q_x, 0) = \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x, \omega')}{\omega'} = \frac{ne^2}{m} \tag{12.12}$$

this means that when the order of limits can be inverted, the system is an insulator:

$$\lim_{\omega \to 0} \lim_{q_x \to 0} \mathrm{Re}\left[\chi^R_{j_x j_x}(q_x, \omega)\right] = \lim_{q_x \to 0} \lim_{\omega \to 0} \mathrm{Re}\left[\chi^R_{j_x j_x}(q_x, \omega)\right]. \tag{12.13}$$

This occurs in particular when there is a gap Δ. In this case, then $\chi''_{j_x j_x}(q_x, \omega) = 0$ for all q_x as long as $\omega < \Delta$. In particular, there can be no contribution from zero frequency since $\chi''_{j_x j_x}(q_x, 0) = 0$ so that the principal part integral and the full integral are equal.

Remark 119 *Gapless insulators: The condition of having a gap is sufficient but not necessary to have an insulator. There are examples where there is no gap in the two-particle excitations but there is a vanishing DC conductivity. [56]*

Remark 120 *Insulators are not completely boring. When there is more than one band, one can have a so-called "topological insulator" that has anomalous Hall effect and metallic surfaces despite being insulator in the bulk. More on this later.*

12.4 What is a superconductor

Finally, *superconductors* are an interesting case. The superconducting state is a state of matter that is thermodynamically stable. It expels magnetic fields whether the fields are applied at a temperature above or below that where the system becomes superconducting. Magnetic fields are either expelled completely by a superconductor (Type I) or they penetrate in quantized units (Type II).[1] Let us not worry about these differences for now.

First, a bit of phenomenology about the Meissner effect. London assumed that the part of the current that depends on gradients did not contribute to the response of the current to an applied vector potential. In other words, he assumed that the wave function was "rigid". So he assumed that only the response was controlled only by the diamagnetic term. Hence, he wrote down

$$\delta \left\langle j^A_a(\mathbf{q},0)^T \right\rangle = -\frac{n_s e^2}{m} A^T_a(\mathbf{q}, 0). \tag{12.14}$$

To simplify the discussion, I take a simple case where the $\mathbf{q}$ dependence of the prefactor n_s can be neglected in the zero-frequency limit, (we keep the zeroth order term in the power series in $\mathbf{q}$). I have written n_s to emphasize that this quantity is in general different from the complete density n. This quantity, n_s is called the superfluid density. The above equation is the so-called London equation. We take the curl on both sides of the Fourier transformed expression,

$$\nabla \times \delta \left\langle \mathbf{j}(\mathbf{r},\omega{=}0) \right\rangle = -\frac{n_s e^2}{m} \mathbf{B}(\mathbf{r}, \omega{=}0) \tag{12.15}$$

[1] The real situation is more complicated. Quantized fluxes can be trapped by impurities, so that in practice there may be differences between applying a magnetic field before or after taking it below T_c.

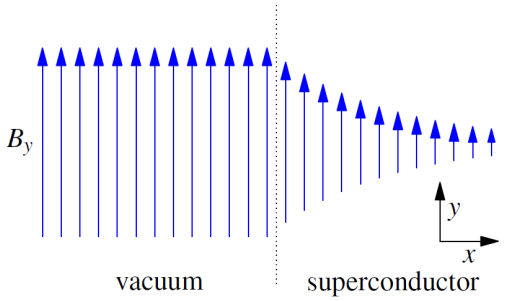


Figure 12-1 Penetration depth in a superconductor

and then multiply by μ_0, the permeability of the vacuum, and use Maxwell's equation $\nabla \times \mathbf{B}(\mathbf{r}, \omega{=}0) = \mu_0 \mathbf{j}(\mathbf{r}, \omega = 0)$ as well as $\nabla \times (\nabla \times \mathbf{B}) = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 (\mathbf{B})$ with $\nabla \cdot \mathbf{B} = 0$. The last equation takes the form,

$$\nabla^2 (\mathbf{B}) = \frac{n_s e^2}{m} \mu_0 \mathbf{B} \tag{12.16}$$

whose solution in the half-plane geometry shown in figure (12-1) is,

$$B_y(x) = B_y(0) e^{-x/\lambda_L}$$

with the London penetration depth

$$\lambda_L^{-2} = \frac{n_s e^2}{m} \mu_0. \tag{12.17}$$

The field is completely expelled from a superconductor[2]. This is perfect diamagnetism.

I now show how the London equation follows from our formalism. Gauge invariance (or $f-$sum rule) implies (11.61) that the following $\omega = 0$ thermodymamic response to a vector potential vanishes:

$$\left[\chi^R_{j_x j_x}(q_x, 0) - \frac{ne^2}{m} \right] = 0. \tag{12.18}$$

Superficially then, it looks as if there can be no response of the current to a pure vector potential. That is a correct assumption, but only for the *longitudinal* part of the vector potential. Gauge invariance does not force the *transverse* response to vanish. Indeed, gauge transformations (11.3) are always longitudinal. Hence, it is possible to have,

$$\left[\chi^R_{j_y j_y}(q_x, 0) - \frac{ne^2}{m} \right] = -\frac{n_s (q_x) e^2}{m} \tag{12.19}$$

where n_s is any density less than n. A superconductor will indeed have such a non-vanishing "transverse Drude weight". We will be interested in the long wave length limit short-coherence length limit (that will be defined later) so that the q_x dependence in $n_s (q_x)$ can be neglected. I will show in Eq.(12.34) below that positivity of the dissipation implies that n_s cannot be larger than n.

Definition 12 *n_s is called the superfluid density.*

[2] At least in so-called type I superconductor. In type II, the field can penetrate in quantized units of flux, $h/(2e)$.

Remark 121 *The term "transverse Drude weight" is a very bad choice of terminology since the order of limits for the Drude weight is very different than for this transverse case.*

A non-vanishing value of n_s in Eq.(12.19) leads to perfect screening of magnetic fields (the Meissner-Oschenfeld effect) in superconductors because, from the general formula for the response to a transverse static electromagnetic field (11.38) ($\omega = 0$), we recover an explicit expression for the London equation:

$$\delta \left\langle j_y^A(q_x,0)^T \right\rangle = \left[\left(\chi^R_{j_y j_y}(q_x,0) \right)^T - \frac{ne^2}{m} \right] A_y^T(q_x,0).$$

Remark 122 *The calculation that we did for the London penetration depth is valid when the superconducting coherence length is smaller than the penetration depth. When this is not the case, the* $\mathbf{q}$ *dependence of* $\chi^R_{j_a j_b}(\mathbf{q},0)$ *cannot be neglected. We have non-local effects that lead to the so-called Pippard penetration depth.*

Remark 123 *Superfluid stiffness: The energy associated with a gradient in the phase of the superconductor, is often written in the form* $\frac{1}{2}\rho_s \left(\nabla\theta\right)^2$*. The quantity* ρ_s *is known as the superfluid stiffness:* $\rho_s \mu_0 = \lambda_L^{-2}$.

Remark 124 *In the case where* $n_s = n$*, which often occurs at zero temperature in BCS-like superconductors, we find*

$$\omega_p^2 \lambda_L^2 = \frac{ne^2}{\varepsilon_0 m} \frac{m}{ne^2\mu_0} = \frac{1}{\varepsilon_0 \mu_0} = c^2. \tag{12.20}$$

Remark 125 *Advantage of S.I. units: The result that we found for the penetration depth Eq.(??) illustrates an advantage of the S.I. units for electromagnetism. Indeed, it is the permeability* μ_0 *that appears in the result. In other units, we would have* $\lambda_L^{-2} = \frac{n_s e^2}{mc^2}$*. Clearly, the velocity of light* c *has nothing to do with the physics we are investigating here, which is all at zero frequency.*

Remark 126 *Since the magnetic induction* $\mathbf{B}$ *obeys* $\mathbf{B} = \boldsymbol{\mu}_0 \left(\mathbf{H} + \mathbf{M}\right)$*, another way to look at this result is that the magnetic field intensity* $\mathbf{H}$ *is cancelled by the magnetization* $\mathbf{M}$ *to yield a vanishing magnetic induction* $\mathbf{B}$**.**

Why are the transverse and longitudinal zero-frequency responses different in a superconductor? By comparing the result of the f-sum rule Eq.(12.18) with the definition of the transverse Drude weight Eq.(12.19) this can happen only if

$$\lim_{q_x \to 0} \chi^R_{j_x j_x}(q_x, 0, \omega = 0) \neq \lim_{q_y \to 0} \chi^R_{j_x j_x}(0, q_y, \omega = 0) \tag{12.21}$$

or in other words

$$\lim_{q_x \to 0} \int dt \int d\mathbf{r} e^{-iq_x x} \chi^R_{j_x j_x}(\mathbf{r}, \omega = 0) \neq \lim_{q_y \to 0} \int dt \int d\mathbf{r} e^{-iq_y y} \chi^R_{j_x j_x}(\mathbf{r}, \omega = 0). \tag{12.22}$$

That is the true definition of a superconductor. A superconductor can have a finite conductivity in the presence of magnetic flux quanta and have no gap like in a d-wave superconductor. The above two limits cannot be inverted in a superconductor because long-range order leads to $\chi^R_{j_x j_x}(\mathbf{r}, \omega = 0)$ that does not decay fast enough for the integral to be uniformly convergent, *i.e.* independent of the order of limits: $\chi^R_{j_x j_x}(\mathbf{r}, \omega = 0)$ does not decay the same way at infinity for $\mathbf{r}$ along the direction x of the current and perpendicular to it. More on this in a later chapter. In an

ordinary metal there is no such long-range order and both limits are identical so that the London penetration depth is infinite, in other words $n_s = 0$ for a metal.

Finally, a superconductor has infinite DC conductivity, namely at $\omega = 0$. While the delta function Drude peak is an idealization in a metal, in a superconductor, the delta function response at $\omega = 0$ is really there. In other words, the full transverse conductivity is

$$\mathrm{Re}\,\sigma_{yy}(q_x,\omega) = \mathcal{P}\frac{1}{\omega}\left[\chi''_{j_y j_y}(q_x,\omega)\right] - \pi\delta(\omega)\left[\mathrm{Re}\,\chi^R_{j_y j_y}(q_x,\omega) - \frac{ne^2}{m}\right] \tag{12.23}$$

12.5 Metal, insulator and superconductor, a summary

In all cases, gauge invariance Eq.(11.61), or equivalently particle conservation, implies that

$$\left[\chi^R_{j_x j_x}(q_x,0) - \frac{ne^2}{m}\right] = 0. \tag{12.24}$$

The difference between a metal, an insulator and a superconductor may be summarized as follows. There are two limits which are relevant. The Drude weight (12.3)

$$\boxed{D(0,\omega) = \pi \lim_{\omega\to 0}\left[\frac{ne^2}{m} - \mathrm{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right]\right]} \tag{12.25}$$

and the transverse analog

$$\boxed{D_S^T(q_x,0) = \pi \lim_{q_x\to 0}\left[\frac{ne^2}{m} - \chi^R_{j_y j_y}(q_x,0)\right]} \tag{12.26}$$

of the $f-$sum rule,

$$\boxed{D_S^L(q_x,0) = \pi \lim_{q_x\to 0}\left[\frac{ne^2}{m} - \chi^R_{j_x j_x}(q_x,0)\right] = 0} \tag{12.27}$$

As we just saw, contrary to its longitudinal analog, (note the order of limits) D_S is not constrained to vanish by gauge invariance. It is instead related to the inverse penetration depth in a superconductor. Since the London penetration depth is generally very long compared with the lattice spacing, the q_x dependense of D_S, or equivalently of the superfluid density, can be neglected. The table summarizes the results.

A superconductor can unambiguously be defined by the non-vanishing of D_S. Indeed, a superconductor has a gap to single-particle excitations, like an insulator, and it has a delta response in the longitudinal direction at zero wave vector, like a metal. On the other hand, D_S vanishes in both metal and insulators.

Remark 127 *It is important to notice that D_S is a thermodynamic quantity. This is apparent from the fact that the $\omega \to 0$ limit is taken first in the correlation function expression Eq. (12.26).*

Remark 128 *Non-standard superconductors: Note that superconductors can be gapless in the presence of magnetic impurities, and they can also have resistance in the so-called mixed-state. These can nevertheless be described by the BCS theory of superconductivity.[62]*

	$D(0,\omega)$	$D^L(q_x,0)$	$D^T(q_x,0)$
Metal	$\neq 0$	0	0
Insulator	0	0	0
Superconductor	$\neq 0$	0	$\neq 0$

Table 12.1 Difference between metal, insulator and superconductor, as seen from the limiting value of correlation functions.

12.6 Finding the London penetration depth from optical conductivity

Let us imagine an experiment at finite temperature where the Drude peak is broadened in the non-superconducting state. It is easier to also use the fact that the $q_x \to 0$ and $q_y \to 0$ limits can be interchanged in a metal and work with the formula Eq. (11.74)

$$\mathrm{Re}\left[\sigma_{yy}(0,\omega)\right] = \frac{\chi''_{j_y j_y}(0,\omega)}{\omega}. \tag{12.28}$$

which is valid even when the Drude peak is broadened.

When the wave vector and the current are in the same direction, the f-sum rule Eq. (11.75), applies, namely

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left[\sigma_{yy}(q_y,\omega)\right] = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega} \left[\chi''_{j_y j_y}(q_y,\omega)\right] = \frac{ne^2}{2m} \tag{12.29}$$

In the long wavelength limit, $\mathbf{q} \to \mathbf{0}$, it does not matter for a metal if $\mathbf{q}$ is along the direction of the current, or perpendicular. The limit is smooth. So we also have

$$\lim_{q_y \to 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left[\sigma_{yy}(q_y,\omega)\right] = \lim_{q_x \to 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left[\sigma_{yy}(q_x,\omega)\right] = \frac{ne^2}{2m}. \tag{12.30}$$

However the f-sum rule strictly applies only when $\mathbf{q}$ and $\mathbf{j}$ are in the same direction since it is only in this case that our derivations using either charge conservation or gauge invariance cannot be dismissed.

In an infrared absorption experiment, the electric field and the current are perpendicular to the direction of propagation towards the material. The experiment can be performed first above the superconducting transition temperature for example and the integral over frequency done, as in the last equation, to find the value of the right-hand side. I will show momentarily that if the objective is to find the penetration depth, it is not necessary to perform this integral in the normal state all the way to infinity.

Now, assume the system becomes a superconductor, then as we just saw a superconductor exhibits a true zero-frequency delta function response at finite wave-vector in the transverse response. We already know that

$$\mathrm{Re}\,\sigma_{yy}(q_x,\omega) = \mathcal{P}\frac{1}{\omega}\left[\chi''_{j_y j_y}(q_x,\omega)\right] - \pi\delta(\omega)\left[\mathrm{Re}\,\chi^R_{j_y j_y}(q_x,\omega) - \frac{ne^2}{m}\right] \tag{12.31}$$

This means that Eq.(12.31) for the transverse conductivity may be written

$$\mathrm{Re}\,\sigma_{yy}(q_x,\omega) = \mathcal{P}\frac{\chi''_{j_y j_y}(q_x,\omega)}{\omega} + D_S(q_x)\,\delta(\omega). \tag{12.32}$$

In that case, a conductivity experiment with electromagnetic radiation will not pick up the piece proportional to $\delta(\omega)$ in the transverse response Eq.(12.32), so

doing the integral we will obtain

$$\lim_{q_x\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\operatorname{Re}\left[\sigma_{yy}(q_x,\omega)\right] = \lim_{q_x\to 0}\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{\omega}\left[\chi''_{j_yj_y}(q_x,\omega)\right]$$

$$= \lim_{q_x\to 0}\frac{1}{2}\operatorname{Re}\chi^R_{j_yj_y}(q_x,0) \tag{12.33}$$

$$= \frac{(n-n_s)\,e^2}{2m} \tag{12.34}$$

where we used the result Eq.(12.19) for $\operatorname{Re}\chi^R_{j_yj_y}(q_x,0)$. Note that there is no difference here between $\operatorname{Re}\chi^R_{j_yj_y}(q_x,0)$ and $\chi^R_{j_yj_y}(q_x,0)$ since this is a thermodynamic quantity (in other words $\omega=0$ first) at small q_x. For the term proportional to D_S the delta function forces us to take the $\omega=0$ limit first. The missing weight for the transverse response is in the delta function at the origin. The weight of that delta function is $D_S/(2\pi)=n_se^2/2m$. It is necessarily less than $ne^2/(2m)$ because the real part of the conductivity is necessarily positive for stability. This means that $n_s<n$ as we had promised to prove. This is called the Ferrell-Glover-Tinkham sum rule [72][230]. It is quite remarkable that the penetration depth can be obtained from an optical conductivity experiment by looking at the missing weight in the *f*-sum rule.

Remark 129 *Since there is no difference between* $\operatorname{Re}\chi^R_{j_yj_y}(q_x,0)$ *and* $\chi^R_{j_yj_y}(q_x,0)$, *one sees that if we include the delta function in the integral over* $\lim_{q_x\to 0}\operatorname{Re}\left[\sigma_{yy}(q_x,\omega)\right]$, *the f-sum rule is obeyed even for the transverse conductivity.*

As a recent example[133] of how this sum rule can be used is shown on Fig. (12-2). The nice aspect is that we do not need the frequency integral up to infinity. Indeed, at sufficiently high frequency, the absorption in the normal and in the superconducting state become identical, so the penetration depth is obtained from the missing area by using our previous result Eq.(12.17), namely $\lambda_L^{-2}=\mu_0 n_s e^2/2m$, to relate the two quantities. In a superconductor, many of the excitations are gapped, in other words they do not contribute to absorption. Let us call the typical gap energy Δ. For frequencies larger than a few times Δ, the results in the superconducting and in the normal state must become identical when $\hbar\omega$ becomes larger than the largest gap. For the example given here, this occurs around 6Δ.

In the cuprates, there is suggestion that there is missing weight when one tries to relate c axis conductivity to penetration depth in the underdoped regime.[22] The in-plane optical conductivity of $YBa_2Cu_3O_{7-x}$ satisfies the sum-rule for the penetration depth but, in the underdoped case, the missing area extends over an unusually broad frequency range, suggesting that simple models based on Fermi liquids do not apply. [96]

Remark 130 *This is a very elegant result that relates two apparently very different experiments. We can obtain the zero frequency penetration depth from a finite-frequency conductivity experiment. This result does not depend on details of the interaction.*

Remark 131 *Other manifestation of delta function response: Note that in the imaginary part of the conductivity, the existence of a non-zero* D_S *has observable consequences at finite frequency since the delta function in the real part gives a long* $1/\omega$ *tail in the imaginary part. More specifically,*

$$\operatorname{Im}\sigma_{yy}(q_x,\omega) = \frac{1}{\omega}\left[\frac{ne^2}{m}-\operatorname{Re}\chi^R_{j_yj_y}(q_x,\omega)\right]-\pi\delta(\omega)\,\chi''_{j_yj_y}(q_x,\omega) \tag{12.35}$$

$$\lim_{\omega\to 0}\omega\operatorname{Im}\sigma_{yy}(q_x,\omega) = \frac{D_S}{\pi} \tag{12.36}$$

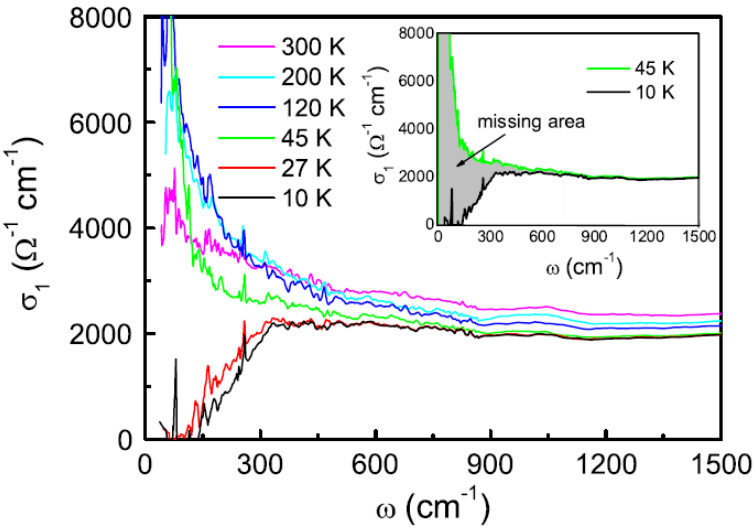


FIG. 3 (color online). T-dependent $\sigma_1(\omega)$ curves. The inset shows $\sigma_1(\omega)$ at 10 and 45 K. The shaded area represents the missing area due to the opening of superconducting energy gap.

Figure 12-2 A penetration depth of $2080\dot{A}$ was obtained from the missing aread in this infrared conductivity experiment on the pnictide $Ba_{0.6}K_{0.4}Fe_2As_2$ with a T_c of 37 K.Figure taken from Ref. [133]

since $\chi''_{j_y j_y}(q_x, 0) = 0$. *That is another way to obtain the London penetration depth. In that case we do not need to know the conductivity at all frequencies, but only its tail in* $1/\omega$ *near* $\omega = 0$. *In practice, the normal state also contributes to* $\mathrm{Im}\,\sigma_{yy}(q_x, \omega)$ *near* $\omega = 0$, *so one must take care of this background correctly to extract the superfluid Drude weight.*

Remark 132 *f-sum rule in a finite band: Note however that the f-sum rule must be modified when the integral is not taken to infinity, which is usually the case. When the integral is taken only across a band, it can be used to define an effective number of carriers. In a single-band tight binding model however, the f-sum rule is related to something close to a kinetic energy. We refer to the literature.[?] This has implications for the sum-rules that I discussed here: [?][?]*

13. *RELATION BETWEEN CONDUCTIVITY AND DIELECTRIC CONSTANT

The relation between dielectric constant and conductivity is a matter of macroscopic electromagnetism. Hence, since we already know the relation beween conductivity and correlation functions, we will be able to relate dielectric constant and correlation functions that we can compute later. The dielectric constant is basic to optical measurements. In infrared spectroscopy for example, one measures the reflectivity or the transmission coefficient, either of which is related to the complex index of refraction which follows from the dielectric constant.

We start from Maxwell's equations. We consider a translationally invariant system, so that it suffices to consider the Fourier-space version

$$i\mathbf{q}\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{13.1}$$

$$i\mathbf{q}\times\mathbf{E} = i\left(\omega+i\eta\right)\mathbf{B} \tag{13.2}$$

$$i\mathbf{q}\cdot\mathbf{B} = 0 \tag{13.3}$$

$$i\mathbf{q}\times\mathbf{B} = \mu_0\mathbf{j} - \frac{i\left(\omega+i\eta\right)}{c^2}\mathbf{E}. \tag{13.4}$$

where $\varepsilon_0 = 8.85\times10^{-12}$ farad/meter is the permittivity of vacuum and μ_0 its permeability is given by $\mu_0 = 4\pi\times10^{-7}$ henry/meter. The speed of light is related to these quantities by $\varepsilon_0\mu_0 = 1/c^2$.

13.1 *Transverse dielectric constant.

Using the definition of transverse conductivity, the last of Maxwell's equations reads,

$$i\mathbf{q}\times\mathbf{B} = \mu_0\overleftrightarrow{\sigma^T}\cdot\mathbf{E} - \frac{i\left(\omega+i\eta\right)}{c^2}\mathbf{E}. \tag{13.5}$$

Using the second Maxwell equation on the left-hand side, as well as $i\mathbf{q}\cdot\mathbf{E} = \mathbf{0}$ for transverse response and $\mathbf{q}\times\left(\mathbf{q}\times\mathbf{E}\right) = \mathbf{q}\left(\mathbf{q}\cdot\mathbf{E}\right) - q^2\mathbf{E}$, we have

$$q^2\mathbf{E} = \mu_0 i\left(\omega+i\eta\right)\overleftrightarrow{\sigma^T}\cdot\mathbf{E} + \frac{\left(\omega+i\eta\right)^2}{c^2}\mathbf{E} \equiv \frac{\left(\omega+i\eta\right)^2}{c^2}\frac{\overleftrightarrow{\epsilon^T}}{\varepsilon_0}\mathbf{E} \tag{13.6}$$

where the last equality is the definition of the dielectric tensor. If there was no coupling to matter, the electric field would have the usual pole for light $\omega = cq$. In general then,

$$\overleftrightarrow{\epsilon^T}\left(\mathbf{q},\omega\right) = \varepsilon_0 + \frac{ic^2\varepsilon_0\mu_0}{\left(\omega+i\eta\right)}\overleftrightarrow{\sigma^T} = \varepsilon_0 + \frac{i}{\left(\omega+i\eta\right)}\overleftrightarrow{\sigma^T} \tag{13.7}$$

In the simple case where the dielectric tensor is diagonal, it is related to the dielectric constant n and the attenuation constant κ through $\sqrt{\epsilon} = n + i\kappa$. Using the Kubo formula for the conductivity in terms of response function Eq.(11.46), we have that

$$\boxed{\overleftrightarrow{\epsilon^T}(\mathbf{q},\omega) = \varepsilon_0 \left(1 - \frac{\omega_p^2}{(\omega+i\eta)^2}\right) \overleftrightarrow{I} + \frac{1}{(\omega+i\eta)^2} \left(\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)\right)^T}. \tag{13.8}$$

Remark 133 *Bound charges: When one can separate the charges into bound and free in the calculation of* $\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)$*, the contribution of the bound charges to* $\frac{1}{(\omega+i\eta)^2}\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)$ *is usually included with the* 1 *and called,* $\overleftrightarrow{\epsilon^T}_{bound}$*.*

Remark 134 *Transverse current and plasmons: The transverse current-current correlation function does not contain the plasmon pole since transverse current does not couple to charge. (One can check this explicitly in diagrammatic calculations: The correlation function between charge and transverse current vanishes in a homogeneous system because the wave-vector for the charge and the vector for the current direction are orthogonal, leaving no possibility of forming a scalar. The equilibrium expectation value of a vector vanishes in a homogenous system. In fact it vanishes even in less general situations which are not enumerated here.)*

Remark 135 *Electromagnetic field and plasmon: One can see from the equation for the electric field (13.6) that in general the electromagnetic field does see the plasmon (negative dielectric constant for* $\omega < \omega_p$ *in Eq.(13.8) means no propagation below the plasma frequency).*

13.2 Longitudinal dielectric constant

Let the system be subjected to some external charge $\rho_e(\mathbf{q},\omega)$**.** The electric field depends on the total charge, including the induced one

$$i\mathbf{q}\cdot\mathbf{E} = \frac{(\rho_e + \delta\langle\rho\rangle)}{\varepsilon_0}. \tag{13.9}$$

The longitudinal dielectric constant is defined by

$$i\mathbf{q}\cdot\overleftrightarrow{\epsilon^L}\cdot\mathbf{E} = \rho_e. \tag{13.10}$$

$\overleftrightarrow{\epsilon^L}$ depends on $\mathbf{q}$ and ω, it is a retarded response function. With a longitudinal applied field, the ratio of the above two equations leads to

$$\left(\epsilon^L\right)^{-1} = \frac{\rho_e + \delta\langle\rho\rangle}{\varepsilon_0\rho_e}. \tag{13.11}$$

In the Landau gauge, where $\nabla\cdot\mathbf{A} = \mathbf{0}$, the linear response to an external charge can be computed from the response to the scalar potential it induces

$$\phi_e(\mathbf{q},\omega) = \frac{1}{\varepsilon_0 q^2}\rho_e(\mathbf{q},\omega). \tag{13.12}$$

As above, linear response to

$$\delta\mathcal{H}(t) = \int d\mathbf{r}\rho(\mathbf{r})\,\phi_e(\mathbf{r},t) \tag{13.13}$$

is given by

$$\delta \langle \rho(\mathbf{q},\omega)\rangle = -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi_e(\mathbf{q},\omega) \tag{13.14}$$

so that simple substitution in the equation for $\left(\epsilon^L\right)^{-1}$ gives,

$$\boxed{\frac{1}{\epsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - \frac{1}{q^2\varepsilon_0}\chi^R_{\rho\rho}(\mathbf{q},\omega)\right)}. \tag{13.15}$$

Remark 136 *Density response and plasmon: The density-density correlation function appearing there still contains the plasmon pole.*

The longitudinal dielectric constant is simply related to the cross section for inelastic electron scattering encountered in Section (7.2). Indeed, the fluctuation-dissipation theorem gives us

$$S_{\rho\rho}(\mathbf{q},\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\,\mathrm{Im}\left[\chi^R_{\rho\rho}(\mathbf{q},\omega)\right] = -\frac{2\hbar}{1-e^{-\beta\hbar\omega}}q^2\,\mathrm{Im}\left[\frac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)}\right]. \tag{13.16}$$

The following properties of the dielectric constants are worthy of interest

Remark 137 *Kramers-Kronig: $\epsilon^T(\mathbf{q},\omega)$ and $\frac{1}{\epsilon^L(\mathbf{q},\omega)} - 1$ obey Kramers-Krönig relations since they are causal. Since they are expressed in terms of correlation functions, they also obey sum rules which follow simply from those already derived, in particular the $f-$sum rule.*

Remark 138 $\epsilon^L(\mathbf{q},\omega) \neq \epsilon^T(\mathbf{q},\omega)$ *in general*

Looking in what follows at the case $\omega << cq$, we assume that $\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t} \approx 0$. Then there are simple things to say about the significance of the poles and zeros of the dielectric constant.

Remark 139 *Collective transverse excitations: The poles of ϵ^T are at the collective transverse excitations. Indeed, let us look since $\nabla\cdot\mathbf{D}$ =0 (no free charge) is garanteed by the fact the excitation is transverse, while $\nabla\times\mathbf{E}$ =0 implies zero electric field in a transverse mode. Nevertheless, $\mathbf{D}^T$≠0 can occur even if the electric field is zero when $\epsilon^T = \infty$. The corresponding poles are those of the transverse part of $\chi^R_{\mathbf{jj}}(\mathbf{q},\omega)$.*

Remark 140 *Collective longitudinal excitations: The zeros of ϵ^L locate the longitudinal collective modes since $\left(\epsilon^L\right)^{-1} = \frac{\rho_e+\delta\langle\rho\rangle}{\varepsilon_0\rho_e} = \infty$ corresponds to internal charge oscillations. Alternatively, $\mathbf{D}^L = 0$ as required by the no-free-charge constraint $\nabla\cdot\mathbf{D}$ =0 but nevertheless $\mathbf{E}^L \neq 0$ is allowed if $\epsilon^L = 0$. ($\nabla\times\mathbf{E}$ =0 is automatic in a longitudinal mode). The corresponding collective modes are also the poles of $\chi^R_{\rho\rho}(\mathbf{q},\omega)$.*

14. EXERCICES FOR PART II

Exercise 14.0.1 *Other derivation of linear response theory: Rederive linear response theory, this time assuming that it is the density matrix instead of the operator that is evolving.*

Exercise 14.0.2 *Derive a Lehmann representation for the fluctuations* $S''_{A_iA_j}(\omega)$*, and by comparing with the Lehmann representation for* $\chi''_{A_iA_j}(\omega)$*, show that the fluctuation-dissipation theorem follows.*

Exercise 14.0.3 *Autre dérivation de la réponse linéaire: Redérivez la théorie de la réponse linéaire mais cette fois-ci en laissant l'Hamiltonien exterieur n'influencer que la matrice densité plutôt que l'operateur dont on veut calculer la réponse.*

Exercise 14.0.4 *Règle de somme f et formule invariante de jauge pour la conductivité longitudinale*

a) En utilisant l'équation de continuité pour la charge électrique et la règle de somme f, démontrez que

$$-i(\omega+i\eta)\chi^R_{j_x\rho}(q_x,\omega)=iq_x\frac{ne^2}{m}-iq_x\chi^R_{j_xj_x}(q_x,\omega) \tag{14.1}$$

b) À partir de

$$\delta\left\langle j^A_a(\mathbf{q},\omega)\right\rangle=\left[\chi^R_{j_aj_b}(\mathbf{q},\omega)-\frac{ne^2}{m}\delta_{ab}\right]A_b(\mathbf{q},\omega)-\chi^R_{j_a\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) \tag{14.2}$$

et du résultat en a), trouvez deux expressions différentes mais équivalentes pour la conductivité longitudinale invariante de jauge.

14.0.1 Lien entre fonctions de réponses, constante de diffusion et dérivées thermodynamiques. Rôle des règles de somme.

Soit un système uniforme de spins 1/2, comme par exemple l'helium ^3He. Les interactions dans le système de spin ne dépendent pas du spin. Donc, l'aimantation totale dans la direction z, que nous noterons M, est conservée, c'est-à-dire que

$$\partial_t M(\mathbf{r},t)+\nabla\cdot\mathbf{j}^M(\mathbf{r},t)=0 \tag{14.3}$$

où $\mathbf{j}^M$ est le courant d'aimantation. Sur une base purement phénoménologique, ce courant dépend du gradient d'aimantation. En d'autres mots, comme M est conservée, il obéit à une dynamique diffusive. Dans un processus hors d'équilibre, (mais pas trop loin de l'équilibre!) et sur des échelles hydrodynamiques, (grand temps et grandes longueurs d'ondes) nous aurons donc

$$\left\langle\mathbf{j}^M(\mathbf{r},t)\right\rangle_{he}=-D\nabla\left\langle M(\mathbf{r},t)\right\rangle_{he} \tag{14.4}$$

où la moyenne fait référence à une moyenne hors d'équilibre.

Soit la fonction de corrélation aimantation-aimantation

$$S_{MM}(\mathbf{r},t)=\left\langle M(\mathbf{r},t)\,M(\mathbf{0},0)\right\rangle \tag{14.5}$$

Cette fonction de corrélation est accessible par exemple par diffusion neutronique.

a) Phénoménologie: En utilisant le fait que le couplage entre aimantation et champ magnétique est donné par

$$H_{int} = -\int d^3\mathbf{r} M(\mathbf{r})\, h \tag{14.6}$$

et que l'Hamiltonien commute avec l'aimantation totale, montrez que

$$\lim_{\mathbf{k}\to 0} S_{MM}(\mathbf{k},t{=}0) = \frac{1}{\beta}\left(\frac{\partial M}{\partial h}\right)_{h=0} \equiv \frac{1}{\beta}\chi_{MM}. \tag{14.7}$$

En supposant ensuite que la dynamique pour $\langle M(\mathbf{r},t)\, M(0,0)\rangle$ avec $t > 0$ est la même que celle obtenue phénoménologiquement pour une perturbation hors d'équilibre et en utilisant la réversibilité, soit

$$\langle M(\mathbf{r},t)\, M(\mathbf{0},0)\rangle = \langle M(\mathbf{0},0)\, M(\mathbf{r},-t)\rangle \tag{14.8}$$

pour déduire le résultat lorsque $t < 0$, montrez qu'aux grandes longueurs d'onde (c'est-à-dire dans la limite hydrodynamique)

$$S_{MM}(\mathbf{k},\omega) = \frac{2Dk^2}{\omega^2 + (Dk^2)^2} S_{MM}(\mathbf{k},t=0) \approx \frac{2Dk^2}{\omega^2 + (Dk^2)^2}\frac{1}{\beta}\chi_{MM} \tag{14.9}$$

- Vous pouvez utiliser l'invariance sous la transformation de parité $\mathbf{r} \to -\mathbf{r}$.
- L'hypothèses menant à ce résultat est connue sous le nom d'hypothèse de régression d'Onsager: "Les fluctuations spontanées à l'équilibre régressent vers l'équilibre de la même façon que les perturbations provoquées de l'extérieur, en autant que ces perturbations ne soient pas trop fortes (réponse linéaire)."

b) Lien entre calcul phénoménologique et microscopique. En utilisant le théorème de fluctuation-dissipation, obtenez une prédiction phénoménologique pour $\chi''_{MM}(\mathbf{k},\omega)$ à partir de $S_{MM}(\mathbf{k},\omega)$. Montrez ensuite que si un calcul microscopique nous donne $\chi''_{MM}(\mathbf{k},\omega)$ alors la constante de diffusion peut être obtenue de ce calcul microscopique en de la façon suivante:

$$D\chi_{MM} = \lim_{\omega\to 0}\left[\lim_{\mathbf{k}\to\mathbf{0}} \frac{\omega}{k^2}\chi''_{MM}(\mathbf{k},\omega)\right] \tag{14.10}$$

tandis que la susceptibilité magnétique uniforme elle, s'obtient de

$$\chi_{MM} = \lim_{\mathbf{k}\to\mathbf{0}} \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{k},\omega)}{\omega} \tag{14.11}$$

c) Règles de somme: La dernière équation ci-dessus est connue comme la règle de somme thermodynamique pour la susceptibilité $\chi''_{MM}(\mathbf{k},\omega)$. Notre expression phénoménologique pour $\chi''_{MM}(\mathbf{k},\omega)$ satisfait cette règle de somme. Considérons maintenant la règle de somme f. L'expression microsopique pour l'aimantation est

$$M(\mathbf{r}) = \sum_{\alpha=1}^{N} 2\mu s_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \tag{14.12}$$

où, dans ce système paramagnétique, $s_\alpha = \pm\frac{1}{2}$ et μ est le moment magnétique, alors que l'expression correspondante pour le courant d'aimantation est

$$\mathbf{j}^M(\mathbf{r}) = \frac{\mu}{m}\sum_{\alpha=1}^{N} s_\alpha\left[\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta(\mathbf{r} - \mathbf{r}_\alpha) + \delta(\mathbf{r} - \mathbf{r}_\alpha)\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\right] \tag{14.13}$$

avec m la masse. Utilisant ces expressions, démontrez la règle de somme f pour ce système de spins, soit

$$\int \frac{d\omega}{\pi}\omega\chi''_{MM}(\mathbf{k},\omega) = \frac{n}{m}\mu^2 k^2 \tag{14.14}$$

où n est la densité. Il suffit de suivre de près la preuve de la règle de somme f faite à la section (10.10.4). Vérifiez ensuite que l'expression phénoménologique trouvée ci-dessus pour $\chi''_{MM}(\mathbf{k},\omega)$ à partir de considérations hydrodynamiques, ne satisfait *pas* la règle de somme f. Laquelle de nos hypothèses phénoménologiques devrait être raffinée pour arriver à satisfaire cette règle de somme?

14.0.2 Fonction de relaxation de Kubo.

Dans la limite classique, le théorème de fluctuation-dissipation devient:

$$\chi''_{A_iA_j}(\mathbf{r},\mathbf{r}';\omega) = \frac{\beta\omega}{2}S_{A_iA_j}(\mathbf{r},\mathbf{r}';\omega).$$

Définissons une fonction $C_{A_iA_j}$ telle que la relation précédente soit toujours vraie, c'est-à-dire que même pour un système quantique on veut que:

$$i\frac{d}{dt}C_{A_iA_j}(\mathbf{r},\mathbf{r}';t) = \frac{2}{\beta}\chi''_{A_iA_j}(\mathbf{r},\mathbf{r}';t).$$

Montrez que cette dernière relation est satisfaite par la définition suivante de $C_{A_iA_j}$

$$C_{A_iA_j}(\mathbf{r},\mathbf{r}';t-t') = \beta^{-1}\int_0^\beta d\beta'[< A_i(\mathbf{r},t)A_j(\mathbf{r}',t'+i\hbar\beta') > - < A_i >< A_j >].$$

Ceci est une autre fonction de corrélation due a Kubo et qui décrit la relaxation.

14.0.3 Constante diélectrique et Kramers-Kronig.

Considérons la constante diélectrique d'un milieu isotrope $\epsilon(t)$ comme une fonction de réponse, sans nous soucier de sa représentation en terme de commutateurs. En utilisant le principe de causalité ($\epsilon(t) = 0$ pour $t < 0$), demontrez que $\epsilon(\omega)$ est analytique dans le plan complexe supérieur. Determinez aussi la parité de ϵ_1 et ϵ_2 ($\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$) sous changement de signe de ω. En utilisant ensuite le théorème de Cauchy sur les intégrales des fonctions analytiques, dérivez deux relations de Kramers-Krönig entre les parties réelles et imaginaires de $\epsilon(\omega)$:

$$\epsilon_1(\omega) - \epsilon_1(\infty) = \frac{2}{\pi}\mathcal{P}\int_0^\infty d\xi\frac{\xi\epsilon_2(\xi)}{\xi^2-\omega^2} \tag{14.15}$$

$$\epsilon_2(\omega) = -\frac{2}{\pi}\omega\mathcal{P}\int_0^\infty d\xi\frac{\epsilon_1(\xi)-\epsilon_1(\infty)}{\xi^2-\omega^2} \tag{14.16}$$

Part III

Introduction to Green's functions. One-body Schrödinger equation

We now know that correlation functions of charge, spin, current etc... allow us to predict the results of various experiments. In quantum mechanics, all these quantities, such as charge, spin, current, are bilinear in the Schrödinger wave function $\Psi(\mathbf{r},t)$, i.e $\rho(\mathbf{r},t) = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t)$ for example. What about correlation functions of the wave function $\Psi(\mathbf{r},t)$ itself? They also are related to experiment, more specifically to photoemission and tunneling experiments for example. We will come back to this later. At this point, it suffices to say that if we do experiments where we actually inject or extract a single electron, then we need to know the correlation function for a single Ψ. These correlation functions are called Green's functions, or propagators. They are absolutely necessary from a theoretical point of view to get a full description of the system, including interference terms that are absent in classical mechanics. They turn out to be easier to compute than correlation functions for transport properties, such as charge-charge or current-current. So we will finally compute this type of correlation function, Green's functions, in this Part. Green's functions share a lot of the general properties of correlation functions: Kramers-Kronig relations, sum rules, high-frequency expansions... But there are also important differences as will become clearer in later chapters.

One can read on this subject in several books[12][71] [69][200]. Here I introduce Green's functions as a simple reformulation of the one-body Schrödinger equation. This will help us, in particular, to develop an intuition for the meaning of Feynman diagrams and of the self-energy in a familiar context. Impurity scattering will be discussed in detail after I present definitions and general properties. Finally, there is an alternate formulation of quantum mechanics, namely Feynman's path integral, that arises naturally when we think about the physical meaning of Green's functions.

From now on, I work in units where $\hbar = 1$.

15. DEFINITION OF THE PROPAGATOR, OR GREEN'S FUNCTION

15.1 Preliminaries: some notation

For a while we work with the continuum normalization for the position $|\mathbf{r}\rangle$ and momentum $|\mathbf{k}\rangle$ eigenstates. The closure relation is

$$\int d\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}| = 1 \tag{15.1}$$

with the normalization

$$\langle\mathbf{r}\,|\mathbf{r}'\rangle = \delta\left(\mathbf{r}-\mathbf{r}'\right). \tag{15.2}$$

Momentum eigenstates are not normalized

$$\langle\mathbf{r}\,|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} \tag{15.3}$$

while the closure and normalization are:

$$\int \frac{d\mathbf{k}}{(2\pi)^3}\,|\mathbf{k}\rangle\,\langle\mathbf{k}| = 1 \tag{15.4}$$

$$\langle\mathbf{k}\,|\mathbf{k}'\rangle = (2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right) \tag{15.5}$$

15.2 Definition of the Green's function and physical meaning

Previously, we needed to know how an operator, such as charge for example, was correlated with another one at another time. The generalization of this idea for a one-body wave function is to know how it correlates with itself at different times. That is also useful because the main idea of perturbation theory is to prepare a state $\Psi_0(\mathbf{r}',t')$ and to let it evolve adiabatically in the presence of the perturbation into the new eigenstate $\Psi(\mathbf{r},t)$.

In our harmonic oscillator example, we found that the displacement was related to the driving force through $x(\omega)=\chi^R(\omega)\,F(\omega)$,so that $\chi^R(\omega)$ is the response to a delta function in time, $F(t)=\delta(t)$ *i.e.* $F(\omega)=1$. Knowing the response for $F(\omega)=1$ allows us to find the response for an arbitrary function of time. In the case of wave functions, the quantity loosely analogous to susceptibility in its version as a function of time is the Green's function or propagator

$$\boxed{\widehat{G}^R(t) = -ie^{-i\widehat{H}t}\theta(t)}. \tag{15.6}$$

Indeed, using Schrödinger's equation, we have that

$$|\Psi(t)\rangle\,\theta(t) = e^{-i\widehat{H}t}\,|\Psi_H\rangle\,\theta(t) \tag{15.7}$$

$$= i\widehat{G}^R(t)\,|\Psi_H\rangle\,. \tag{15.8}$$

Acting on this last equation with $i\frac{\partial}{\partial t}$ on both sides, one finds that since $|\Psi_H\rangle$ is arbitrary, $\widehat{G}^R(t)$ must obey the differential equation

$$\boxed{\left(i\tfrac{\partial}{\partial t} - \widehat{H}\right)\widehat{G}^R(t) = \delta(t)\,.} \tag{15.9}$$

Remark 141 *Notations: Note that in reality, I should write $\widehat{I}\delta(t)$ and $\widehat{I}\frac{\partial}{\partial t}$ with $\widehat{I}$ the identity operator in Hilbert space. This $\widehat{I}$ is omitted most of the time. Also, the $-i$ in the definition of $\widehat{G}^R(t)$ was introduced so that the right-hand side of the last equation is $\delta(t)$ which is the usual way that Green's functions are defined in the context of differential equations.*

The Green's function was proposed by Green in the nineteenth century to solve partial differential equations in electrodynamics. We know that Schrödinger's point of view is concerned with waves. And in classical physics, waves obey Huygens principle, namely that the amplitude of a wave at one point is the sum of all wavelets generated by scatters that act as point sources. The Green's function describes these wavelets, as I proceed to show. Inserting complete sets of states in the operator relation between state and Green's function, we find

$$\boxed{\langle\mathbf{r}\,|\Psi(t)\rangle\,\theta(t) = i\int d\mathbf{r}'\,\langle\mathbf{r}|\,\widehat{G}^R(t)\,|\mathbf{r}'\rangle\,\langle\mathbf{r}'\,|\Psi_H\rangle.} \tag{15.10}$$

If the initial wave function is an eigenstate of position, $|\mathbf{r}''\rangle$, since $\langle\mathbf{r}'\,|\mathbf{r}''\rangle = \delta(\mathbf{r}-\mathbf{r}'')$, this leads to

$$\Psi(\mathbf{r},t)\theta(t) = \langle\mathbf{r}\,|\Psi(t)\rangle\,\theta(t) = i\,\langle\mathbf{r}|\,\widehat{G}^R(t)\,|\mathbf{r}''\rangle\,. \tag{15.11}$$

In other words, an eigenstate of position spreads in time in a way described by the propagator. For a general state $|\Psi_H\rangle$, each of the components on position eigenstates must be superposed with

$$\boxed{\langle\mathbf{r}|\,\widehat{G}^R(t)\,|\mathbf{r}'\rangle \equiv G^R(\mathbf{r},\mathbf{r}';t)} \tag{15.12}$$

to find the value of $\Psi(\mathbf{r},t)$, in a manner similar to that proposed by Huygens for classical waves.

The differential equation obeyed by $G^R(\mathbf{r},\mathbf{r}';t)$ is easy to find by taking matrix elements of the operator differential equation Eq. (15.9)

$$\boxed{\int d\mathbf{r}'\left(i\tfrac{\partial}{\partial t}\delta(\mathbf{r}-\mathbf{r}') - \langle\mathbf{r}|\,\widehat{H}\,|\mathbf{r}'\rangle\right)\langle\mathbf{r}'|\,\widehat{G}^R(t)\,|\mathbf{r}''\rangle = \delta(t)\,\delta(\mathbf{r}-\mathbf{r}'').} \tag{15.13}$$

This is indeed the definition of the Green's function for the Schrödinger equation seen as a differential equation.

Remark 142 *Historical remark: Green was born over two centuries ago. At age 35, George Green, the miller of Nottingham, published his first and most important work: "An Essay on the Applications of Mathematical Analysis to the Theory of Electricity and Magnetism" dedicated to the Duke of Newcastle. It is in trying to solve the differential equations of electromagnetism that Green developed the propagator idea. Ten years after his first paper, he had already moved from the concept of the static three-dimensional Green's function in electrostatics to the dynamical concept. Green had no aristocratic background. His work was way ahead of his time and it was noticed mainly because of the attention that Kelvin gave it.*

Note that formally, we can invert the equation for the Green's function as follows:

$$\boxed{\widehat{G}^R(t) = \left[i\frac{\partial}{\partial t} - \widehat{H}\right]^{-1} \delta(t)} \tag{15.14}$$

In this form, it looks more like the response to a delta function perturbation. I will come back to what this inverse means, but if you think in matrix language, you can already guess. The above is meaningless unless we specify that the boundary condition is that $G^R(-\infty) = 0$, (which, by the way, is satisfied by $G^R(t) = \int \frac{d\omega}{2\pi} e^{-i(\omega+i\eta)t} G^R(\omega)$). This should be compared with Eq. (16.8) below.

This may look like a useless exercise in definitions, but in fact there are many reasons to work with the retarded Green's function $G^R(\mathbf{r}, \mathbf{r}'; t)$.

- $G^R(\mathbf{r}, \mathbf{r}'; t)$ does not depend on the initial condition $\Psi_0(\mathbf{r}', t')$.
- $G^R(\mathbf{r}, \mathbf{r}'; t)$ contains for most purposes all the information that we need. In other words, from it one can extract wave-functions, eigenenergies etc... Obviously, the way we will want to proceed in general is to express all observables in terms of the Green's function so that we do not need to explicitly return to wave functions. This function $G^R(\mathbf{r}, \mathbf{r}'; t)$ provides an alternate formulation of quantum mechanics due to Feynman that we discuss in the last chapter of this part.
- $G^R(\mathbf{r}, \mathbf{r}'; t)$ is the analog of the Green's function used in the general context of differential equations (electromagnetism for example).
- Perturbation theory for $G^R(\mathbf{r}, \mathbf{r}'; t)$ can be developed in a natural manner.
- $G^R(\mathbf{r}, \mathbf{r}'; t)$ is generalizable to the many-body context where it keeps the same physical interpretation (but not exactly the same mathematical definition).
- Suppose we want to know the expectation value of two one-body operators at different times. The calculation will involve $G^R(\mathbf{r}, \mathbf{r}'; t)$.

Definition 13 *$G^R(\mathbf{r}, \mathbf{r}'; t)$ is called a* propagator, *(or* Green's function*), since it gives the wave function at any time, as long as the initial condition is given. In other words, it propagates the initial wave function, like Huygens wavelets describe the propagation of a wave as a sum of individual contributions from point scatterers.*

15.3 *The initial condition can be at some arbitrary time

Up to now, I have evolved the wave function from $t = 0$ where Heisenberg and Schrödinger pictures coincide. Clearly, the initial time could be anywhere. If it is at t', then the Green's function depends on $t - t'$ if the Hamiltonian is time independent. That is that simple. Nevertheless, let me go through a proof in case you are skeptic. We know that $\Psi(\mathbf{r}, t) = \langle \mathbf{r} | e^{-iHt} | \Psi_H \rangle$. If instead of knowing the state $|\Psi_H\rangle$ in the Heisenberg picture, we known the initial value of the state in the Schrödinger picture, namely

$$|\Psi_0(t')\rangle = e^{-iHt'} |\Psi_H\rangle, \tag{15.15}$$

we can write the wave function $\Psi(\mathbf{r},t)$ in terms of the initial state in the Schrödinger picture

$$\Psi(\mathbf{r},t) = \langle \mathbf{r}| \, e^{-iH\left(t-t'\right)} \, |\Psi_0(t')\rangle \, . \tag{15.16}$$

To rewrite the same thing in terms of the initial wave function,

$$\Psi_0(\mathbf{r}',t') = \langle \mathbf{r}'| \, \Psi_0 \left(t'\right)\rangle \tag{15.17}$$

it suffices to use a complete set of states

$$\Psi(\mathbf{r},t)\theta\left(t-t'\right) = \int d\mathbf{r}' \, \langle \mathbf{r}| \, e^{-iH\left(t-t'\right)} \, |\mathbf{r}'\rangle \, \langle \mathbf{r}'| \, \Psi_0 \left(t'\right)\rangle \, \theta\left(t-t'\right) \tag{15.18}$$

where the $\theta\left(t-t'\right)$ is added to make causality explicit. This last equation may be rewritten as

$$\Psi(\mathbf{r},t)\theta\left(t-t'\right) = i \int d\mathbf{r}' G^R \left(\mathbf{r},t;\mathbf{r}',t'\right) \Psi_0(\mathbf{r}',t') \tag{15.19}$$

if I introduce the following definition of the retarded Green's function in the position basis:

$$\boxed{G^R \left(\mathbf{r},t;\mathbf{r}',t'\right) = -i \, \langle \mathbf{r}| \, e^{-iH\left(t-t'\right)} \, |\mathbf{r}'\rangle \, \theta\left(t-t'\right)}. \tag{15.20}$$

16. VARIOUS WAYS OF REPRESENTING THE ONE-BODY PROPAGATOR, THEIR PROPERTIES AND THE INFORMATION THEY CONTAIN

In this section, we show various representations of the one-body propagator, as operator, or as solution to a differential equation. We will encounter the analogs of Kramers-Kronig relations, sum-rules, high-frequency expansion that we saw previously and how the propagator allows us to compute transport and fluctuations in the simplest case.

16.1 Representation in frequency space and Lehmann representation

It is very useful to work with the Fourier transform in time of $G^R(\mathbf{r},\mathbf{r}';t)$ because it contains information about the energy spectrum

$$G^R(\mathbf{r},\mathbf{r}';\omega) = -i\int_0^\infty d(t-t')\, e^{i(\omega+i\eta)(t-t')} \langle \mathbf{r}| e^{-iH\left(t-t'\right)} |\mathbf{r}'\rangle . \tag{16.1}$$

In this expression, I have used the $\theta(t-t')$ and the corresponding $\omega + i\eta$ in Fourier space to insure causality. Insert in this equation a complete set of energy eigenstates

$$H|n\rangle = E_n|n\rangle \tag{16.2}$$

$$\langle n| e^{-iH\left(t-t'\right)} |m\rangle = e^{-iE_n\left(t-t'\right)}\delta_{n,m} \tag{16.3}$$

to obtain for the Green's function

$$G^R(\mathbf{r},\mathbf{r}';\omega) = -i\sum_n \langle \mathbf{r}|\, n\rangle \int_0^\infty dt e^{i(\omega+i\eta-E_n)t} \langle n\, |\mathbf{r}'\rangle \tag{16.4}$$

or using $\Psi_n(\mathbf{r}) = \langle \mathbf{r}|\, n\rangle$

$$\boxed{G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \frac{\langle \mathbf{r}|\, n\rangle\langle n\, |\mathbf{r}'\rangle}{\omega+i\eta-E_n} = \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*\left(\mathbf{r}'\right)}{\omega+i\eta-E_n}} \tag{16.5}$$

$$\boxed{= \sum_n \langle \mathbf{r}|\, n\rangle \langle n| \frac{1}{\omega+i\eta-E_n} |n\rangle \langle n\, |\mathbf{r}'\rangle \equiv \langle \mathbf{r}| \frac{1}{\omega+i\eta-\widehat{H}} |\mathbf{r}'\rangle}. \tag{16.6}$$

We thus see more clearly what is meant by the inverse operator.

Let us evaluate explicitly the Green's function for a simple case. Let us take a free particle. The eigenstates are momentum eigenstates, $H|\mathbf{k}\rangle = \varepsilon_{\mathbf{k}}|\mathbf{k}\rangle$ .Then,

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = \langle \mathbf{k}| \frac{1}{\omega + i\eta - \widehat{H}} |\mathbf{k}'\rangle = \frac{\langle \mathbf{k}|\ \mathbf{k}'\rangle}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \tag{16.7}$$

From the form Eq. (16.6), one can clearly see that

- The poles of $G^R(\mathbf{r}, \mathbf{r}'; \omega)$ are at the eigenenergies.
- The residue at the pole is related to the corresponding energy eigenstate.
- This is the analog of a Lehmann representation, that we will encounter later.

Remark 143 *Significance of the poles: It would be more accurate to say that the poles are located at the energy $\hbar\omega$ for a transition from the vacuum to a state containing a single-particle. This will come out more clearly in second quantization and is in accord with Bohr's correpondence principle.*

16.2 *Operator representation in frequency space

As can be seen from the last equation of the previous section, in frequency space, the expression for the Green operator is thus,

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega + i\eta - \widehat{H}} = \left(\omega + i\eta - \widehat{H}\right)^{-1}.} \tag{16.8}$$

That operator is also called the *resolvent* operator. The following

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \langle \mathbf{r}| \widehat{G}^R(\omega) |\mathbf{r}'\rangle . \tag{16.9}$$

is a generalization of what we have already seen in real time, Eq. (15.12).

The advanced propagator is defined by

$$\boxed{\widehat{G}^A(t) = ie^{-iHt}\theta(-t)} \tag{16.10}$$

$$\boxed{\widehat{G}^A(\omega) = \frac{1}{\omega - i\eta - \widehat{H}}} \tag{16.11}$$

Remark 144 *Boundary condition in time vs pole location in frequency space: From the equation for the propagator (15.13) it appears that one can add to $G^R(\mathbf{r}, \mathbf{r}'; t)$ any solution of the homogeneous form of the differential equation (right-hand side equal to zero). The boundary condition that $G^R(\mathbf{r}, \mathbf{r}'; t)$ vanishes for all $t < 0$ (the $i\eta$) and is equal to $-i$ at $t = 0$ makes the solution unique. For a first-order differential equation, one boundary condition at $t = 0^+$ suffices to know the function at $t > 0$. We will not know then the value before $t = 0$ but we specify that it is equal to zero as long as $t < 0$. In frequency space, this latter assumption moves the poles away from the real axis. To be more explicit, the general solution of the differential equation is $\widehat{G}(t) = -ie^{-i\widehat{H}t}\theta(t) - iCe^{-i\widehat{H}t}$, where the constant C multiplies the solution of the homogeneous equation. Taking into account the initial condition $\widehat{G}(0) = -i$, which follows from the definition of $\widehat{G}(0)$, as well as the vanishing of $\widehat{G}^R(t)$ for negative times, implies that $C = 0$ for the retarded function. Correspondingly, for $G^A(\mathbf{r}, \mathbf{r}'; t)$ we need to specify the vanishing of the function at*

$t > 0$ and we can find its value at all times prior to $t = 0^-$ by stating that it is equal to $+i$ at that time. Indeed, in that case $C = -1$ in $\widehat{G}(t) = -ie^{-i\widehat{H}t}\theta(t) - iCe^{-i\widehat{H}t}$ so that $\widehat{G}^A(t) = -ie^{-i\widehat{H}t}\theta(t) + ie^{-i\widehat{H}t} = ie^{-i\widehat{H}t}\theta(-t)$, as in the earlier definition Eq.(16.10).

16.3 Observables can be obtained from the Green's function

Knowing the Green's function is equivalent to having the solution of Schrödinger's equation. In fact for an arbitrary state that has evolved from a given initial condition, we can use the relation between Green's function and wave function, Eq. (15.10), to build any time-dependent expectation value using the usual rules of quantum mechanics to find observables from Green's functions. There are a few observables that can be obtained in a simple manner directly from the Green's function.

This can be seen from the spectral representation Eq. (16.5)

$$-\frac{1}{\pi}\operatorname{Im} G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')\,\delta(\omega - E_n)\,. \tag{16.12}$$

The quantity,

$$\rho(\mathbf{r},\omega) = -\frac{1}{\pi}\operatorname{Im} G^R(\mathbf{r},\mathbf{r};\omega) \tag{16.13}$$

is called the local density of states, a quantity relevant in particular when there is no translational invariance. If we have a tip whose density of states is structureless, to a good approximation, the local density of states is what is measured by scanning tunneling microscopes. The local density of states can be interpreted as the probability that an electron in an eigenstate of energy $\omega = E_n$ is at position $\mathbf{r}$, namely $\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r})$ summed over all eigenstates with the same energy

Integrating over all positions, we obtain the density of states

$$\boxed{-\tfrac{1}{\pi}\textstyle\int d\mathbf{r}\operatorname{Im} G^R(\mathbf{r},\mathbf{r};\omega) = \sum_n \int d\mathbf{r}\,\langle n\,|\mathbf{r}\rangle\,\langle\mathbf{r}|\,n\rangle\,\delta(\omega - E_n)} \tag{16.14}$$

$$\boxed{= \rho(\omega) = \textstyle\sum_n \delta(\omega - E_n)}\,. \tag{16.15}$$

This can be rewritten in a manner which does not refer to the explicit representation (such as $|\mathbf{r}\rangle$ above) by using Eq.(16.6) that defines the Green function

$$\boxed{\rho(\omega) = -\tfrac{1}{\pi}\mathrm{Tr}\left[\operatorname{Im}\widehat{G}^R(\omega)\right]}\,. \tag{16.16}$$

Clearly, this procedure can be used for any other observable. Suppose we want to know the total kinetic energy in a given energy eigenstate. Then using the expression for the imaginary part of the Green's funtion Eq. (16.12) at the beginning of this section, and assuming no degeneracy, we find, in the case where

we have discrete energy levels separated by less than ε,

$$K_n = \int d\mathbf{r} \left[-\frac{\nabla^2}{2m} \Psi_n(\mathbf{r}) \right] \Psi_n^*(\mathbf{r}) \tag{16.17}$$

$$= \int d\mathbf{r} \int_{E_n-\varepsilon}^{E_n+\varepsilon} d\omega \sum_{n'} \left[-\frac{\nabla^2}{2m} \Psi_{n'}(\mathbf{r}) \right] \Psi_{n'}^*(\mathbf{r}) \, \delta(\omega - E_{n'}) \tag{16.18}$$

$$= -\frac{1}{\pi} \int d\mathbf{r} \int_{E_n-\varepsilon}^{E_n+\varepsilon} d\omega \, -\frac{\nabla^2}{2m} \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}'; \omega) \Big|_{\mathbf{r}'=\mathbf{r}}. \tag{16.19}$$

If there is a potential term, $V(\mathbf{r})$, the total potential energy can also be computed.

$$V_n = -\frac{1}{\pi} \operatorname{Im} \int d\mathbf{r} \int_{E_n-\varepsilon}^{E_n+\varepsilon} V(\mathbf{r}) \, G^R(\mathbf{r}, \mathbf{r}; \omega) \, d\omega. \tag{16.20}$$

The imaginary part can be taken before or after the integration.

Remark 145 *Trace representation: Formally, the above observables can be represented as partial traces.*

16.4 *Spectral representation, Kramers-Kronig, sum rules and high frequency expansion

Green's functions are response functions for the wave function, hence they have many formal properties that are analogous to those of response functions that we saw earlier. We discuss some of them here.

16.4.1 Spectral representation and Kramers-Kronig relations.

Returning to the explicit representation in energy eigenstates, (16.5), it can be written in a manner which reminds us of the spectral representation

$$\boxed{G^R(\mathbf{r}, \mathbf{r}'; \omega)} = \sum_n \frac{\Psi_n(\mathbf{r}) \, \Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} = \int \frac{d\omega'}{2\pi} \frac{\sum_n \Psi_n(\mathbf{r}) \, \Psi_n^*(\mathbf{r}') \, 2\pi\delta(\omega' - E_n)}{\omega + i\eta - \omega'} \tag{16.21}$$

$$\boxed{= \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} = \int \frac{d\omega'}{2\pi} \frac{-2 \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} = \int d\omega' \frac{\rho(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'}} \tag{16.22}$$

which defines the spectral weight

$$A(\mathbf{r}, \mathbf{r}'; \omega') = \sum_n \Psi_n(\mathbf{r}) \, \Psi_n^*(\mathbf{r}') \, 2\pi\delta(\omega' - E_n) \tag{16.23}$$

for the one-particle Green's functions. $\rho(\mathbf{r}, \mathbf{r}'; \omega')$ is a generalization of the density of states. The *diagonal* piece is usually what we call the local density of states. Note that in momentum space we would have, for a translationally invariant system,

$$\boxed{G^R(\mathbf{k}; \omega) = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}; \omega')}{\omega + i\eta - \omega'}} \tag{16.24}$$

with

$$\boxed{A(\mathbf{k};\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{k};\omega')} \tag{16.25}$$

$$A(\mathbf{k};\omega') = \sum_n \Psi_n(\mathbf{k})\,\Psi_n^*(\mathbf{k})\,2\pi\delta(\omega'-E_n) \tag{16.26}$$

$$= \sum_n \langle\mathbf{k}|\,n\rangle\,\langle n\,|\mathbf{k}\rangle\,2\pi\delta(\omega'-E_n)\,. \tag{16.27}$$

In the case of free particles, there is only a single eigenstate $|n\rangle = |\mathbf{k}\rangle$ that contributes to the sum and we have a single delta function for the spectral weight. That occurs whenever we are in an eigenbasis.

Remark 146 *Assumptions in relating A to $\mathrm{Im}\,G^R$: It is only in the presence of a time-reversal invariant system that the Schrödinger wave functions $\Psi_n(\mathbf{r})$ can always be chosen real. In such a case, it is clear that we are allowed to write $A(\mathbf{r},\mathbf{r}';\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r}';\omega')$ as we did in Eq.(16.22).*

Remark 147 *Analogies with ordinary correlation functions. Contrary to the spectral representation for correlation functions introduced earlier, there is $\frac{d\omega'}{2\pi}$ instead of $\frac{d\omega'}{\pi}$. That is why there is a factor of two in relating the imaginary part of the Green's function to the spectral weight. Furthermore, the denominator involves $\omega+i\eta-\omega'$ instead of $\omega'-\omega-i\eta$, which explains the minus sign in $A(\mathbf{k};\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{k};\omega')$, Eq.(16.25). Apart from these differences, it is clear that $A(\mathbf{k};\omega')$ here is analogous to $\chi''(\mathbf{k};\omega')$ for correlation functions.*

Analyticity in the upper half-plane implies Kramers-Kronig relations as before. In fact, the spectral representation itself leads immediately to

$$\mathrm{Re}\left[G^R(\mathbf{r},\mathbf{r}';\omega)\right] = \mathcal{P}\int\frac{d\omega'}{\pi}\frac{\mathrm{Im}\left[G^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega'-\omega}. \tag{16.28}$$

The other reciprocal Kramers-Kronig relation follows as before.

$$\mathrm{Im}\left[G^R(\mathbf{r},\mathbf{r}';\omega)\right] = -\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\mathrm{Re}\left[G^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega'-\omega} \tag{16.29}$$

16.4.2 *Sum rules

As before, the imaginary part, here equal to the local density of states, obeys sum rules

$$\int\frac{d\omega'}{2\pi}\left(-2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r}';\omega')\right) = \int\frac{d\omega'}{2\pi}\sum_n\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')\,2\pi\delta(\omega'-E_n) \tag{16.30}$$

$$= \sum_n\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \tag{16.31}$$

so that

$$\int d(\mathbf{r}-\mathbf{r}')\int\frac{d\omega'}{2\pi}\left(-2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r}';\omega')\right) = 1. \tag{16.32}$$

More sum rules are trivially derived. For example,

$$\boxed{\int d\mathbf{r}\int\tfrac{d\omega'}{2\pi}\omega'\left(-2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r};\omega')\right)} = \int d\mathbf{r}\int d\omega'\omega'\rho(\mathbf{r},\omega') = \int d\mathbf{r}\sum_n E_n\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}) \tag{16.33}$$

$$\boxed{= \int d\mathbf{r} \left\langle \mathbf{r} \right| \widehat{H} \left| \mathbf{r} \right\rangle}. \tag{16.34}$$

This relates the Green's function to another observable, the energy.

In operator form, all of the above results are trivial

$$\boxed{\int \tfrac{d\omega}{2\pi} \omega^n \mathrm{Tr}\left[-2\,\mathrm{Im}\left(\widehat{G}^R\right)\right]} = \int \frac{d\omega}{2\pi} \omega^n \mathrm{Tr}\left[-2\,\mathrm{Im}\left(\frac{1}{\omega + i\eta - \widehat{H}}\right)\right] \tag{16.35}$$

$$\boxed{= \int d\omega \omega^n \mathrm{Tr}\delta\left(\omega - \widehat{H}\right) = \mathrm{Tr}\left(\widehat{H}^n\right)}$$

Evaluating the trace in the position representation, we recover previous results. Special cases include

$$\int d\mathbf{r} \int \frac{d\omega'}{2\pi} \left(\omega'\right)^n \left(-2\,\mathrm{Im}\, G^R\left(\mathbf{r}, \mathbf{r}; \omega'\right)\right) = \int d\mathbf{r} \left\langle \mathbf{r} \right| \widehat{H}^n \left| \mathbf{r} \right\rangle \tag{16.36}$$

$$\int \frac{d\mathbf{k}}{\left(2\pi\right)^3} \int \frac{d\omega'}{2\pi} \left(\omega'\right)^n \left(-2\,\mathrm{Im}\, G^R\left(\mathbf{k}, \mathbf{k}; \omega'\right)\right) = \int \frac{d\mathbf{k}}{\left(2\pi\right)^3} \left\langle \mathbf{k} \right| \widehat{H}^n \left| \mathbf{k} \right\rangle$$

You may be uneasy with the formal manipulations of operators we did in this section. If so, you should to back to the derivations at the beginning of this section which clearly explain what is meant by the formal manipulations.

Remark 148 *Recall that in the case of sum rules for χ'', there was also an implicit trace since we were computing equilibrium expectation values.*

16.4.3 *High frequency expansion.

Once we have established sum rules, we can use them for high frequency expansions. Consider the spectral representation in the form

$$G^R\left(\mathbf{k}, \mathbf{k}; \omega\right) = \int \frac{d\omega'}{2\pi} \frac{-2\,\mathrm{Im}\, G^R\left(\mathbf{k}, \mathbf{k}; \omega'\right)}{\omega + i\eta - \omega'}. \tag{16.37}$$

Then for ω sufficiently large that $\mathrm{Im}\, G^R\left(\mathbf{k}, \mathbf{k}; \omega\right) = 0$ (see remark below), the Green's function becomes purely real and one can expand the denominator so that at asymptotically large frequencies,

$$G^R\left(\mathbf{k}, \mathbf{k}; \omega\right) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\omega'}{2\pi} \left(\omega'\right)^n \left(-2\,\mathrm{Im}\, G^R\left(\mathbf{k}, \mathbf{k}; \omega'\right)\right) \tag{16.38}$$

Integrating on both sides and using sum rules, we obtain,

$$\int \frac{d\mathbf{k}}{\left(2\pi\right)^3} G^R\left(\mathbf{k}, \mathbf{k}; \omega\right) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\mathbf{k}}{\left(2\pi\right)^3} \left\langle \mathbf{k} \right| \widehat{H}^n \left| \mathbf{k} \right\rangle \tag{16.39}$$

or in more general terms,

$$\mathrm{Tr}\left[\widehat{G}^R\left(\omega\right)\right] \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \mathrm{Tr}\left(\widehat{H}^n\right) \tag{16.40}$$

which is an obvious consequence of the high-frequency expansion of (16.8)

$$\widehat{G}^R(\omega) = \frac{1}{\omega + i\eta - \widehat{H}} \tag{16.41}$$

Remark 149 $\operatorname{Im} G^R(\mathbf{k},\mathbf{k};\omega)=0$ *at high frequency: Indeed consider the relation of this quantity to the spectral weight Eq.(16.25) and the explicit representation of the spectral weight Eq.(16.27). Only high energy eigenstates can contribute to the high-frequency part of* $\operatorname{Im} G^R(\mathbf{k},\mathbf{k};\omega)=0$. *The contribution of these high-energy eigenstates is weighted by matrix elements* $\langle n|\mathbf{k}\rangle$. *It is a general theorem that the higher the energy, the larger the number of nodes in* $\langle n|$. *Hence, for* $|\mathbf{k}\rangle$ *fixed, the overlap* $\langle n|\mathbf{k}\rangle$ *must vanish in the limit of infinite energy.*

Remark 150 *The leading high-frequency behavior is in* $1/\omega$, *contrary to that of correlation functions which was in* $1/\omega^2$.

16.5 *Relation to transport and fluctuations

The true many-body case is much more complicated, but for the single-particle Schrödinger equation, life is easy. I work schematically here to show that, in this case, transport properties may be related to single-particle propagators in a simple manner. This example is taken from Ref.[12].

Let $S_{\rho\rho}(\mathbf{k},\omega)$ be the charge structure factor for example.

$$S_{\rho\rho}(\mathbf{k},\omega)=\frac{1}{\mathcal{V}}\int dt e^{i\omega t}\left\langle \rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}\right\rangle=\frac{1}{\mathcal{V}}\int dt e^{i\omega t}\left\langle e^{iHt}\rho_{\mathbf{k}}e^{-iHt}\rho_{-\mathbf{k}}\right\rangle. \tag{16.42}$$

The real-time retarded propagator was

$$\widehat{G}^R(t)=-ie^{-iHt}\theta(t) \tag{16.43}$$

while the advanced propagator was

$$\widehat{G}^A(t)=ie^{-iHt}\theta(-t).$$

The charge structure factor is then expressed in terms of the propagators

$$S_{\rho\rho}(\mathbf{k},\omega)=\frac{-1}{\mathcal{V}}\int dt e^{i\omega t}\left\langle \left(\widehat{G}^R(-t)-\widehat{G}^A(-t)\right)\rho_{\mathbf{k}}\left(\widehat{G}^R(t)-\widehat{G}^A(t)\right)\rho_{-\mathbf{k}}\right\rangle. \tag{16.44}$$

Because of the θ functions, $\widehat{G}^R(-t)\,\widehat{G}^R(t)=0$.

Remark 151 *Alternate proof: We can also see this in the Fourier transform version using the convolution theorem*

$$S_{\rho\rho}(\mathbf{k},\omega)=\frac{-1}{\mathcal{V}}\int \frac{d\omega'}{2\pi}\left\langle \left(\widehat{G}^R(\omega')-\widehat{G}^A(\omega')\right)\rho_{\mathbf{k}}\left(\widehat{G}^R(\omega'+\omega)-\widehat{G}^A(\omega'+\omega)\right)\rho_{-\mathbf{k}}\right\rangle. \tag{16.45}$$

Integrals such as $\int \frac{d\omega'}{2\pi}G^R(\omega')\,G^R(\omega'-\omega)$ *vanish because poles are all in the same half-plane.*

The only terms left then are

$$\boxed{S_{\rho\rho}(\mathbf{k},\omega)=\tfrac{1}{\mathcal{V}}\int\tfrac{d\omega'}{2\pi}\left\langle \widehat{G}^R(\omega')\rho_{\mathbf{k}}\widehat{G}^A(\omega'+\omega)\rho_{-\mathbf{k}}+\widehat{G}^A(\omega')\rho_{\mathbf{k}}\widehat{G}^R(\omega'+\omega)\rho_{-\mathbf{k}}\right\rangle} \tag{16.46}$$

In a specific case, to compute matrix elements in the energy representation, one recalls that

$$G^R(n,n';E)=\langle n|\frac{1}{E-\widehat{H}+i\eta}|n'\rangle=\delta_{nn'}\frac{1}{E-E_n+i\eta} \tag{16.47}$$

$$G^A(n,n';E) = \langle n| \frac{1}{E-\widehat{H}-i\eta} |n'\rangle \tag{16.48}$$

17. A FIRST PHENOMENOLOGICAL ENCOUNTER WITH SELF-ENERGY

In this short Chapter, we want to develop an intuition for the concept of self-energy. The concept is simplest to understand if we start from a non-interacting system and assume that we add interactions with a potential or whatever that changes the situation a little. We will be guided by simple ideas about the harmonic oscillator.

Let us start then from the Green function for a non-interacting particle in Eq.(16.7)

$$\langle \mathbf{k}| \, \widehat{G}_0^R(\omega) \, |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) = \langle \mathbf{k}| \, \frac{1}{\omega + i\eta - \widehat{H}} \, |\mathbf{k}'\rangle = \frac{\langle \mathbf{k}| \, \mathbf{k}'\rangle}{\omega + i\eta - \varepsilon_{\mathbf{k}}}. \tag{17.1}$$

Since the momentum states are orthogonal, it is convenient to define $G_0^R(\mathbf{k},\omega)$ by

$$G_0^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \varepsilon_{\mathbf{k}}}.$$

The corresponding spectral weight is particularly simple,

$$A_0(\mathbf{k},\omega) = -2\,\mathrm{Im}\, G_0^R(\mathbf{k},\omega) = 2\pi\delta(\omega - \varepsilon_{\mathbf{k}}). \tag{17.2}$$

We should think of the frequency as the energy. It is only for a non-interacting particle that specifying the energy specifies the wave vector, since it is only in that case that $\omega = \varepsilon_{\mathbf{k}}$.

In general, if momentum is not conserved, the spectral representation Eq.(16.24)

$$G^R(\mathbf{k};\omega) = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k};\omega')}{\omega + i\eta - \omega'} \tag{17.3}$$

and the explicit expression for the spectral weight Eq.(16.27)

$$A(\mathbf{k};\omega') = \sum_n \langle \mathbf{k}| \, n\rangle \, \langle n \, |\mathbf{k}\rangle \, 2\pi\delta(\omega' - E_n) \tag{17.4}$$

tells us that a momentum eigenstate has non-zero projection on several true eigenstates and hence $A(\mathbf{k};\omega')$ is not a delta function.

Intuitively, for weak perturbations, we simply expect that $A(\mathbf{k};\omega')$ will broaden in frequency around $\omega = \widetilde{\varepsilon}_{\mathbf{k}}$ where $\widetilde{\varepsilon}_{\mathbf{k}}$ is close to $\varepsilon_{\mathbf{k}}$.We take this intuition from the damped harmonic oscillator where the resonance is broadened and shifted by damping. If we take a Lorentzian as a phenomenological form for the spectral weight

$$A(\mathbf{k};\omega') = \frac{2\Gamma}{(\omega - \widetilde{\varepsilon}_{\mathbf{k}})^2 + \Gamma^2} \tag{17.5}$$

then the Green's function can be computed from the spectral representation Eq.(17.3) by using Cauchy's residue theorem. The result is

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega - \widetilde{\varepsilon}_{\mathbf{k}} + i\Gamma}. \tag{17.6}$$

We have neglected $i\eta$ in front of $i\Gamma$. It is easy to verify that $-2\,\mathrm{Im}\,G^R(\mathbf{k},\omega)$ gives the spectral weight we started from.

With a jargon that we shall explain momentarily, we define the one-particle irreducible self-energy by

$$G^R(\mathbf{k},\omega)=\frac{1}{\omega+i\eta-\varepsilon_{\mathbf{k}}-\Sigma^R(\mathbf{k},\omega)}=\frac{1}{G_0^R(\mathbf{k},\omega)^{-1}-\Sigma^R(\mathbf{k},\omega)}. \tag{17.7}$$

Its physical meaning is clear. The imaginary part $\mathrm{Im}\,\Sigma^R(\mathbf{k},\omega)=-\Gamma$ corresponds to the scattering rate, or inverse lifetime, whereas the real part, $\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)=\widetilde{\varepsilon}_{\mathbf{k}}-\varepsilon_{\mathbf{k}}$ leads to the shift in the position of the resonance in the spectral weight. In other words, $\Sigma^R(\mathbf{k},\omega)$ contains all the information about the interactions.

With the simple approximation that we did for the self-energy,

$$\Sigma^R(\mathbf{k},\omega)=\widetilde{\varepsilon}_{\mathbf{k}}-\varepsilon_{\mathbf{k}}-i\Gamma, \tag{17.8}$$

one notices that the second moment $n=2$ in Eq.(16.36) diverges because the second moment of a Lorentzian does. Hence, the high-frequency expansion becomes incorrect already at order $1/\omega^3$. We need to improve the approximation to recover higher frequency moments. Nevertheless, in the form

$$G^R(\mathbf{k},\omega)^{-1}=G_0^R(\mathbf{k},\omega)^{-1}-\Sigma^R(\mathbf{k},\omega) \tag{17.9}$$

equivalent to that given above, there is no loss in generality. The true self-energy is defined as the difference between the inverse of the non-interacting propagator and the inverse of the true propagator. Lifetimes and shifts must in general be momentum and frequency dependent.

Remark 152 *The time dependence of the retarded Green's function shows the damping: Indeed, note that the Fourier transform of* $G^R(\mathbf{k},\omega)$ *is, for* $t>0$,

$$G^R(\mathbf{k},t)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\frac{1}{\omega-\widetilde{\varepsilon}_{\mathbf{k}}+i\Gamma}=-i\theta(t)\,e^{-i\widetilde{\varepsilon}_{\mathbf{k}}t-\Gamma t} \tag{17.10}$$

which shows that when Γ *tends to zero, then we have the expected oscillatory behavior in time for the evolution of an eigenstate of renormalized energy* $\widetilde{\varepsilon}_{\mathbf{k}}$. *Taking the square gives a time-independent result (apart from the* $\theta(t)$*) for the probability. On the other hand, a finite* Γ *means that the amplitude to stay in state* $\mathbf{k}$ *decays with time, as does the probability (twice as fast). That probability can be constructed as follows. By construction, the operator* $\widehat{G}^R(t)$ *allows us to find the wave function at time* t*, given the initial condition* $|\mathbf{k}\rangle$ *at time zero, or as an equation,* $\langle\mathbf{k}|\,\widehat{G}^R(t)\,|\mathbf{k}\rangle=\langle\mathbf{k}|\,\psi(t)\rangle$. *Using the Born rule, the probatility that there is still a particle in state* $|\mathbf{k}\rangle$ *at time* t *is the absolute value of the projection of the state at time* t *on the state* $|\mathbf{k}\rangle$*, or in other words,*

$$|\langle\mathbf{k}|\,\psi(t)\rangle|^2=\left|G^R(\mathbf{k},t)\right|^2=\theta(t)\,e^{-2\Gamma t}. \tag{17.11}$$

18. *PERTURBATION THEORY FOR ONE-BODY PROPAGATOR

Feynman diagrams in their most elementary form appear naturally in perturbation theory for a one-body potential. We will also be able to introduce more precisely the notion of self-energy and point out that the definition given above for the self-energy, $G^R(\mathbf{k},\omega)^{-1} = G_0^R(\mathbf{k},\omega)^{-1} - \Sigma^R(\mathbf{k},\omega)$ is nothing but the so-called Dyson's equation. As an example, we will treat in more details the propagation of an electron in a random potential.

18.1 Perturbation theory in operator form

If we can diagonalize H, then we know the propagator

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega - \widehat{H} + i\eta}} \tag{18.1}$$

from the identities we developed above,

$$G^R(n,n';E) = \langle n| \frac{1}{E - \widehat{H} + i\eta} |n'\rangle = \delta_{nn'} \frac{1}{E - E_n + i\eta} \tag{18.2}$$

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \frac{\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n}. \tag{18.3}$$

This last equation shows that if we can diagonalize the Hamiltonian, we know the Green's function. It can happen that one part of the Hamiltonian, say H_0 can be diagonalized while the other part, say $\widehat{V}$, cannot be diagonalized in the same basis. For example, H_0 could be a free particle Hamiltonian diagonal in momentum space while $\widehat{V}$ could be a potential diagonal in real space. In this situation, we know that we can still find wave functions and eigenenergies using perturbation theory. But since it will be natural to formulate everything with Green's functions, it is desirable to develop perturbation methods directly for the propagator. The easiest manner to proceed (when $\widehat{V}$ is independent of time) is using the operator methods that follow.

First, write

$$\left(\omega + i\eta - \widehat{H}_0 - \widehat{V}\right)\widehat{G}^R(\omega) = 1. \tag{18.4}$$

$\widehat{G}^R(\omega)$ is an operator that we will explicitly write later in terms of its matrix elements, just as $\widehat{H}_0$ and $\widehat{V}$ are operators in the Hilbert space. It is customary to omit the identity matrix that multiplies $(\omega + i\eta)$. I hope this does not confuse you. Just recall that we are working with abstract operators for now. Putting the perturbation $\widehat{V}$ on the right-hand side, and using

$$\widehat{G}_0^R(\omega) = \frac{1}{\omega + i\eta - \widehat{H}_0} \tag{18.5}$$

we have

$$\left(\widehat{G}_0^R(\omega)\right)^{-1}\widehat{G}^R(\omega)=1+\widehat{V}\widehat{G}^R(\omega)\,. \tag{18.6}$$

Multiplying by $\widehat{G}_0^R(\omega)$ on both sides, we write the equation in the form

$$\boxed{\widehat{G}^R(\omega)=\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}^R(\omega)}\,. \tag{18.7}$$

Perturbation theory is obtained by iterating the above equation.

$$\widehat{G}^R(\omega)=\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)+\ldots \tag{18.8}$$

In scattering theory, this is the propagator version of the Lippmann-Schwinger equation. It looks as if we have done much progress. We cannot invert the large matrix H to compute $\widehat{G}^R(\omega)$ but we have expressed it in terms of quantities we know, namely $\widehat{G}_0^R(\omega)$ and $\widehat{V}$. We know $\widehat{G}_0^R(\omega)$ because by hypothesis $\widehat{H}_0$ can be diagonalized. At first sight, if we want to know the propagator to a given order, we just stop the above expansion at some order. Stopping the iteration at an arbitrary point may however lead to misleading results, as we shall discuss after discussing a simple representation of the above series in terms of pictures, or, let us call them, (baby) Feynmann diagrams.

But before this, we point out that perturbation theory here can be seen as resulting from the following matrix identity,

$$\boxed{\tfrac{1}{X+Y}=\tfrac{1}{X}-\tfrac{1}{X}Y\tfrac{1}{X+Y}} \tag{18.9}$$

To prove this identity, multiply by $X+Y$ either from the left or from the right. For example

$$\frac{1}{X+Y}(X+Y)=\frac{1}{X}X+\frac{1}{X}Y-\frac{1}{X}Y\frac{1}{X+Y}(X+Y)=1 \tag{18.10}$$

18.2 Feynman diagrams for a one-body potential and their physical interpretation.

The Lippmann-Schwinger equation Eq.(18.7) may be represented by diagrams. The thick line stands for $\widehat{G}^R(\omega)$ while the thin line stands for $\widehat{G}_0^R(\omega)$ and the dotted line with a cross represents the action of $\widehat{V}$.

- Iterating the basic equation (18.7), one obtains the series -

  $$\widehat{G}^R(\omega)=\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)\,\widehat{V}\widehat{G}_0^R(\omega)+\ldots \tag{18.11}$$

  which we represent diagrammatically by Fig.(18-1). Physically, one sees that the full propagator is obtained by free propagation between scatterings off the potential.

18.2.1 A basis with plane wave states normalized to unity

We will want to express the Lippmann-Schwinger equation in position and momentum spaces. We change our definitions a bit. Until we mention a change, we

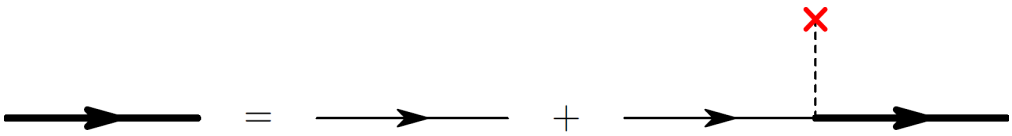


Figure 18-1 Diagrammatic representation of the Lippmann-Schwinger equation for scattering.

work with the following mixed representation where wave vectors are discrete and space is continuous. We assume that plane waves are normalized to unity in a box of volume $\mathcal{V}$.

$$\langle \mathbf{r} \left| \mathbf{k}_i \right\rangle = \frac{1}{\mathcal{V}^{1/2}} e^{i\mathbf{k}_i \cdot \mathbf{r}} \tag{18.12}$$

The discrete momenta are defined by imagining that we have discretized space with $N_x = L_x/a$ points in the x direction, a being the lattices spacing. Similar discretization is done in the other directions. We then have, with periodic boundary conditions,

$$\mathcal{V} = L_x L_y L_z \quad ; \quad k_x = \frac{2\pi n_x}{L_x} ... \quad ; \tag{18.13}$$

$$n_x = -\frac{N_x}{2} + 1, ..., -1, 0, 1, ..., \frac{N_x}{2} \tag{18.14}$$

$$\text{or } n_x = 1, 2, ..., N_x \tag{18.15}$$

The closure relation and normalization in position space are

$$\int d\mathbf{r} \left| \mathbf{r} \right\rangle \langle \mathbf{r}| = 1 \tag{18.16}$$

$$\langle \mathbf{r} \left| \mathbf{r}' \right\rangle = \delta \left(\mathbf{r} - \mathbf{r}' \right). \tag{18.17}$$

One can check that $\left(\int d\mathbf{r} \left| \mathbf{r} \right\rangle \langle \mathbf{r}| \right) \left| \mathbf{r}' \right\rangle = \left| \mathbf{r}' \right\rangle$.

The normalization to unity of the plane waves follows from

$$\begin{aligned} \langle \mathbf{k} \left| \mathbf{k}' \right\rangle &= \langle \mathbf{k}| \left(\int d\mathbf{r} \left| \mathbf{r} \right\rangle \langle \mathbf{r}| \right) \left| \mathbf{k}' \right\rangle \\ &= \int d\mathbf{r} \frac{1}{\mathcal{V}} e^{i\left(\mathbf{k}' - \mathbf{k}\right) \cdot \mathbf{r}} = \delta_{\mathbf{k},\mathbf{k}'} \end{aligned} \tag{18.18}$$

where $\delta_{\mathbf{k},\mathbf{k}'}$ is a Kronecker delta. Consistent with this normalization, the closure relation is

$$\sum_{\mathbf{k}} \left| \mathbf{k} \right\rangle \langle \mathbf{k}| = 1. \tag{18.19}$$

As usual, one changes from a discrete sum to an integral using the formula

$$\int \frac{d\mathbf{k}}{(2\pi)^3} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \tag{18.20}$$

A potential term in the Hamiltonian is diagonal in position space, which means

$$\langle \mathbf{r}| \widehat{V} \left| \mathbf{r}' \right\rangle = v\left(\mathbf{r}\right) \langle \mathbf{r} \left| \mathbf{r}' \right\rangle = V\left(\mathbf{r}\right) \delta \left(\mathbf{r} - \mathbf{r}' \right) \tag{18.21}$$

and in the momentum basis

$$\langle \mathbf{k}| \widehat{V} \left| \mathbf{k}' \right\rangle = \int d\mathbf{r} \int d\mathbf{r}' \langle \mathbf{k} \left| \mathbf{r} \right\rangle \langle \mathbf{r}| \widehat{V} \left| \mathbf{r}' \right\rangle \langle \mathbf{r}' \left| \mathbf{k}' \right\rangle \tag{18.22}$$

$$= \int d\mathbf{r} \langle \mathbf{k} \left| \mathbf{r} \right\rangle \langle \mathbf{r} \left| \mathbf{k}' \right\rangle v\left(\mathbf{r}\right) = \int d\mathbf{r} \frac{1}{\mathcal{V}} e^{-i\left(\mathbf{k} - \mathbf{k}'\right) \cdot \mathbf{r}} v\left(\mathbf{r}\right) \tag{18.23}$$

$$= \frac{1}{\mathcal{V}} V\left(\mathbf{k} - \mathbf{k}'\right) \tag{18.24}$$

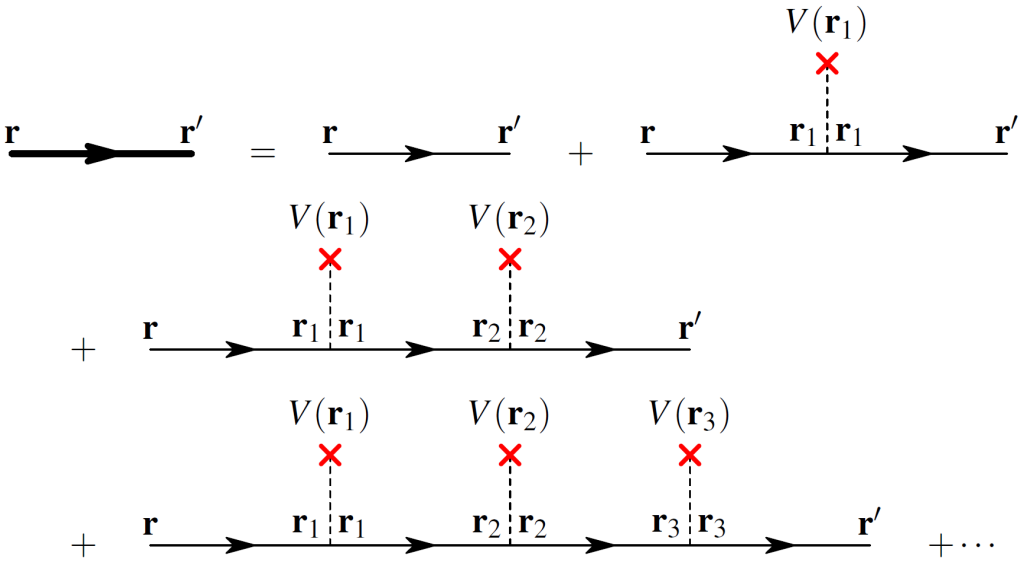


Figure 18-2 Perturbation series for the progagator for free electrons scattering-off impurities in the position-space basis.

18.2.2 Diagrams in position space

To do an actual computation, we have to express the operators in some basis. This is simply done by inserting complete sets of states. Using the fact that the potential is diagonal in the position representation, $\langle \mathbf{r}_1 | \widehat{V} | \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle \mathbf{r}_1 | \widehat{V} | \mathbf{r}_1 \rangle$, we have that

$$\langle \mathbf{r} | \widehat{G}^R(\omega) | \mathbf{r}' \rangle = \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | \widehat{V} | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + ... \tag{18.25}$$

$$= \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | \widehat{V} | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + ... \tag{18.26}$$

Remark 153 *Physical interpretation and path integral: Given that* $\langle \mathbf{r} | \widehat{G}^R(\omega) | \mathbf{r}' \rangle$ *is the amplitude to propagate from* $\langle \mathbf{r}|$ *to* $|\mathbf{r}'\rangle$*, the last result may be interpreted as saying that the full propagator is obtained by adding up the amplitudes to go with free propagation between* $\langle \mathbf{r}|$ *and* $|\mathbf{r}'\rangle$*, then with two free propagations and one scattering at all possible intermediate points, then with three free propagations and two scatterings at all possible intermediate points etc... The Physics is the same as that seen in Feynman's path integral formulation of quantum mechanics that we discuss below. Multiple scatterings on the same impurity are possible.*

One can read off the terms of the perturbation series from the diagrams above by using the following simple diagrammatic rules which go with the following figure (18-2).

- Let each thin line with an arrow stand for $\langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle$. One end of the arrow represents the original position $\mathbf{r}$ while the other represents the final position $\mathbf{r}'$ so that the line propagates from $\mathbf{r}$ to $\mathbf{r}'$. Strictly speaking, from the way we have defined the retarded propagator in terms of propagation of wave functions, this should be the other way around. But the convention we are using now is more common.

- The X at the end of a dotted line stands for a potential $\langle \mathbf{r}_1 | \widehat{V} | \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_1)$.
- Diagrams are built by attaching each potential, represented by an X, to the end of a propagator line and the beginning of another propagator line by a dotted line.
- The intersection of a dotted line with the two propagator lines is called a vertex.
- There is one dummy integration variable $\int d\mathbf{r}_1$ over coordinates for each vertex inside the diagram.
- The beginning point of each continuous line is $\langle \mathbf{r}|$ and the last point is $|\mathbf{r}'\rangle$. These coordinates are not integrated over.
- The propagator is obtained by summing all diagrams formed with free propagators scattering off one or more potentials. Clearly, I used some artistic liberty in drawing these diagrams. You could bend the individual lines, rotate the whole diagram if you wish, it does not change its algebraic meaning, as long as you deform the lines in a continuous way, not cutting any of them. In other words it is only the topology of the diagram that counts. And all topologically distinct possibilities must be considered in the sum. One scattering is distinct from two etc...

18.2.3 Diagrams in momentum space

Since the propagator for a free particle is diagonal in the momentum space representation, this is often a convenient basis to write the perturbation expansion in (18.11). Using complete sets of states again, as well as the definition $\langle \mathbf{k}| \widehat{G}_0^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) \langle \mathbf{k}|\ \mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega)\delta_{\mathbf{k},\mathbf{k}'}$ we have that for a particle with a quadratic dispersion law, or a Hamiltonian $H_0 = p^2/2m$,

$$G_0^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \frac{k^2}{2m}}. \tag{18.27}$$

In this basis, the perturbation series becomes

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}'\rangle + \sum_{\mathbf{k}_1} G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}_1\rangle \langle \mathbf{k}_1| \widehat{G}^R(\omega) |\mathbf{k}'\rangle . \tag{18.28}$$

Solving by iteration to second order, we obtain,

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}'\rangle + G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}'\rangle G_0^R(\mathbf{k}',\omega) \tag{18.29}$$

$$+ \sum_{\mathbf{k}_1} G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}_1\rangle G_0^R(\mathbf{k}_1,\omega)\langle \mathbf{k}_1| \widehat{V} |\mathbf{k}'\rangle G_0^R(\mathbf{k}',\omega) + ... \tag{18.30}$$

The diagrams shown in the following figure Fig.(18-3) are now labeled differently. The drawing is exactly the same as well as the rule of summing over all topologically distinct diagrams.

However,

- Each free propagator has a label $\mathbf{k}$,ω. One can think of momentum $\mathbf{k}$ flowing along the arrow.

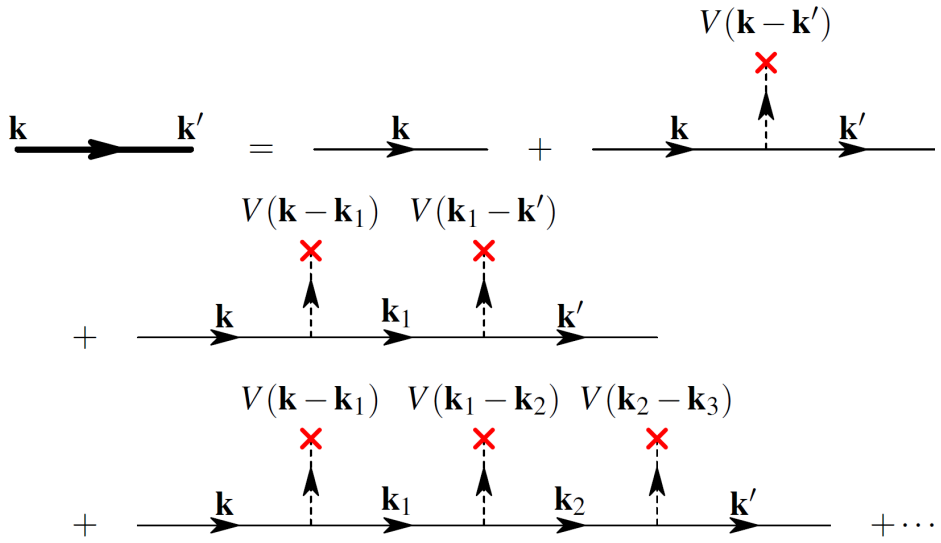


Figure 18-3 Perturbation series for the progagator for free electrons scattering-off impurities in the momentum-space basis. (before impurity averaging).

- Each dotted line now has two momentum indices associated with it. One for the incoming propagator, say $\mathbf{k}$, and one for the outgoing one, say $\mathbf{k}''$. The potential contributes a factor $\langle \mathbf{k}| \widehat{V} |\mathbf{k}''\rangle$. One can think of momentum $\mathbf{k} - \mathbf{k}''$ flowing along the dotted line, and being lost into the X.
- One must sum $\sum_{\mathbf{k}_1}$ over momenta not determined by momentum conservation. If there are n potential scatterings, there are $n-1$ momenta to be integrated over.

18.3 Dyson's equation, irreducible self-energy

Here I show that to make physical sense of the power series, we need to rearrange it so that it becomes a power series not for the Green's function, but for the self-energy that we introduced earlier. In other words, we must rearrange the series and resum infinite subsets. This idea will come back over and over again. We discuss it here in the simple context of scattering off impurities. Even in this simple context we would need in principle to introduce the impurity averaging technique, but we can avoid this.

The Green's function describes how a wave propagates through a medium. We know from experience that even in a random potential, such as that which light encounters when going through glass, the wave can be scattered forward, i.e. if it comes in an eigenstate of momentum, a plane wave, it has a probability to come out in the same eigenstate of momentum. So let us compute the amplitude for propagating from $\langle \mathbf{k}|$ to $|\mathbf{k}\rangle$ using perturbation theory. Suppose we truncate the perturbation expansion to some finite order. For example, take only the $\mathbf{k}_1 = \mathbf{k}$ term in the integral $\sum_{\mathbf{k}_1}$ appearing in the perturbation expansion Eq.(18.30) and consider the truncated series for the diagonal element $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| \mathbf{k}\rangle + G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| \mathbf{k}\rangle . \quad (18.31)$$

This step makes more sense in terms of discrete momenta but can be rationalized with integrals as well. The missing terms in the sum will be included later. Stopping this last series to any finite order does not make much sense for most calculations of interest. For example, the above series will give for $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$ simple and double poles at frequencies strictly equal to the unperturbed energies, while we know from the spectral representation that $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$ should have only simple poles at the true one-particle eigenenergies. Even more disturbing, we know from Eqs.(16.25) and (16.27) that the imaginary part of the retarded Green's function should be negative while these double poles lead to positive contributions. These positive contributions come from the fact that

$$\mathrm{Im}\frac{1}{\left(\omega+i\eta-\frac{k^2}{2m}\right)^2} = -\frac{\partial}{\partial\omega}\mathrm{Im}\frac{1}{\omega+i\eta-\frac{k^2}{2m}} \tag{18.32}$$

$$= \pi\frac{\partial}{\partial\omega}\delta\left(\omega-\frac{k^2}{2m}\right) \tag{18.33}$$

This derivative of a delta function can be positive or negative depending from which side it is approached, a property that is more easy to see with a Lorentzian or Gaussian representation of the delta function. Clearly, the perturbation expansion truncated to any finite order does not seem very physical. It looks as if we are expanding in powers of

$$\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle G_0^R(\mathbf{k},\omega) = \frac{\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle}{\omega+i\eta-\frac{k^2}{2m}} \tag{18.34}$$

a quantity which is not small for ω near the unperturbed energies $\frac{k^2}{2m}$.

If instead we consider a subset of the terms appearing in the *infinite* series, namely

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}\rangle \tag{18.35}$$

$$+ G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}\rangle + ... \tag{18.36}$$

which may be generated by

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\langle \mathbf{k}|\ \mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle \tag{18.37}$$

then things start to make more sense since the solution

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle = \frac{\langle \mathbf{k}|\ \mathbf{k}\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1} - \langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle} \tag{18.38}$$

has simple poles corresponding to eigenenergies shifted from $\frac{k^2}{2m}$ to $\frac{k^2}{2m}+\langle \mathbf{k}| \widehat{V} |\mathbf{k}\rangle$ as given by ordinary first-order perturbation theory for the energy. To get the first-order energy shift, we needed an infinite-order expansion for the propagator.

Remark 154 **The simple procedure above gave $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$ that even satisfies the first sum rule $\int \frac{d\omega}{2\pi}\mathrm{Tr}\left[-2\,\mathrm{Im}\left(\widehat{G}^R(\omega)\right)\right] = 1$ as well as the second $\int \frac{d\omega}{2\pi}\omega\mathrm{Tr}\left[-2\,\mathrm{Im}\left(\widehat{G}^R\right)\right] = \mathrm{Tr}[H]$.*

Even though we summed an infinite set of terms, we definitely did not take into account all terms of the series. We need to rearrange it in such a way that it can be resummed as above, with increasingly accurate predictions for the positions of the shifted poles.

Figure 18-4 Dyson's equation and irreducible self-energy.

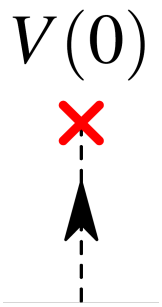


Figure 18-5 First-order irreducible self-energy.

We know how to do this from our previous phenomenological encounter with the concept of self-energy in Sec.17. Here we define the *irreducible self-energy* $\sum(\mathbf{k},\omega)$ by the equation

$$\boxed{\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\,\Sigma^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle}. \quad (18.39)$$

This is the so-called *Dyson equation* whose diagrammatic representation is given in Fig.(18-4) and whose solution can be found algebraically

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = \frac{\langle\mathbf{k}|\,\mathbf{k}\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1} - \Sigma^R(\mathbf{k},\omega)}. \quad (18.40)$$

The definition of the self-energy is found in principle by comparing with the exact result Eq.(18.28) obtained from the Lippmann-Schwinger equation. The algebraic derivation is discussed in the following section, but diagrammatically one can see what to do. The self-energy $\sum(\mathbf{k},\omega)$ should contain all possible diagrams that start with an interaction vertex with entering momentum $\mathbf{k}$, and end with an interaction vertex with outgoing momentum $\mathbf{k}$ and never have in the intermediate states $G_0^R(\mathbf{k}',\omega)$ with $\mathbf{k}'$ equal to the value of $\mathbf{k}$ we are studying. The entering vertex and outgoing vertex is the same to first order. One can convince oneself that this is the correct definition by noting that iteration of the Dyson equation (18.39) will give back all missing $G_0^R(\mathbf{k},\omega)$ in intermediate states.

$\sum(\mathbf{k},\omega)$ is called *irreducible* because a diagram in the self-energy cannot be cut in two separate pieces by cutting one $G_0^R(\mathbf{k},\omega)$ with the same $\mathbf{k}$. In the context of self-energy, one usually drops the term *irreducible* since the *reducible* self-energy $\widetilde{\Sigma}^R(\omega)$, defined by $\widehat{G}^R(\omega) = \widehat{G}_0^R(\omega) + \widehat{G}_0^R(\omega)\,\widetilde{\Sigma}^R(\omega)\,\widehat{G}_0^R(\omega)$, does not have much interest from the point of view of calculations. The last factor in that last equation is $\widehat{G}_0^R(\omega)$ instead of the full $\widehat{G}^R(\omega)$. Hence $\widetilde{\Sigma}^R$ contains diagrams that can be cut in two pieces by cutting one $G_0^R(\mathbf{k},\omega)$.

To first order then, $\sum(\mathbf{k},\omega)$ is given by the diagram in Fig.(18-5) whose algebraic expression can be read off

$$\Sigma^{R(1)}(\mathbf{k},\omega) = \langle\mathbf{k}|\,\widehat{V}\,|\mathbf{k}\rangle. \quad (18.41)$$

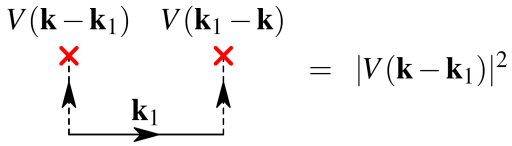


Figure 18-6 Second order irreducible self-energy (before impurity averaging). Note that $\mathbf{k}_1 \neq \mathbf{k}$.That is why this diagram is irreducible.

This is the first-order shift to the energies we had found above. To second order, the diagram is given in Fig.(18-6) and its algebraic expression is

$$\Sigma^{R(2)}(\mathbf{k},\omega) = \sum_{\mathbf{k}_1 \neq \mathbf{k}} \langle \mathbf{k}| \widehat{V} |\mathbf{k}_1\rangle G_0^R(\mathbf{k}_1,\omega) \langle \mathbf{k}_1| \widehat{V} |\mathbf{k}\rangle . \tag{18.42}$$

The result is now frequency dependent and less trivial than the previous one. There will be a non-zero imaginary part, corresponding to the finite lifetime we described previously in our introduction to the self-energy in Chap.17

What have we achieved? We have rearranged the series in such a way that simple expansion in powers of $\widehat{V}$ is possible, but for the irreducible self-energy.

Remark 155 *Locator expansion: The choice of H_0 is dictated by the problem. One could take $\widehat{V}$ as the unperturbed Hamiltonian and the hopping as a perturbation. One then has the "locator expansion".*

Remark 156 *Strictly speaking the irreducible self-energy starting at order three will contain double poles, but at locations different from $\varepsilon_{\mathbf{k}}$ and in addition these will have negligible weight in integrals so they will not damage analyticity properties.*

19. *FORMAL PROPERTIES OF THE SELF-ENERGY

We will come back in the next chapter on the properties of the self-energy and of the Green function but we give a preview. Given the place where the self-energy occurs in the denominator of the full Green function Eq.(18.40), we see that its imaginary part has to be negative if we want the poles of $\widehat{G}^R(\omega)$ to be in the lower half-plane. Also, from the Dyson equation (18.39), the self-energy is analytic in the upper half-plane since $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$ itself is. Analyticity in the upper half-plane means that $\Sigma^R(\mathbf{k},\omega)$ obeys Kramers-Kronig equations analogous to those found before for response functions,

$$\mathrm{Re}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega) - \Sigma^R(\mathbf{r},\mathbf{r}';\infty)\right] = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega'-\omega}. \tag{19.1}$$

$$\mathrm{Im}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega') - \Sigma^R(\mathbf{r},\mathbf{r}';\infty)\right]}{\omega'-\omega} \tag{19.2}$$

One motivation for the definition of the self-energy is that to compute the shift in the energy associated with $\mathbf{k}$, we have to treat exactly the free propagation with $G_0^R(\mathbf{k},\omega)$.

The self-energy itself has a spectral representation, and obeys sum rules. To find its formal expression, let us first define projection operators:

$$\mathcal{P} = |\mathbf{k}\rangle\langle\mathbf{k}| \quad ; \quad \mathcal{Q} = 1-\mathcal{P} = \int \frac{d\mathbf{k}'}{(2\pi)^3} |\mathbf{k}'\rangle\langle\mathbf{k}'| - |\mathbf{k}\rangle\langle\mathbf{k}| \tag{19.3}$$

with the usual properties for projection operators

$$\mathcal{P}^2 = \mathcal{P} \quad ; \quad \mathcal{Q}^2 = \mathcal{Q} \quad ; \quad \mathcal{P}+\mathcal{Q} = 1 \tag{19.4}$$

The following manipulations will illustrate methods widely used in projection operator techniques.[**?**]

Since H_0 is diagonal in this representation, we have that

$$\mathcal{P}G_0^R(\mathbf{k},\omega)\,\mathcal{Q} = \mathcal{Q}G_0^R(\mathbf{k},\omega)\,\mathcal{P} = 0 \tag{19.5}$$

We will use the above two equations freely in the following calculations.

We want to evaluate the full propagator in the subspace $|\mathbf{k}\rangle$. Let us thus project the Lippmann-Schwinger equation

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\widehat{V}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\widehat{V}\mathcal{P}\widehat{G}^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\widehat{V}\mathcal{Q}\widehat{G}^R\mathcal{P}. \tag{19.6}$$

To close the equation, we need $\mathcal{Q}\widehat{G}^R\mathcal{P}$, which can also be evaluated,

$$\mathcal{Q}\widehat{G}^R\mathcal{P} = \mathcal{Q}\widehat{G}_0^R\widehat{V}\widehat{G}^R\mathcal{P} = \mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{P}\widehat{G}^R\mathcal{P} + \mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{Q}\widehat{G}^R\mathcal{P} \tag{19.7}$$

$$\mathcal{Q}\widehat{G}^R\mathcal{P} = \frac{1}{1-\mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{P}\widehat{G}^R\mathcal{P}. \tag{19.8}$$

Substituting in the previous result, we find

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\widehat{V}\left[1+\frac{1}{1-\mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R\widehat{V}\right]\mathcal{P}\widehat{G}^R\mathcal{P} \tag{19.9}$$

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\mathcal{P}\widehat{V}\left[1 + \frac{1}{1-\mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R\widehat{V}\mathcal{P}\right]\mathcal{P}\widehat{G}^R\mathcal{P} \tag{19.10}$$

This means that the self-energy operator is defined algebraically by

$$\boxed{\widehat{\Sigma}^R = \mathcal{P}\widehat{V}\mathcal{P} + \mathcal{P}\widehat{V}\mathcal{Q}\frac{1}{1-\mathcal{Q}\widehat{G}_0^R\mathcal{Q}\widehat{V}\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R\mathcal{Q}\widehat{V}\mathcal{P}}. \tag{19.11}$$

This is precisely the algebraic version of the diagrammatic definition which we gave before. The state $\mathbf{k}$ corresponding to the projection $\mathcal{P}$ never occurs in intermediate states, but the initial and final states are in $\mathcal{P}$.

Remark 157 *Self-energy as a response function: Spectral representation, sum rules and high frequency expansions could be worked out from here. In particular, the first-order expression for the self-energy suffices to have a propagator which satisfies the first two sum rules. Note that we could continue the process started here and decide that for the self-energy we will take into account exactly the propagation in a given state and project out everything else. This eventually generates a continued fraction expansion.[**?**]*

Remark 158 *High-frequency behavior of self-energy and sum rules: Given the $1/\omega$ high-frequency behavior of $\widehat{G}_0^R$, one can see that the infinite frequency limit of the self-energy is a constant given by $\mathcal{P}\widehat{V}\mathcal{P} = |\mathbf{k}\rangle\langle\mathbf{k}|\widehat{V}|\mathbf{k}\rangle\langle\mathbf{k}|$ and that the next term in the high-frequency expansion is $\mathcal{P}\widehat{V}\mathcal{Q}\frac{1}{\omega}\mathcal{Q}\widehat{V}\mathcal{P}$ as follows from the high-frequency behavior of $\widehat{G}_0^R$. We will see in the interacting electrons case that the Hartree-Fock result is the infinite-frequency limit of the self-energy.*

Remark 159 *Projection vs frequency dependence: By projecting out in the subspace $|\mathbf{k}\rangle\langle\mathbf{k}|$, we have obtained instead of the time-independent potential $\widehat{V}$, a self-energy Σ^R which plays the role of an effective potential which is diagonal in the appropriate subspace, but at the price of being frequency dependent. This is a very general phenomenon. In the many-body context, we will want to remove instantaneous two-body potentials to work only in the one-body subspace. When this is done, a frequency dependent self-energy appears: it behaves like an effective frequency dependent one-body potential. This kind of Physics is beyond band structure calculations which always work with a frequency independent one-body potential.*

20. *ELECTRONS IN A RANDOM POTENTIAL: IMPURITY AVERAGING TECHNIQUE.

We treat in detail the important special case of an electron being scattered by a random distribution of impurities. This serves as a model of the residual resistivity of metals. It is the Green's function version of the Drude model for elastic impurity scattering. One must however add the presence of the Fermi sea. When this is done in the many-body context, very little changes compared with the derivation that follows. The many-body calculation will also allow us to take into account inelastic scattering. We start by discussing how to average over impurities, and then we apply these results to the averaging of the perturbation series for the Green's function.

Note that we return to the continuum normalization of Sec.15.1

20.1 *Impurity averaging

Assume that electrons scatter from the potential produced by uniformly distributed impurities

$$V_C(\mathbf{r}) = \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) \tag{20.1}$$

where each of the N_i impurities produces the same potential v but centered at a different position $\mathbf{R}_i$. We have added the index C to emphasize the fact that at this point the potential depends on the actual configuration of impurities. We want to work in momentum space since after averaging over impurities translational invariance will be recovered. This means that the momentum representation will be the most convenient one for the Green's functions.

$$V_C(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) = \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \int d\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_i)} v(\mathbf{r} - \mathbf{R}_i) \tag{20.2}$$

$$= v(\mathbf{q}) \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \tag{20.3}$$

We assume that the impurities are distributed in a uniform and statistically independent manner (The joint probability distribution is a product of a factor $1/\mathcal{V}$ for each impurity). Denoting the average over impurity positions by an overbar, we have for this distribution of impurities,

$$\overline{V_C(\mathbf{q})} = v(\mathbf{q}) \sum_{i=1}^{N_i} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}} \right) = v(\mathbf{q}) \sum_{i=1}^{N_i} \frac{1}{\mathcal{V}} \int d\mathbf{R}_i e^{-i\mathbf{q}\cdot\mathbf{R}_i} = v(\mathbf{q}) \frac{N_i}{\mathcal{V}} (2\pi)^3 \delta(\mathbf{q}) \tag{20.4}$$

$$= n_i v\left(\mathbf{0}\right)\left(2\pi\right)^3 \delta\left(\mathbf{q}\right) \tag{20.5}$$

where n_i is the impurity concentration. We will also need to consider averages of products of impurity potentials,

$$\overline{V_C\left(\mathbf{q}\right) V_C\left(\mathbf{q}'\right)} = v\left(\mathbf{q}\right) v\left(\mathbf{q}'\right) \overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \sum_{j=1}^{N_i} e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}. \tag{20.6}$$

To compute the average, we need to know the joint probability distribution for having an impurity at site i and an impurity at site j. The most simple-minded model takes no correlations, in other words, the probability is the product of probabilities for a single impurity, which in the present case were uniform probability distributions. (This is not such a bad approximation in the dilute-impurity case). So for $i \neq j$, we write

$$\overline{\sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} e^{-i\mathbf{q}'\cdot\mathbf{R}_j}} = \sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}} \quad \overline{e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}\right) = \frac{\left(N_i^2 - N_i\right)}{\mathcal{V}^2}\left(2\pi\right)^3 \delta\left(\mathbf{q}\right)\left(2\pi\right)^3 \delta\left(\mathbf{q}'\right). \tag{20.7}$$

When $i = j$ however, we are considering only one impurity so that

$$\overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} e^{-i\mathbf{q}'\cdot\mathbf{R}_i}} = n_i \left(2\pi\right)^3 \delta\left(\mathbf{q}+\mathbf{q}'\right). \tag{20.8}$$

Gathering the results, and using the result that for a real potential $\left|v\left(\mathbf{q}\right)\right|^2 = v\left(\mathbf{q}\right) v\left(-\mathbf{q}\right)$ we find

$$\overline{V_C\left(\mathbf{q}\right) V_C\left(\mathbf{q}'\right)} = \frac{\left(N_i^2 - N_i\right)}{\mathcal{V}^2}\left(v\left(\mathbf{0}\right)\left(2\pi\right)^3 \delta\left(\mathbf{q}\right)\right)\left(v\left(\mathbf{0}\right)\left(2\pi\right)^3 \delta\left(\mathbf{q}'\right)\right) + n_i \left|v\left(\mathbf{q}\right)\right|^2 \left(2\pi\right)^3 \delta\left(\mathbf{q}+\mathbf{q}'\right). \tag{20.9}$$

20.2 *Averaging of the perturbation expansion for the propagator

Let us return to the perturbation expansion in momentum space to second order Eq.(18.30).Using

$$\left\langle \mathbf{k}\right| V_C \left|\mathbf{k}'\right\rangle = \int d\mathbf{r}\left\langle \mathbf{k}\right|\left.\mathbf{r}\right\rangle V_C\left(\mathbf{r}\right)\left\langle \mathbf{r}\right|\left.\mathbf{k}'\right\rangle = V_C\left(\mathbf{k}-\mathbf{k}'\right) \tag{20.10}$$

and $\left\langle \mathbf{k}\right|\left.\mathbf{k}'\right\rangle = \left(2\pi\right)^3 \delta\left(\mathbf{k}-\mathbf{k}'\right)$, we rewrite the perturbation expansion and average it,

$$\overline{\left\langle \mathbf{k}\right| \widehat{G}^R\left(\omega\right)\left|\mathbf{k}'\right\rangle} = G_0^R\left(\mathbf{k},\omega\right)\left(2\pi\right)^3 \delta\left(\mathbf{k}-\mathbf{k}'\right) + G_0^R\left(\mathbf{k},\omega\right)\overline{V_C\left(\mathbf{k}-\mathbf{k}'\right)} G_0^R\left(\mathbf{k}',\omega\right) \tag{20.11}$$

$$+ \int \frac{d\mathbf{k}_1}{\left(2\pi\right)^3} G_0^R\left(\mathbf{k},\omega\right)\overline{V_C\left(\mathbf{k}-\mathbf{k}_1\right) G_0^R\left(\mathbf{k}_1,\omega\right) V_C\left(\mathbf{k}_1-\mathbf{k}'\right)} G_0^R\left(\mathbf{k}',\omega\right) + ... \tag{20.12}$$

Using what we have learned about impurity averaging, this is rewritten as,

$$\left\langle \mathbf{k}\right| \widehat{G}^R\left(\omega\right)\left|\mathbf{k}'\right\rangle = \quad \left\{G_0^R\left(\mathbf{k},\omega\right) + G_0^R\left(\mathbf{k},\omega\right)\left[n_i v\left(\mathbf{0}\right)\right] G_0^R\left(\mathbf{k},\omega\right)\right.$$

$$+G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)$$
$$-G_0^R(\mathbf{k},\omega)\left[n_i\left|v(\mathbf{0})\right|^2\frac{1}{\mathcal{V}}\right]G_0^R(\mathbf{k},\omega)G_0^R(\mathbf{k},\omega)$$
$$+G_0^R(\mathbf{k},\omega)\int\frac{d\mathbf{k}_1}{(2\pi)^3}G_0^R(\mathbf{k}_1,\omega)\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]G_0^R(\mathbf{k},\omega)+\ldots\}(2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \tag{20.13}$$

Recalling the relation between discrete sums and integrals,

$$\int\frac{d\mathbf{k}_1}{(2\pi)^3}=\frac{1}{\mathcal{V}}\sum_{\mathbf{k}_1} \tag{20.14}$$

we see that the term with a negative sign above removes the $\mathbf{k}=\mathbf{k}_1$ term from the integral. We are thus left with the series

$$\langle\mathbf{k}|\widehat{G}^R(\omega)|\mathbf{k}'\rangle = \quad\{G_0^R(\mathbf{k},\omega)+G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)$$
$$+G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)$$
$$+G_0^R(\mathbf{k},\omega)\left(\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}G_0^R(\mathbf{k}_1,\omega)\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\right)G_0^R(\mathbf{k},\omega)+\ldots\}(2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \tag{20.15}$$

The diagrams corresponding to this expansion are illustrated in Fig.(20-1)

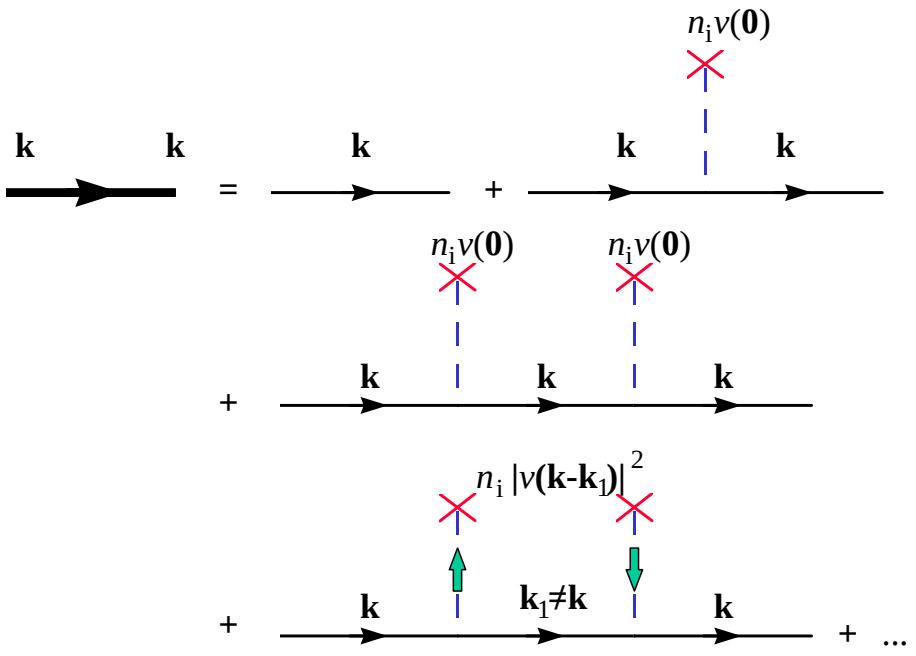


Figure 20-1 Direct iterated solution to the Lippmann-Schwinger equation after impurity averaging.

The diagrammatic rules have changed a little bit. Momentum is still conserved at every vertex, but this time,

- No momentum can flow through an isolated X (in other words, at the vertex the momentum continues only along the line.)
- A factor $[n_i v(\mathbf{0})]$ is associated with every isolated X.

- Various X can be joined together, accounting for the fact that in different X the impurity can be the same.
- When various X are joined together, some momentum can flow along the dotted lines. Each dotted line has a factor $v(\mathbf{k}-\mathbf{k}_1)$ associated with it, with the momentum determined by the momentum conservation rule (which comes from the fact that if in $\int d\mathbf{r} f_1(\mathbf{r}) f_2(\mathbf{r}) f_3(\mathbf{r})$ we replace each function by its Fourier representation, the integral $\int d\mathbf{r}$ will lead to a delta function of the Fourier variables, i.e. $\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0$.)
- The overall impurity concentration factor associated with a single X linking many dotted lines, is n_i, however many dotted lines are associated with it.
- There is an integral over all momentum variables that are not purely determined by the momentum conservation.

Once again, one cannot truncate the series to any finite order since this leads to double poles, triple poles and the other pathologies discussed above. One must resum infinite subsets of diagrams. Clearly, one possibility is to write a self-energy so that

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = \frac{\langle \mathbf{k}|\ \mathbf{k}'\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1} - \Sigma^R(\mathbf{k},\omega)}. \tag{20.16}$$

If we take the diagrams in Fig.(20-2) for the self-energy, expansion of the last equation for the Green's function, or iteration of Dyson's equation in diagrammatic Fig.(18-4), regive the terms discussed above in the straightforward expansion since the algebraic expression for the self-energy we just defined is

$$\boxed{\Sigma^R(\mathbf{k},\omega) = [n_i v(\mathbf{0})] + \int_{\mathbf{k}_1\neq\mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i |v(\mathbf{k}-\mathbf{k}_1)|^2\right] G_0^R(\mathbf{k}_1,\omega)}. \tag{20.17}$$

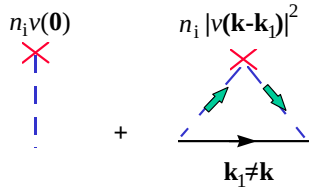


Figure 20-2 Second-order irreducible self-energy in the impurity averaging technique.

Remark 160 *Energy shift: This self-energy gives us the displacements of the poles to linear order in the impurity concentration and to second order in the impurity potential. The displacement of the poles is found by solving the equation*

$$E = \frac{k^2}{2m} + \mathrm{Re}\left[\Sigma^R(\mathbf{k},E)\right]. \tag{20.18}$$

Remark 161 *Lifetime: Taking the Fourier transform to return to real time, it is easy to see that a constant imaginary self-energy corresponds to a life-time, in other words to the fact that the amplitude for being in state* $\mathbf{k}$ *"leaks out" as other states become populated. Indeed, take* $\Sigma^R(\mathbf{k},\omega) = a - i/\tau$ *for example, as an approximation for the self-energy. The corresponding spectral weight is a Lorenzian and the corresponding propagator in time is* $G^R(\mathbf{k},\omega) = -ie^{-i\left(k^2/2m-a\right)t}e^{-t/\tau}$. *We see that the probability of being in state* $\mathbf{k}$ *decreases exponentially. One can*

also check explicitly that the formula found for the lifetime by taking the imaginary part of the self-energy corresponds to what would be obtained from Fermi's Golden rule. For example, the second order contribution from the self-energy expression Eq.(20.17) is

$$\begin{aligned} \operatorname{Im}\Sigma^R(\mathbf{k},\omega) &= -\pi\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\delta\left(\omega-\frac{k_1^2}{2m}\right) \quad (20.19)\\ &= -\pi\int d\varepsilon N(\varepsilon)\frac{d\Omega}{4\pi}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\delta(\omega-\varepsilon) \quad (20.20)\end{aligned}$$

where in the last expression, $N(\varepsilon)$ is the density of states, and Ω the solid angle. One recognizes the density of states at the frequency of interest ω that will come in and the square of the matrix element. We have an overall factor of π instead of 2π because $-\operatorname{Im}\Sigma^R(\mathbf{k},\omega)$ is the scattering rate for the amplitude instead of the probability. In the continuum, we do not need to worry about $\mathbf{k}_1\neq\mathbf{k}$ for this calculation.

Remark 162 *Self-energy and sum rules: One can check that this self-energy is explicitly analytic in the upper half-plane and that the corresponding Green's function satisfies the first sum rule $\int\frac{d\omega}{2\pi}Tr\left[-2\operatorname{Im}\left(\widehat{G}^R(\omega)\right)\right]=Tr\left[H^0\right]=1$ as well as the second $\int\frac{d\omega}{2\pi}\omega Tr\left[-2\operatorname{Im}\left(\widehat{G}^R\right)\right]=Tr\left[H\right]$. However, at this level of approximation, none of the other sum rules are satisfied because the second and higher moments of a Lorentzian are not defined.*

Remark 163 *Average self-energy and self-averaging: We could have obtained precisely the same result by directly averaging the self-energies (18.41)(18.42) defined in the previous subsection (18.39). Indeed, since the rule there was that $G_0^R(\mathbf{k},\omega)$ could not occur in the intermediate states, impurity averaging of the second-order diagram (18.42) would have given only the correlated contribution $\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]G_0^R(\mathbf{k}_1,\omega)$. A $G_0^R(\mathbf{k},\omega)$ in the intermediate state would be necessary to obtain a contribution $\left[n_iv(\mathbf{0})\right]^2$. It is possible to average directly the self-energy in the Dyson equation Eq.(18.39) only if $\langle\mathbf{k}|\widehat{G}^R(\omega)|\mathbf{k}\rangle$ is itself not a random variable. What the present demonstration shows is that indeed, forward scattering, i.e. $\langle\mathbf{k}|\widehat{G}^R(\omega)|\mathbf{k}'\rangle$ with $\mathbf{k}=\mathbf{k}'$, is a self-averaging quantity, in other words, its fluctuations from one realization of the disorder to another may be neglected. Forward scattering remains coherent.*

Remark 164 *Correlations in the impurity distribution: If we had taken into account impurity-impurity correlations in the joint average (20.7),*

$$\overline{\sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i}e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}, \quad (20.21)$$

then we would have found that instead of two delta functions leading eventually to forward scattering only, $(2\pi)^3\delta(\mathbf{k}-\mathbf{k}')$, off-diagonal matrix elements of $\langle\mathbf{k}|\widehat{G}^R(\omega)|\mathbf{k}'\rangle$ would have been generated to order n_i^2 by the Fourier transform of the impurity-impurity correlation function. In other words, correlations in the impurity distribution lead to coherent scattering off the forward direction. In optics, this effect is observed as laser speckle pattern.

Remark 165 *Strong impurity potential: It is easy to take into account the scattering by a single impurity more carefully in the self-energy. The set of diagrams*

in Fig.(20-3) are all first-order in impurity concentration. Their summation corresponds to summing the full Born series. In other words, the summation would correspond to replacing the Born cross section entering the expression for the imaginary part of the Green's function by the full T-matrix expression. The cross section for the impurity is then evaluated beyond the Born approximation. This is important when the phase shifts associated with scattering from the impurity are important.

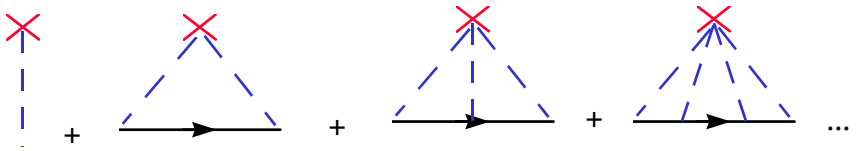


Figure 20-3 Taking into account multiple scattering from a single impurity.

Remark 166 *Irreversibility and infinite volume limit: We have proven that the poles of the Green's function are infinitesimally close to the real axis. In particular, suppose that $|n\rangle$ labels the true eigenstates of our one-body Schrödinger equation in the presence of the impurity potential. Then, our momentum space Green's function will be given by Eq.(16.5)*

$$G^R(\mathbf{k},\mathbf{k};\omega) = \sum_n \frac{\langle \mathbf{k}|\ n\rangle\ \langle n\ |\mathbf{k}\rangle}{\omega + i\eta - E_n} \tag{20.22}$$

$$-\frac{1}{\pi}\,\mathrm{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right] = \sum_n \langle \mathbf{k}|\ n\rangle\ \langle n\ |\mathbf{k}\rangle\ \delta(\omega - E_n)\,. \tag{20.23}$$

In the case we are considering here, $\mathbf{k}$ is no longer a good quantum number. Hence, instead of a single delta function, the spectral weight $-\frac{1}{\pi}\,\mathrm{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right]$ contains a sum of delta functions whose weight is determined by the projection of the true eigenstate on $\mathbf{k}$ states. However, if we go to the infinite volume limit, or equivalently assume that the level separation is smaller than η, the discrete sum over n can be replaced by an integral, and we obtain a continuous function for the spectral weight. As long as the Green's function has discrete poles, the Fourier transform in time of G^R is an oscillatory function and we have reversibility (apart from the damping η). Going to the infinite volume limit, (level spacing goes to zero before η), we obtained instead a continuous function of frequency instead of a sum over discrete poles. The Fourier transform of this continuous function will in general decay in time. In other words, we have obtained irreversibility by taking the infinite volume limit before the $\eta \to 0$ limit.

Remark 167 *Origin of poles far from the real axis: We come back to the phenomenological considerations on the self-energy in Chap.17. In the case of a continuous spectral weight, when we start to do approximations there may appear poles that are not infinitesimally close to the real axis. Indeed, return to our calculation of the imaginary part of the self-energy above. If we write*

$$-\frac{1}{\pi}\,\mathrm{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right] = \frac{1}{\pi}\,\frac{-\,\mathrm{Im}\left[\Sigma^R(\mathbf{k},\omega)\right]}{\left(\omega - \frac{k^2}{2m} - \mathrm{Re}\left[\Sigma^R(\mathbf{k},\omega)\right]\right)^2 + \left(\mathrm{Im}\left[\Sigma^R(\mathbf{k},\omega)\right]\right)^2} \tag{20.24}$$

then there are many cases, such as the one of degenerate electrons scattering off impurities, where for small ω we can approximate $\mathrm{Im}\left(\Sigma^R(\mathbf{k},\omega)\right)$ by a constant and $\mathrm{Re}\left[\Sigma^R(\mathbf{k},\omega)\right]$ by a constant plus a linear function of frequency. Then $G^R(\mathbf{k},\mathbf{k};\omega)$

has a single pole, far from the real axis. In reality, we see from the spectral representation Eq.(16.24) that this single pole is the result of the contribution of a series of poles near the real axis, each of which gives a different residue contribution to the spectral weight. (In the impurity problem, $\mathbf{k}$ *is not a good quantum number anymore so that several of the true eigenstates* E_n *entering the spectral weight Eq.(16.27) have a non-zero projection* $\langle \mathbf{k}| \, n\rangle$ *on momentum eigenstates* $\langle \mathbf{k}| \, .$*) It is because the spectral weight here is approximated by a Lorentzian that the resulting retarded Green's function looks as if it has a single pole. It is often the case that the true Green's function is approximated by functions with a few poles that are not close to the real axis. This can be done not only for the Green's function, but also for general response functions. Poles far from the real axis will arise in general when the spectral weight, or equivalently the self-energy, is taken as a continuous function of frequency, in other words when the infinite size limit is taken before the limit* $\eta \to 0$*.*

21. *OTHER PERTURBATION RESUMMATION TECHNIQUES: A PREVIEW

The ground state energy may be obtained by the first sum rule. But in the more general case, one can develop a perturbation expansion for it. The corresponding diagrams are a sum of connected diagrams. The so-called "linked cluster theorem" is a key theorem that will come back over and over again.

Given the expression we found above for the density-density correlation, the reader will not be surprised to learn that the diagrams to be considered are, before impurity averaging, of the type illustrated in Fig.(21-1). The density operators act at the far left and far right of these diagrams.

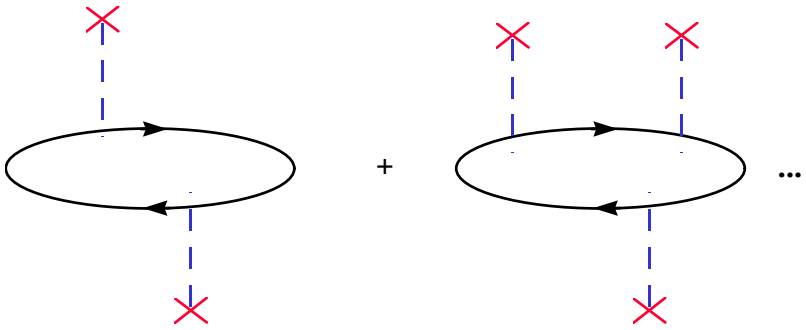


Figure 21-1 Some diagrams contributing to the density-density correlation function before impurity averaging.

After impurity averaging, we obtain for example diagrams of the form illustrated in Fig.(21-2)

Subset of diagrams corresponding to dressing internal lines with the self-energy can be easily resummed. The corresponding diagrams are so-called skeleton diagrams. The first two diagrams in Fig.(21-2) could be generated simply by using lines that contain the full self-energy. The diagrams that do not correspond to self-energy insertions, such as the last on in Fig.(21-2), are so-called vertex corrections.

Subsets of vertex corrections that can be resummed correspond to ladders or bubbles. Ladder diagrams, illustrated in Fig.(21-3) correspond to the so-called Bethe-Salpeter equation, or T-matrix equation. They occur in the problem of superconductivity and of localization.

The bubbles illustrated in Fig.(21-4) are useful especially for long-range forces. They account for dielectric screening, and either renormalize particle-hole excitations or give new collective modes: excitons, plasmons, spin wave, zero sound and the like.

Finally, self-consistent Hartree-Fock theory can be formulated using skeleton diagrams, as illustrated in Fig.(21-5). The self-consistency contained in Hartree-Fock diagrams is crucial for any mean-field type of approximation, such as the BCS theory for superconductivity and Stoner theory for magnetism.

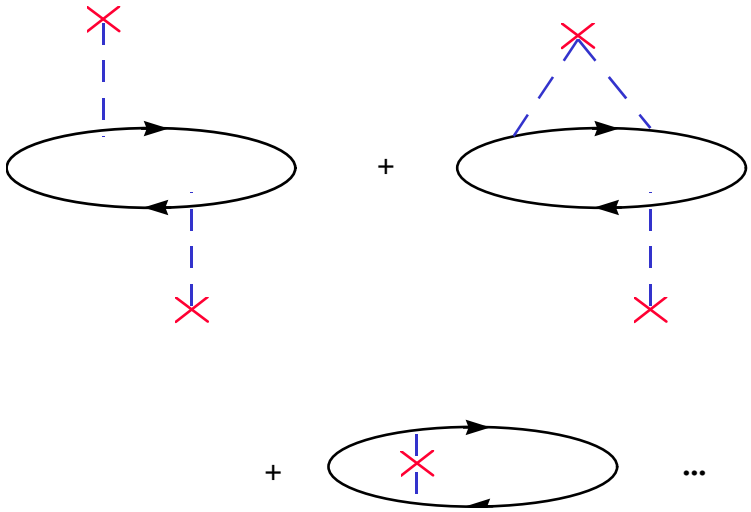


Figure 21-2 Some of the density-density diagrams after impurity averaging.

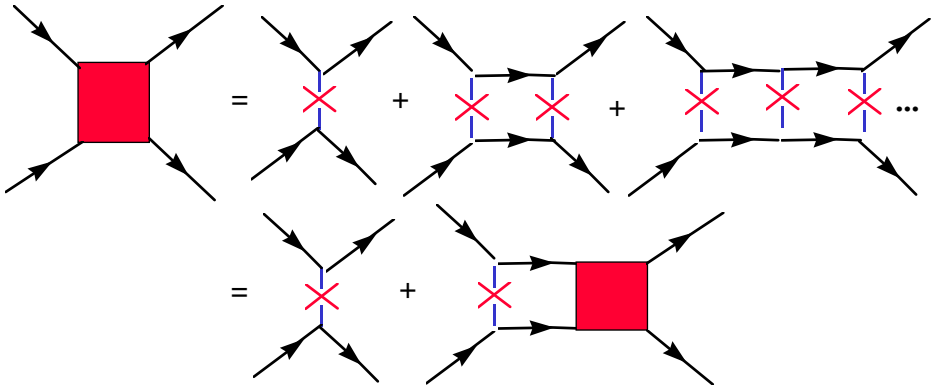


Figure 21-3 Ladder diagrams for T-matrix or Bethe-Salpeter equation.

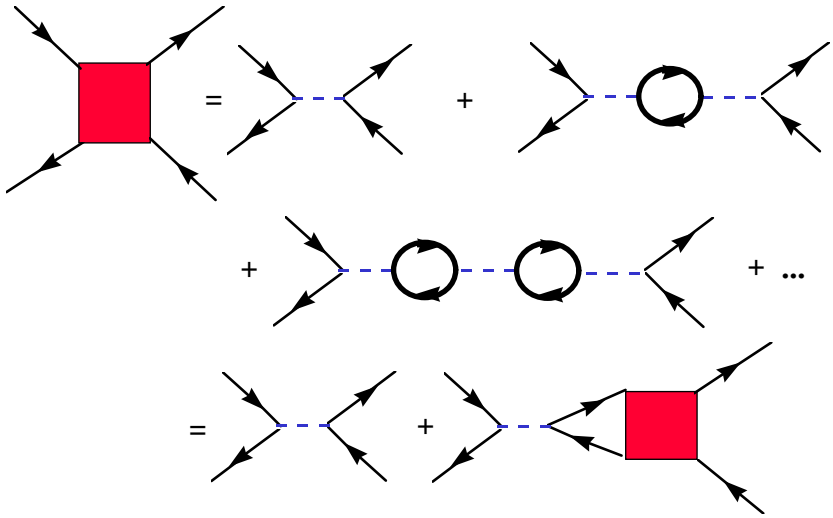


Figure 21-4 Bubble diagrams for particle-hole exitations.

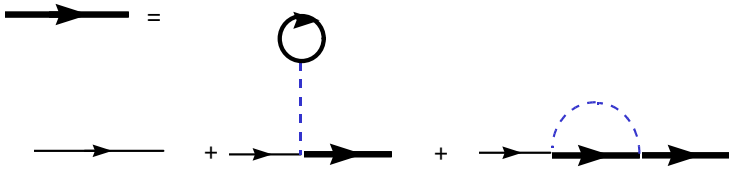


Figure 21-5 Diagrammatic representation of the Hartree-Fock approximation.

Parquet diagrams sum bubble and ladder simultaneously. They are essential if one wants to formulate a theory at the two-particle level which satisfies fully the antisymmetry of the many-body wave-function. In diagrammatic language, this is known as crossing symmetry.

We come back on all these notions as in the context of the "real" many-body problem that we now begin to discuss.

22. *FEYNMAN PATH INTEGRAL FOR THE PROPAGATOR, AND ALTERNATE FORMULATION OF QUANTUM MECHANICS

We have seen that all the information is in the one-particle propagator. It is thus possible to postulate how the propagator is calculated in quantum mechanics and obtain a new formulation that is different from Schrödinger's, but that can be proven equivalent. This formulation is Feynman's path integral,[**?**] that came from ideas of Dirac.[68] The final outcome will be that the amplitude to go from one point to another is equal to the sum over all possible ways of going between the points, each path being weighted by a term proportional to $e^{iS(\dot{x},x)}$ where S is the action. To understand that all intermediate paths are explored, it suffices to think of Young's interference through two slits. If we add more and more slits, we see that the wave must go everywhere. In quantum mechanics there is no trajectory, one of the most surprising results of that theory. However, if the action is large, as in the classical limit, the most likely path will be that which minimizes the action, just as we know from the least action principle in classical mechanics. That is one of the ways in which the classical limit comes out most clearly.

Remark 168 *As emphasized by Dirac, if matter is made of elementary constituents, there must be an absolute notion of smallness, otherwise there is no end into the question "what is inside". That absolute quantity is not a size, it is an action, Planck's constant h.That is why macroscopic objects can behave quantum mechanically, as long as the physical processes involved have an action that is comparable to Planck's constant. And vice-versa, why classical mechanics comes out if the action is large, as we proceed to see.*

Instead of postulating Feynman's path integral, here I derive the path integral formulation from Schrödinger's quantum mechanics. In practice, this method is now used mostly for numerical calculations and for deriving semi-classical approximations. It is conceptually very useful and has generalizations to the many-body case that often used in contemporary work.

We take a single particle in one dimension to simplify the discussion. The relevant object is the amplitude for a particle to go from position x_i to position x_f in a time t. Feynman calls that the probability amplitude or the kernel $K\left(x_f,t;x_i,0\right)$. I will use the notation $G^{>}\left(x_f,t;x_i,0\right)$ for reasons that will be come clear when we discuss propagators in second quantized notation. Mathematically then,

$$G^{>}\left(x_f,t;x_i,0\right)\equiv\left\langle x_f\right|e^{-iHt/\hbar}\left|x_i\right\rangle. \tag{22.1}$$

It is the basic object of this section.

22.1 *Physical interpretation

There are several ways to physically understand the quantity defined above. From the basic postulates of quantum mechanics, squaring $G^{>}(x_f,t;x_i,0)$ gives the probability $\left|\langle x_f|\, e^{-iHt/\hbar}\,|x_i\rangle\right|^{2.}$ that we are in eigenstate of position x_f at time t if the starting state is a position eigenstate x_i. Also, if we know $G^{>}(x_f,t;x_i,0)$ we know the amplitude to go from any state to any other one. Indeed, inserting complete sets of position eigenstates we find that

$$\langle\psi_f|\, e^{-iHt/\hbar}\,|\psi_i\rangle = \int dx_i dx_f \psi_f^*(x_f)\,\psi_i(x_i)\,\langle x_f|\, e^{-iHt}\,|x_i\rangle \tag{22.2}$$

Another way to see how to use $G^{>}(x_f,t;x_i,0)$ is to relate it to the retarded propagator,

$$G^R(x_f,t;x_i,0) \equiv -i\,\langle x_f|\, e^{-iHt}\,|x_i\rangle\,\theta(t) = -iG^{>}(x_f,t;x_i,0)\,\theta(t) \tag{22.3}$$

where $\theta(t)$ is the heaviside step function. Inserting a complete set of energy eigenstates, we find

$$\begin{aligned} G^R(x_f,t;x_i,0) &\equiv -i\sum_n \langle x_f|\, n\rangle\, e^{-iE_nt}\,\langle n\,|x_i\rangle\,\theta(t) \\ &= -i\sum_n \psi_n(x_f)\,\psi_n^*(x_i)\,e^{-iE_nt}\theta(t) \end{aligned} \tag{22.4}$$

As we saw before, the Fourier transform of this quantity with η a positive real number is

$$\int_{-\infty}^{\infty} dt e^{i(z+i\eta)t} G^R(x_f,t;x_i,0) = \sum_n \frac{\psi_n(x_f)\,\psi_n^*(x_i)}{z+i\eta-E_n}. \tag{22.5}$$

The poles of this function, as we already know, give the eigenenergies and the residues are related to the wave functions. In the many-body context, a generalization of the propagator occurs very naturally in perturbation theory.

Remark 169 *In statistical physics, $\langle x_f|\,\rho\,|x_i\rangle$ is a quantity of interest. Using the known form of the density matrix, we have $\langle x_f|\,\rho\,|x_i\rangle = \langle x_f|\, e^{-\beta H}\,|x_i\rangle/Z$. Hence, computing these matrix elements is like computing the propagator in imaginary time τ with the substitution $t\to -i\tau$. This analogy holds also in the many-body context. The density matrix is much better behaved in numerical evaluations of the path integral than the equivalent in real time because it does not have unpleasant oscillations as a function of time.*

22.2 *Computing the propagator with the path integral

In general, H contains non-commuting pieces. The potential energy V is diagonal in position space, but the kinetic energy K is diagonal in momentum space. Hence, computing the action of e^{-iHt} on $|x_i\rangle$ is non-trivial since we need to diagonalize the Hamiltonian to compute the value of the exponential of an operator and that

Hamiltonian contains two non-commuting pieces that are diagonal in different basis. The key observation is that if the time interval t is very small, say ε, then the error that we do in writing the exponential as a product of exponentials is of order ε^2 since it depends on the commutator of $K\varepsilon$ with $V\varepsilon$

$$e^{-iH\varepsilon} \sim e^{-iK\varepsilon}e^{-iV\varepsilon} + O\left(\varepsilon^2\right). \tag{22.6}$$

In fact the error of order ε^2 is in the argument of the exponential, as one can see from the Baker-Campbell-Hausdorff formula $e^A e^B = e^M$ with

$$M = A + B + \frac{1}{2}\left[A, B\right] + a_2\left[A, \left[A, B\right]\right] + \ldots \tag{22.7}$$

where a_2 is a numerical coefficient. In numerical calculations it is important to keep the exponential form since this garantees unitarity.

Other factorizations give errors of even higher order. For example,

$$e^{-iH\varepsilon} \sim e^{-iV\varepsilon/2}e^{-iK\varepsilon}e^{-iV\varepsilon/2} \tag{22.8}$$

gives an error of order ε^3. In practice, for numerical simulations it is quite useful to use factorizations that lead to higher order errors. To continue analytically however, the simplest factorization suffices.

In the factorized form, we can take advantage of the fact that we can introduce complete sets of states where the various pieces of the Hamiltonian are diagonal to compute the propagator for an infinitesimal time

$$\left\langle x_f\right| e^{-iK\varepsilon}e^{-iV\varepsilon}\left|x_i\right\rangle = \int \frac{dp}{2\pi}\left\langle x_f\right| e^{-iK\varepsilon}\left|p\right\rangle\left\langle p\right| e^{-iV\varepsilon}\left|x_i\right\rangle \tag{22.9}$$

$$= \int \frac{dp}{2\pi}e^{i\left[-\varepsilon\frac{p^2}{2m}+p(x_f-x_i)-\varepsilon V(x_i)\right]} \tag{22.10}$$

where, reverting to our earlier continuum normalization in Sec. 15.1, I used $\left\langle x\right| \left.p\right\rangle = e^{ipx}$. The last formula can be rewritten

$$\int \frac{dp}{2\pi}e^{i(p\dot{x}-H)\varepsilon} \tag{22.11}$$

where

$$\dot{x} \equiv \frac{x_f - x_i}{\varepsilon}. \tag{22.12}$$

The argument of the exponential is the Lagrangian times the time interval. It thus has the units of action and is made dimensionless by dividing by the quantum of action $\hbar$ that we have set to unity.

For a finite time interval, we simply split the time evolution operator into evolution pieces that evolve over an infinitesimal time interval

$$e^{-iHt} = \prod_{i=1}^{N} e^{-iH\varepsilon} \tag{22.13}$$

where $\varepsilon = t/N$. There is no approximation here. Inserting $N-1$ complete sets of states, we have

$$\left\langle x_f\right| e^{-iHt}\left|x_i\right\rangle = \int \prod_{j=1}^{N-1} dx_j \left\langle x_f\right| e^{-iH\varepsilon}\left|x_{N-1}\right\rangle\left\langle x_{N-1}\right| e^{-iH\varepsilon}\left|x_{N-2}\right\rangle\left\langle x_2\right|\ldots$$
$$\left|x_1\right\rangle\left\langle x_1\right| e^{-iH\varepsilon}\left|x_i\right\rangle. \tag{22.14}$$

Each of the N matrix elements can be evaluated now using the previous trick so that the propagator is given by the formally exact expression

$$\begin{aligned}\left\langle x_f\right| e^{-iHt}\left|x_i\right\rangle &= \lim_{N\to\infty}\int\prod_{j=1}^{N-1}dx_j\int\prod_{j=1}^{N}\frac{dp_j}{2\pi}\exp\left[i\left(p_N\frac{x_f-x_{N-1}}{\varepsilon}-\frac{p_N^2}{2m}-V\left(x_{_{N-1}}\right)\right)\varepsilon\right.\\ &+i\left(p_{N-1}\frac{x_{N-1}-x_{N-2}}{\varepsilon}-\frac{p_{N-1}^2}{2m}-V\left(x_{_{N-2}}\right)\right)\varepsilon\\ &+\ldots\\ &\left.+\,i\left(p_1\frac{x_1-x_i}{\varepsilon}-\frac{p_1^2}{2m}-V\left(x_{_i}\right)\right)\varepsilon\right] \qquad (22.15)\end{aligned}$$

To do the calculation, this is what one has to do. Formally however, the final expression is quite nice. It can be written as a path integral in phase space

$$\begin{aligned}\left\langle x_f\right| e^{-iHt}\left|x_i\right\rangle &= \int[DxDp]\exp\left\{i\int dt\left[p\dot{x}-H\left(p,x\right)\right]\right\} \qquad (22.16)\\ &= \int[DxDp]\exp iS\left(x,p\right) \qquad (22.17)\end{aligned}$$

where the definition of the measure $[DxDp]$ is clear by comparison and where S is the action.

It is more natural to work in configuration space where the Lagrangian is normally defined. This comes out automatically by doing the integral over all the intermediate momenta. They can be done exactly since they are all Gaussian integrals that are easily obtained by completing the square

$$\begin{aligned}\int\frac{dp}{2\pi}\exp i\left(p_{N-1}\frac{x_{N-1}-x_{N-2}}{\varepsilon}-\frac{p_{N-1}^2}{2m}\right)\varepsilon &= \sqrt{\frac{m}{2\pi i\varepsilon}}\exp\left[\frac{im}{2}\left(\frac{x_{N-1}-x_{N-2}}{\varepsilon}\right)^2\varepsilon\right]\\ &= \sqrt{\frac{m}{2\pi i\varepsilon}}\exp\left[\frac{im}{2}\dot{x}_{N-1}^2\varepsilon\right]. \qquad (22.18)\end{aligned}$$

Remark 170 *The above is the propagator for a free particle. In that case, the time interval could be arbitrary and the result could also be obtained using our earlier decomposition on energy eigenstates since*

$$\sum_n\phi_n\left(x_f\right)\phi_n^*\left(x_i\right)e^{-iE_nt}=\int\frac{dp}{2\pi}e^{ip(x_f-x_i)-it\frac{p^2}{2m}}. \qquad (22.19)$$

Once the integrals over momenta have been done, we are left with

$$\begin{aligned}\left\langle x_f\right| e^{-iHt}\left|x_i\right\rangle &= \lim_{N\to\infty}\int\prod_{j=1}^{N-1}dx_j\left(\sqrt{\frac{mN}{2\pi it}}\right)^N\exp\left[i\varepsilon\left(\frac{m}{2}\left(\frac{x_f-x_{N-1}}{\varepsilon}\right)^2-V\left(x_{_{N-1}}\right)\right)\right.\\ &+i\varepsilon\left(\frac{m}{2}\left(\frac{x_{N-1}-x_{N-2}}{\varepsilon}\right)^2-V\left(x_{_{N-2}}\right)\right)\\ &+\ldots\\ &\left.+\,i\varepsilon\left(\frac{m}{2}\left(\frac{x_1-x_i}{\varepsilon}\right)^2-V\left(x_{_i}\right)\right)\right] \qquad (22.20)\\ &= \int_{x_i}^{x_f}Dx\exp\left(i\int_0^t dt'\left(\frac{1}{2}m\dot{x}^2-V\left(x\right)\right)\right)=\int_{x_i}^{x_f}Dxe^{iS(\dot{x},x)} \qquad (22.21)\end{aligned}$$

where the formal expression makes clear only that it is the integral of the Lagrangian, hence the action, that comes in the argument of the exponential. The

integration measure here is different from the one we had before. This form is particularly useful for statistical physics where all the integrals are clearly convergent, as opposed to the present case where they oscillate rapidly and do not always have a clear meaning.

The physical interpretation of this result is quite interesting. It says that the amplitude for going from one point to another in a given time is given by the sum amplitudes for all possible ways of going between these two points in the given time, each path, or trajectory, being weighted by an exponential whose phase is the classical action measured in units of the action quantum $\hbar$.

Remark 171 *Classical limit: The classical limit is obtained when the action is large compared with the quantum of action. Indeed, in that case the integral can be evaluated in the stationary phase approximation. In that approximation, one expands the action to quadratic order around the trajectory that minimizes the action. That trajectory, given by the Euler-Lagrange equation, is the classical trajectory according to the principle of least action. By including gaussian fluctuations around the classical trajectory, one includes a first set of quantum corrections.*

Remark 172 *The exponentials in the path integral are time-ordered, i.e. the ones corresponding to later times are always to the left of those with earlier times. This time-ordering feature will be very relevant later for Green functions.*

23. EXERCICES FOR PART III

23.0.1 Fonctions de Green retardées, avancées et causales.

Soit la fonction de Green pour des particules libres:

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2m}\nabla^2\right]G\left(\mathbf{r}-\mathbf{r}';t\right)=\delta^3\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t\right)$$

a) Calculez $G\left(\mathbf{k},\omega\right)$ en prenant la transformée de Fourier de cette équation d'abord dans l'espace, puis dans le temps. Pour la transformée de Fourier spatiale, on peut supposer que $G\left(\mathbf{r}-\mathbf{r}';t\right)=0$ à $\mathbf{r}-\mathbf{r}'=\pm\infty$. Dans le cas de la transformée de Fourier dans le temps, intégrez par parties et montrez que le choix $\pm i\eta$ est déterminé par l'endroit où G s'annulle, soit à $t=\infty$ ou à $t=-\infty$. Une de ces fonctions de Green est la fonction dite avancée.

b) Rajoutez à la fonction retardée une solution de la version homogène de l'équation différentielle pour obtenir une fonction de Green qui ne s'annule ni à $t=\infty$ ni à $t=-\infty$ et qui est le plus symétrique possible sous le changement $(t\rightarrow -t)$, plus spécifiquement $G_c^*\left(\mathbf{k},t\right)=G_c\left(\mathbf{k},-t\right)$. C'est la fonction de Green "Causale" (Time-ordered).

c) Calculez la fonction de Green retardée $G^R\left(\mathbf{r}-\mathbf{r}';t\right)$ pour une particule libre en trois dimensions en prenant la transformée de Fourier de $G^R\left(\mathbf{k},\omega\right)$.

23.0.2 Partie imaginaire de la self-énergie et règle d'or de Fermi

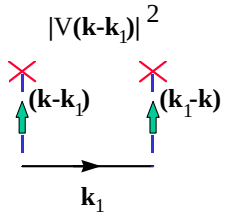


Figure 23-1 Second order irreducible self-energy (before impurity averaging). Note that $\mathbf{k}_1\neq\mathbf{k}$.That is why this diagram is irreducible.

Supposons un potentiel delta, $\langle\mathbf{r}|\,V\,|\mathbf{r}'\rangle=v\left(\mathbf{r}\right)\langle\mathbf{r}\,|\mathbf{r}'\rangle=v\delta\left(\mathbf{r}\right)\langle\mathbf{r}\,|\mathbf{r}'\rangle=v\delta\left(\mathbf{r}\right)\delta\left(\mathbf{r}-\mathbf{r}'\right)$ dans un milieu uniforme. De plus, on suppose que

$$G_0^R\left(\mathbf{k}_1,\omega\right)=\frac{1}{\omega+i\eta-\frac{k^2}{2m}} \tag{23.1}$$

a) Montrez que

$$\begin{aligned}\langle\mathbf{k}|\,V\,|\mathbf{k}_1\rangle &= \int d^3\mathbf{r}\int d^3\mathbf{r}'\,\langle\mathbf{k}\,|\mathbf{r}\rangle\,\langle\mathbf{r}|\,V\,|\mathbf{r}'\rangle\,\langle\mathbf{r}'\,|\mathbf{k}_1\rangle &(23.2)\\ &= \langle\mathbf{k}\,|\mathbf{r}=\mathbf{0}\rangle\,\langle\mathbf{r}=\mathbf{0}\,|\mathbf{k}_1\rangle\,v &(23.3)\\ &= \frac{v}{\mathcal{V}}. &(23.4)\end{aligned}$$

b) Montrez qu'au premier ordre en V, la self-énergie ne fait que déplacer le zéro d'énergie. (Négligez ce changement de zéro d'énergie dans la suite).

c) Évaluez la partie imaginaire de la self-énergie au deuxième ordre

$$\Sigma^{R(2)}(\mathbf{k},\omega) = \sum_{\mathbf{k}_1 \neq \mathbf{k}} \langle \mathbf{k}| V |\mathbf{k}_1\rangle G_0^R(\mathbf{k}_1,\omega) \langle \mathbf{k}_1| V |\mathbf{k}\rangle \tag{23.5}$$

et montrez que l'on retrouve ce que la règle d'or de Fermi nous aurait donné pour une collision élastique. (Passez de la somme discrète à une intégrale en utilisant un facteur $\mathcal{V}^{-1}$ et utilisez la densité d'états pour réécrire le résultat et remarquez que la restriction $\mathbf{k}_1 \neq \mathbf{k}$ est de mesure négligeable). Pour faire le lien entre le temps de vie trouvé avec la self et la règle d'or, vous pouvez transformer l'amplitude $\langle \mathbf{k}| G^R(t) |\mathbf{k}\rangle$ en probabilité en prenant le module carré. Vous pouvez prendre la partie imaginaire de la self-énergie comme une constante pour calculer $\langle \mathbf{k}| G^R(t) |\mathbf{k}\rangle$. Il y aura une décroissance exponentielle en temps de cette probabilité. Ce taux de décroissance est relié à celui trouvé avec la règle d'or de Fermi. Pouvez-vous expliquer le facteur 2?

d) Discutez de l'interprétation de la partie imaginaire de la self-énergie comme d'un temps de vie (vous pouvez faire l'approximation que la densité d'états est indépendante de la fréquence).

e) Discutez de la partie réelle de la self-énergie en lien avec la formule standard pour le déplacement des niveaux d'énergie en théorie des perturbations au deuxième ordre.

f) Montrez que la relation ci-dessus pour la self-énergie est cohérente avec le fait que parties réelles et imaginaires de la self-énergie soient reliées par une relation de Kramers-Kronig.

23.0.3 Règles de somme dans les systèmes désordonnés.

La seconde quantification est prérequise à cet exercice. Soit l'Hamiltonien de liaisons fortes pour une chaîne unidimensionnelle:

$$H = \sum_i \epsilon_i a_i^+ a_i + t \sum_i \left(a_i^+ a_{i+1} + a_{i+1}^+ a_i \right)$$

où a_i est un opérateur de destruction sur le site i. Les énergies ϵ_i des sites ont une valeur ϵ_0 avec une probabilité x et une valeur ϵ_1 avec une probabilité $1-x$. Il n'y a qu'une particule.

a) Utilisez les règles de somme pour calculer la valeur moyenne sur le désordre du moment d'ordre 0 et du moment d'ordre 1 de la densité d'états totale $\rho(\omega)$, i.e. calculez la valeur moyenne sur le désordre de $\int d\omega \omega^n \rho(\omega)$ pour $n = 0, 1$.

b) Calculez aussi $\rho(\omega)$ lorsque la chaîne est ordonnée, i.e. $x = 1$.

23.0.4 Développement du locateur dans les systèmes désordonnés.

Soit une particule sur un réseau où l'énergie potentielle sur chaque site i est aléatoire (L'espace des positions est maintenant discret et les intégrales peuvent être remplacées par des sommes).

a) Décrivez dans l'espace des positions les diagrammes pour la théorie des perturbations permettant de calculer G_{ii} lorsque le potentiel joue le rôle de H_0

—diagonal dans l'espace des positions i— et les éléments de matrice H_{ij} de la perturbation sont non-nuls seulement lorsque deux sites i et j sont premiers voisins. Il n'est pas nécessaire de faire la moyenne sur le désordre.

b) Comment définirait-on la self-énergie de Dyson pour G_{ii}, toujours sans faire la moyenne sur le désordre?

23.0.5 Une impureté dans un réseau: état lié, résonnance, matrice T.

Considérons des électrons qui n'interagissent pas l'un avec l'autre mais qui sautent d'un site à l'autre sur un réseau. Les intégrales sur la position deviennent des sommes discrètes. On suppose ce réseau invariant sous translation et on note les éléments de matrice de l'Hamiltonien $\langle i| H |j\rangle = t_{ij}$ sauf pour une impureté, située à l'origine, caractérisée par un potentiel V local. À partir de l'équation de Lippmann-Schwinger, on voit que l'équation du mouvement pour la fonction de Green retardée dans ce cas est

$$\sum_{\ell} \left(\delta_{i,\ell}\left(\omega + i\eta\right) - t_{i\ell}\right) G^R\left(\ell, j; \omega\right) = \delta_{i,j} + \delta_{i,0} V G^R\left(0, j; \omega\right) \tag{23.6}$$

On suppose qu'on connaît la solution du problème lorsque l'impureté est absente, *i.e.* qu'on connaît

$$\sum_{\ell} \left(\delta_{i,\ell}\left(\omega + i\eta\right) - t_{i\ell}\right) G_0^R\left(\ell, j; \omega\right) = \delta_{i,j} \tag{23.7}$$

a) Utilisant ce dernier résultat, montrez que

$$G^R\left(i, j; \omega\right) = G_0^R\left(i, j; \omega\right) + G_0^R\left(i, 0; \omega\right) V G^R\left(0, j; \omega\right) \tag{23.8}$$

b) Résolvez l'équation précédente pour $G^R\left(0, j; \omega\right)$ en posant $i = 0$ puis démontrez que dans le cas général

$$G^R\left(i, j; \omega\right) = G_0^R\left(i, j; \omega\right) + G_0^R\left(i, 0; \omega\right) T^R\left(0, 0; \omega\right) G_0^R\left(0, j; \omega\right) \tag{23.9}$$

où la matrice T est définie par

$$T^R\left(0, 0; \omega\right) = \frac{V}{1 - V G_0^R\left(0, 0; \omega\right)} \tag{23.10}$$

La matrice T tient compte exactement de la diffusion provoquée par l'impureté. Dans le cas de l'approximation de Born, il n'y aurait eu que le numérateur pour la matrice T.

Nous allons calculer maintenant la densité d'états locale sur l'impureté.

c) Démontrez d'abord que les pôles $G_0^R\left(0, 0; \omega\right)$ du problème sans impureté n'apparaissent plus directement dans ceux du nouveau propagateur $G^R\left(0, 0; \omega\right)$ et que les pôles de ce dernier sont plutôt situés là où

$$1 - V G_0^R\left(0, 0; \omega\right) = 0 \tag{23.11}$$

d) Posons ($\hbar = 1$)

$$G_0^R\left(0, 0; \omega\right) = \frac{1}{N} \sum_{\mathbf{k}=\mathbf{1}}^{N} \frac{1}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \tag{23.12}$$

où les $\varepsilon_{\mathbf{k}}$ sont les énergies propres du système sans impureté. En ne dessinant qu'un petit nombre des valeurs de $\varepsilon_{\mathbf{k}}$ possibles et en notant que celles-ci sont très près

l'une de l'autres (distantes de $O(1/N)$), montrez graphiquement que les nouveaux pôles donnés par la solution de $1 - V \operatorname{Re} G_0^R(0,0;\omega) = 0$ ne sont que légèrement déplacés par rapport à la position des anciens pôles, sauf pour un nouvel état lié (ou anti-lié) qui peut se situer loin de l'un ou de l'autre des bords de l'ancienne bande à condition que $V \geq V_0$ ou $V \leq V_0'$. Pour ce dernier calcul, on utilise la limite $N = \infty$,

$$\frac{1}{N} \sum_{\mathbf{k=1}}^{N} \rightarrow \int N(\varepsilon)\, d\varepsilon \tag{23.13}$$

et les définitions

$$\frac{1}{V_0} \equiv \int \frac{N(\varepsilon)\, d\varepsilon}{\omega_B - \varepsilon} \quad ; \quad \frac{1}{V_0'} \equiv \int \frac{N(\varepsilon)\, d\varepsilon}{\omega_{B'} - \varepsilon} \tag{23.14}$$

ω_B et $\omega_{B'}$ étant respectivement définies comme les fréquences supérieures et inférieures des bords de la bande .

e) Montrez que la densité d'états locale sur l'impureté est donnée par

$$\frac{N(\omega)}{\left[1 - V\mathcal{P}\int \frac{N(\varepsilon)d\varepsilon}{\omega - \varepsilon}\right]^2 + V^2\pi^2 N(\omega)^2} \tag{23.15}$$

Par rapport à la densité d'états $N(\omega)$ de la bande originale, cette densité d'états est donc augmentée ou réduite, selon que le dénominateur est plus petit ou plus grand que l'unité. En particulier, même lorsqu'il n'y a pas d'état lié ou anti-lié, il est quand même possible qu'il y ait une forte augmentation de la densité d'états pour une énergie située à l'intérieur de la bande. La position de la résonnance ω_r est donnée par

$$1 - V\mathcal{P}\int \frac{N(\varepsilon)\, d\varepsilon}{\omega_r - \varepsilon} = 0 \tag{23.16}$$

et sa largeur est approximativement donnée par $V\pi N(\omega_r)$.

f) À partir du résultat précédent, montrez qu'en dehors de l'ancienne bande, c'est-à-dire là où $N(\omega) \rightarrow 0$, une fonction delta apparaît dans la densité d'états lorsqu'il y a un état lié ou anti-lié et calculez le poids de cette fonction delta. Laissez les résultats sous forme d'intégrale sans les évaluer explicitement.

23.0.6 Diffusion sur des impuretés. Résistance résiduelle des métaux.

Continuons le problème de la diffusion d'une particule sur des impuretés abordé précédemment. Supposez qu'on s'intéresse à des quantités de mouvement et des énergies près de la surface de Fermi d'un métal. ($d = 3$) Mesurant l'énergie par rapport à la surface de Fermi, on a alors comme propagateur non-perturbé

$$G_0^R(\mathbf{k}, \omega) = \frac{1}{\omega + i\eta - \xi(\mathbf{k})}$$

où $\xi(\mathbf{k}) \equiv (\epsilon(\mathbf{k}) - \mu)$ avec $\epsilon(\mathbf{k}) = k^2/2m$ et μ le potentiel chimique.

Dans tous les calculs qui suivent vous pouvez faire l'approximation que les contributions principales viennent des énergies près du niveau de Fermi. Cela veut dire que vous pouvez partout faire la substitution

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \approx N(0) \int_{-\infty}^{\infty} d\xi$$

où $N(0)$ est la densité d'états au niveau de Fermi, que l'on prend constante. Dans le cas où l'intégrale sur ξ ne converge pas, on régularise de la façon suivante

$$N(0)\int_{-E_0}^{E_0} d\xi$$

où E_0 est une coupure de l'ordre de l'énergie de Fermi.

a) Calculez explicitement la valeur de la règle de somme $Tr[H]$ pour ce problème de diffusion sur un potentiel aléatoire.

b) Calculez les parties réelle et imaginaire de $\sum^R(\mathbf{k},\omega)$ dans l'approximation illustrée sur la figure 23-2

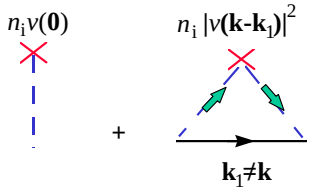


Figure 23-2 Second-order irreducible self-energy in the impurity averaging technique.

en prenant une fonction delta ($v(\mathbf{r}) = u\boldsymbol{\delta}(\mathbf{r})$) pour le potentiel diffuseur. Exprimez le résultat en fonction de la densité d'états.

c) En négligeant toute dépendance en $\mathbf{k}$ et ω de $\sum(\mathbf{k},\omega)$, vérifiez que dans cette approximation, les deux règles de somme sur $G^R(\mathbf{k},\omega)$ correspondant à $Tr\left[H^0\right] = Tr[1]$ et à $Tr[H]$ sont satisfaites, mais qu'aucune autre ne l'est.

d) En approximant encore la self-énergie par une constante indépendante de $\mathbf{k}$ et ω, prenez la transformée de Fourier du résultat que vous avez trouvé pour $G^R(\mathbf{k},\omega)$ et calculez $G^R(\mathbf{k},t)$. (N.B. Il est utile de définir un temps de relaxation pour votre résultat en vous basant sur des considérations dimensionnelles.) Donnez une interprétation physique de votre résultat pour $G^R(\mathbf{k},t)$.

e) Supposons que dans le diagramme de ci-haut qui contient une fonction de Green, on fait une approximation auto-cohérente, i.e. on utilise la fonction de Green "habillée" plutôt que la fonction de Green des particules libres. Montrez que, moyennant des hypothèse raisonnables, les résultats précédents ne sont pas vraiment modifiés.

f) Dessinez quelques-uns des diagrammes de la série de perturbation originale pour la self-énergie que l'approximation auto-cohérente décrite ci-dessus resomme automatiquement.

Part IV

The one-particle Green's function at finite temperature

In the many-body context we need to find a generalization of the Green's function that will reduce to that found for the one-body Schrödinger equation in the appropriate limit. This object comes in naturally from two perspectives. From the experimental point of view, a photoemission experiment probes the Green's function in the same way that our scattering experiment at the very beginning probed the density-density correlation function. Just from an experimental point of view then, it is important to define that quantity. From the theoretical point of view, any quantum mechanical calculation of a correlation function involves the Green's function as an intermediate step. That is one more reason to want to know more about it.

I will begin with a brief recall of second quantization and then move on to show that to predict the results of a photoemission experiment, we need a Green's function. We will establish the correspondance with the Green's function we already know. When there are interactions, one needs perturbation theory to treat the problem. Time-ordered products come in naturally in that context. Such time-ordered products motivate the definition of the Matsubara Green's function at finite temperature. The finite temperature formalism is more general and not more difficult than the zero-temperature one. We will once more spend some time on the interpretation of the spectral weight, develop some formulas for working with the Fourier series representation of the imaginary time functions (Matsubara frequencies). This should put us in a good position to start doing perturbation theory, which is all based on Wick's theorem. Hence, we will spend some time proving this theorem as well as the very general linked-cluster theorem that is very useful in practice.

24. MAIN RESULTS FROM SECOND QUANTIZATION

One of the most important results of quantum mechanics is that identical particles are indistinguishible: we cannot tell that a specific electron is at a given coordinate, we can just say that one electron is at that coordinate. Even in statistical mechanics, this indistinguishibility is important. This means that the wave function, say $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ behaves in s specific way if coordinates are interchanged: If $\mathbf{r}_1$ takes any particular value, say $\mathbf{a}$, and $\mathbf{r}_2$ takes another value, say $\mathbf{b}$, then they are indistinguishible, i.e. $\psi(\mathbf{a}, \mathbf{b}, \mathbf{r}_3) = \psi(\mathbf{b}, \mathbf{a}, \mathbf{r}_3)$. But that is not the only possibility since the only thing we know for sure is that if we exchange twice the coordinates of two particles then we should return to the same wave function. This means that under one permutation of two coordinates (exchange), the wave function can not only stay invariant, or have an eigenvalue of $+1$ as in the example we just gave, it can also have an eigenvalue of -1. These two cases are clearly the only possibilities and they correspond respectively to bosons and fermions. There are more possibilities in two dimensions, but that is beyond the scope of this chapter.

When dealing with many identical particles, a basis of single-particle states is most convenient. Given what we just said however, it is clear that a simple direct product such as $|\alpha_1\rangle \otimes |\alpha_2\rangle$ cannot be used without further care because many-particle states must be symmetrized or antisymmetrized depending on whether we deal with bosons or fermions. For example, for two fermions an acceptable wave function would have the form $\sqrt{2}^{-1} \langle \mathbf{r}_1| \otimes \langle \mathbf{r}_2| \left[|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle \right]$. Second quantization allows us to take into account these symmetry or antisymmetry properties in a straightforward fashion. To take matrix elements directly between wave functions would be very cumbersome.

The single-particle basis state is a complete basis that is used most often. Note however that a simple wave-function such as

$$\psi(x, y) = (x - y) N e^{-|x-y|/a} \tag{24.1}$$

for two electrons in one dimension, with N and a constants, is a perfectly acceptable antisymmetric wave function. To expand it in a single-particle basis state however requires a sum over many (in general an infinite number of) antisymmetrized one-particle states. There are cases, such as the quantum Hall effect, where working directly with wave functions is desirable, but for our purposes this is not so.

Remark 173 *Second quantization as we introduce it in this chapter looks like just a convenient trick to work with many particles. Second and first quantization are completely equivalent. In first quantization, we start with particles, set up commutation relations between position and momentum, and end up with a wave function. Second quantization can be seen as starting from a wave function, or field , setting up commutation relations with the conjugate field and ending up with particles, or excitations of that field. With the electromagnetic field, in a sense we do not have the choice to do this. The next chapter will introduce the formal way to set up second quantization from first principles.*

Remark 174 *In some ways, second quantization is the perfect formalism to see*

wave-particle duality. A state will be defined by having an integer number of creation operator acting on the vacuum. Each operator creates a particle, but that particle is in a state that can be a plane wave for example. And even "worse". The many-body state can be a superposition of N particles in momentum eigenstates plus N particles in position eigenstates, to take an extreme example.

24.1 Fock space, creation and annihilation operators

As is often the case in mathematics, working in a space that is larger than the one we are interested in may simplify matters. Think of the use of functions of a complex variable to do integrals on the real axis. Here we are interested most of the time in Hamiltonians that conserve the number of particles. Nevertheless, it is easier to work in a space that contains an arbitrary number of particles. That is Fock space. Annihilation and creation operators allow us to change the number of particles while preserving indistinguishability and antisymmetry. In this representation, a three-electron state comes out as three excitations of the same vacuum state $|0\rangle$, a rather satisfactory state of affairs since it looks very much from what we know from the quantized harmonic oscillator. Particles in that context correpond simply to transitions from the ground state to excited states. To go to the third excited state, we need three particles.

It will be very helpful if you review creation-annihilation operators, also called ladder operators, in the context of the harmonic oscillator.

24.1.1 Creation-annihilation operators for fermion wave functions

For the time being our fermions *are spinless, it will be easy to add spin later on.* We assume that the one-particle states $|\alpha_i\rangle$ form an orthonormal basis for one particle, namely $\langle\alpha_i|\,\alpha_j\rangle = \delta_{i,j}$. The notation is that α denotes the basis whose components are labeled by the index. α_1 is the first state, α_2 the second state etc.

What concerns us here are many-body states. The state $|\alpha_1\alpha_2\rangle$ with two fermions is antisymmetrized, namely

$$|\alpha_1\alpha_2\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle\right).$$

The first Hilbert space on the right of the above expression can be either in state α_1 or α_2. Antisymmetry means that $|\alpha_1\alpha_2\rangle = -\,|\alpha_2\alpha_1\rangle$.

We define a vaccum $|0\rangle$ that contains no particle. Then, we define $a^\dagger_{\alpha_1}$ that creates a particle from the vacuum to put it in state $|\alpha_1\rangle$ and for fermions it antisymmetrizes that state will all others. In other words, $a^\dagger_{\alpha_1}|0\rangle = |\alpha_1\rangle$. Up to now, there is nothing to antisymmetrize with, but if we add another particle,

$$a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}|0\rangle = |\alpha_1\alpha_2\rangle$$

then that state has to be antisymmetric. In other words, we need to have $|\alpha_2\alpha_1\rangle = -\,|\alpha_1\alpha_2\rangle$, or

$$|\alpha_2\alpha_1\rangle = a^\dagger_{\alpha_2}a^\dagger_{\alpha_1}|0\rangle = -\,|\alpha_1\alpha_2\rangle = -a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}|0\rangle.$$

Clearly this will automatically be the case if we impose that the creation operators anticommute, i.e. $a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} = -a^\dagger_{\alpha_j} a^\dagger_{\alpha_i}$ or

$$\left\{a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \equiv a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j} a^\dagger_{\alpha_i} = 0. \tag{24.2}$$

This property is a property of the operators, independently of the specific state they act on. The anticommutation property garantees the Pauli exclusion principle as we know it, since if $i = j$ then the above leads to

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_i} = -a^\dagger_{\alpha_i} a^\dagger_{\alpha_i}. \tag{24.3}$$

The only operator that is equal to minus itself is zero. Hence we cannot create two particles in the same state.

If we want the whole formalism to make sense, we want to have a sign change to occur whenever we interchange two fermions, wherever they are in the list. In other words, we want $|\alpha_i \alpha_j \dots \alpha_k \dots \alpha_l \dots \alpha_m\rangle = -|\alpha_i \alpha_j \dots \alpha_l \dots \alpha_k \dots \alpha_m\rangle$. To see that our formalism works, you can write the state to the left in terms of creation operators on the vacuum

$$|\alpha_i \alpha_j \dots \alpha_k \dots \alpha_l \dots \alpha_m\rangle = a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} \dots a^\dagger_{\alpha_k} \dots a^\dagger_{\alpha_l} \dots a^\dagger_{\alpha_m} |0\rangle . \tag{24.4}$$

If there are n operators between $a^\dagger_{\alpha_k}$ and $a^\dagger_{\alpha_l}$, we pay a $(-1)^n$ to place $a^\dagger_{\alpha_k}$ to the left of $a^\dagger_{\alpha_l}$. Then there is a (-1) to interchange $a^\dagger_{\alpha_k}$ and $a^\dagger_{\alpha_l}$, and finally another $(-1)^n$ to take $a^\dagger_{\alpha_l}$ where $a^\dagger_{\alpha_k}$ was. Since $(-1)^{2n} = 1$, there is only the minus sign from the "local" interchange $a^\dagger_{\alpha_k}$ and $a^\dagger_{\alpha_l}$ that is left.

Note that with fermions we need to determine an initial order of operators for the states. That is totally arbitrary because of the phase arbitrariness of quantum mechanics. But then, during the calculations we need to keep track of the minus signs.

Now that we know how to create, let us move to destruction. The destruction operators are the adjoints of $a^\dagger_{\alpha_i}$. Their anticommutation property follows by taking the adjoint of $\left\{a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right\} = 0$:

$$\left\{a_{\alpha_i}, a_{\alpha_j}\right\} \equiv a_{\alpha_i} a_{\alpha_j} + a_{\alpha_j} a_{\alpha_i} = 0. \tag{24.5}$$

These adjoint operators are defined as follows

$$\langle \alpha_1| = \langle 0| a_{\alpha_1}. \tag{24.6}$$

They create and antisymmetrize in bras instead of kets. When they act on kets instead of bras, they remove a particle instead of adding it. In particular,

$$a_{\alpha_1} |0\rangle = 0. \tag{24.7}$$

This is consistent with $\langle \alpha_1|\, 0\rangle = 0 = \langle 0| a_{\alpha_1} |0\rangle$.

Since we also want states to be normalized, we need

$$\langle \alpha_i|\, \alpha_j\rangle = \langle 0| a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = \delta_{i,j}. \tag{24.8}$$

Since we already know that $a_{\alpha_1} |0\rangle = 0$, that will automatically be satisfied if we write the following anticommutation relation between creation and annihilation operators

$$\left\{a_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \equiv a_{\alpha_i} a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j} a_{\alpha_i} = \delta_{i,j} \tag{24.9}$$

because then $\langle 0| a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = -\langle 0| a^\dagger_{\alpha_j} a_{\alpha_i} |0\rangle + \langle 0| \delta_{i,j} |0\rangle = 0 + \delta_{i,j}$. The above three sets of anticommutation relations are called canonical.

At this point one may ask why anticommutation instead of commutation. Well, two reasons. The first one is that given the previous anticommutation rules, this choice seems elegant. The second one is that with this rule, we can define the very useful operator, the number operator

$$\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{24.10}$$

That operator just counts the number of particles in state α_i. To see that this is so and that anticommutation is needed for this to work, we look at a few simple cases. First note that if $\widehat{n}_{\alpha_i}$ acts on a state where α_i is not occupied, then

$$\widehat{n}_{\alpha_i} |\alpha_j\rangle = \widehat{n}_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = -a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_i} |0\rangle = 0. \tag{24.11}$$

In an arbitrary many-particle state $|\alpha_j, \alpha_k, \ldots\rangle$, if the state α_i does not appear in the list, then when I compute $\widehat{n}_{\alpha_i} |\alpha_j, \alpha_k, \ldots\rangle$, I will be able to anticommute the destruction operator all the way to the vacuum and obtain zero. On the other hand, if α_i appears in the list then

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots \widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle . \tag{24.12}$$

I have been able to move the operator all the way to the indicated position without any additional minus sign because both the destruction and the annihilation operators anticommute with the creation operators that do not have the same labels. The minus signs from the creation and from the annihilation operators in $a^\dagger_{\alpha_i} a_{\alpha_i}$ cancel each other. This would not have occured if a_{α_i} and $a^\dagger_{\alpha_j}$ had commuted instead of anticommuted while a_{α_i} and a_{α_j} had anticommuted. Now, let us focus on $\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i}$ in the last equation. Using our anticommutation properties, one can check that

$$\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} \left(1 - a^\dagger_{\alpha_i} a_{\alpha_i} \right) . \tag{24.13}$$

Since there are never two fermions in the same state, now the destruction operator in the above equation is free to move and annihilate the vacuum state, and

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) . \tag{24.14}$$

This means that $\widehat{n}_{\alpha_i}$ does simply count the number of particles. It gives one or zero depending on whether the state is occupied or not.

Remark 175 *We define the bra* $\langle \alpha_1 \alpha_2 |$ *by*

$$\langle \alpha_1 \alpha_2 | = \left(|\alpha_1 \alpha_2\rangle \right)^\dagger = \left(a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle \right)^\dagger = \langle 0 | a_{\alpha_2} a_{\alpha_1}. \tag{24.15}$$

Notice the change in the order of labels between $\langle \alpha_1 \alpha_2 |$ *and* $\langle 0 | a_{\alpha_2} a_{\alpha_1}$.

24.1.2 Creation-annihilation operators for boson wave functions

In the case of bosons, the state must be symmetric. Following Negele and Orland[173] we introduce the symmetrized many-body state

$$|\alpha_1 \alpha_2 ... \alpha_N \} . \tag{24.16}$$

The state is not normalized at this point, which explains the unusual notation. The state is symmetric means that $|\alpha_1 \alpha_2 \} = |\alpha_2 \alpha_1 \} = a^\dagger_{\alpha_2} a^\dagger_{\alpha_1} |0\rangle$. Hence in this

case, the creation operators and their corresponding annihilation operators must commute:

$$\left[a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right] \equiv a^\dagger_{\alpha_i}a^\dagger_{\alpha_j} - a^\dagger_{\alpha_j}a^\dagger_{\alpha_i} = 0 \tag{24.17}$$

$$\left[a_{\alpha_i}, a_{\alpha_j}\right] \equiv a_{\alpha_i}a_{\alpha_j} - a_{\alpha_j}a_{\alpha_i} = 0. \tag{24.18}$$

This time there is no Pauli exclusion principle. Several particles can occupy the same state. So what happens when we exchange creation and annihilation operators. By analogy with the fermions, it is natural to expect that they must commute, namely

$$\left[a_{\alpha_i}, a^\dagger_{\alpha_j}\right] \equiv a_{\alpha_i}a^\dagger_{\alpha_j} - a^\dagger_{\alpha_j}a_{\alpha_i} = \delta_{i,j} \tag{24.19}$$

The above set of commutation relations is called canonical. The same considerations as before tell us that annihilation operators destroy the vacuum.

And again the number operator is defined by

$$\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i}a_{\alpha_i}. \tag{24.20}$$

Why is that true? If the state α_i is unoccupied or occupied only once, one can check the effect of the operator $\widehat{n}_{\alpha_i}$ the same way we did it for fermions. And note that when there are many other particles around, one must take commutation and not anticommutation between creation and annihilation operators to make sure that the many-particle state is an eigenstate of $\widehat{n}_{\alpha_i}$ with eigenvalue unity when a single state is occupied.

What happens if the same state is occupied multiple times? Then,

$$\widehat{n}_{\alpha_i}a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i}a_{\alpha_i}a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i}\left(1 + a^\dagger_{\alpha_i}a_{\alpha_i}\right) \tag{24.21}$$

$$= a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i}\widehat{n}_{\alpha_i}. \tag{24.22}$$

The destruction operator in $\widehat{n}_{\alpha_i}$ will not be able to complete its journey to the vacuum to annihilate it. Every time it encounters an operator $a^\dagger_{\alpha_i}$ it leaves it behind and adds a new term $a^\dagger_{\alpha_i}\widehat{n}_{\alpha_i}$ just like above. Once we have done that repeatedly, the destruction operator accomplishes its task and we are left with n_{α_i} times the original state, where n_{α_i} is the number of times the label α_i appeared in the list. So $\widehat{n}_{\alpha_i}$ really has the meaning of a number operator, i.e. an operator that counts the number of times a given label appears in a many-body state. All that we are left to do is normalize the symmetrized state.

24.1.3 Number operator and normalization

To fix the normalization in the case of bosons, it suffices to consider a single state that can be multiply occupied and then to generalize. Let us drop then all indices and ask how the state $\left(a^\dagger\right)^n|0\rangle$ can be normalized. First, notice that Eq.(24.22) above can be written as

$$\boxed{\left[\widehat{n}, a^\dagger\right] = a^\dagger} \tag{24.23}$$

By the way, using the fact that $\left(a^\dagger\right)^2 = 0$ on the right-hand side of Eq.(24.13) we see that the latter equation is true for fermions as well. Taking the adjoint of the above equation we find

$$\boxed{\left[\widehat{n}, a\right] = -a} \tag{24.24}$$

The above two equations are very important identities that we will use over and over again.

We can now use a very useful theorem that is trivial to prove. We will call it the theorem on commutators of ladder operators.

Theorem 14 *Let $|n\rangle$ be an eigenstate of $\widehat{n}$ with eigenvalue n. If $\left[\widehat{n}, a^\dagger\right] = Ba^\dagger$ with B a real or complex number, then $a^\dagger |n\rangle$ is an eigenstate of $\widehat{n}$ with eigenvalue $n + B$.*

Proof: $\left[\widehat{n}, a^\dagger\right] |n\rangle = \widehat{n}\left(a^\dagger |n\rangle\right) - a^\dagger n |n\rangle = Ba^\dagger |n\rangle$, so that $\widehat{n}\left(a^\dagger |n\rangle\right) = (n + B)\left(a^\dagger |n\rangle\right)$ Q.E.D.

Using this theorem with our result for the commutator of the number operator with the creation operator Eq.(24.23) we have that $\widehat{n}\left(a^\dagger |n\rangle\right) = (n+1)\left(a^\dagger |n\rangle\right)$ hence $a^\dagger |n\rangle = C |n+1\rangle$. Assuming that $|n\rangle$ and $|n+1\rangle$ are normalized we can find the normalization constant as follows

$$\begin{aligned} \langle n| aa^\dagger |n\rangle &= |C|^2 \langle n+1 |n+1\rangle = |C|^2 \\ &= \langle n| 1 + a^\dagger a |n\rangle = (n+1) \langle n |n\rangle = (n+1). \end{aligned} \tag{24.25}$$

We are free to choose the phase real so that $C = \sqrt{n+1}$. We thus have recursively

$$\begin{aligned} a^\dagger |0\rangle &= |1\rangle \\ \left(a^\dagger\right)^2 |0\rangle &= \sqrt{2} |2\rangle \\ \left(a^\dagger\right)^3 |0\rangle &= \sqrt{3}\sqrt{2} |3\rangle \end{aligned} \tag{24.26}$$

and

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a^\dagger\right)^n |0\rangle. \tag{24.27}$$

From this we conclude that for a general many-body state,

$$\boxed{|\alpha_i \alpha_j ... \alpha_m\rangle = \frac{1}{\sqrt{\Pi_i\, n_{\alpha_i}!}} |\alpha_i \alpha_j ... \alpha_m\} = \frac{1}{\sqrt{\Pi_i\, n_{\alpha_i}!}} a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} \ldots a^\dagger_{\alpha_m} |0\rangle} \tag{24.28}$$

where the product in the denominator is over the indices that label the occupied one-particle states and n_{α_i} counts the number of times a given one-particle state appears.

Remark 176 *Since with fermions a state is occupied only once, we did not need to worry about the $n_{\alpha_i}!$.*

Remark 177 *By recalling the theorem proven in this section, it is also easy to remember that $\left[\widehat{n}, a^\dagger\right] = a^\dagger$ and $[\widehat{n}, a] = -a$.*

24.2 Change of basis

24.2.1 General case

Creation-annihilation operators change basis in a way that is completely determined by the way one changes basis in single-particle states. Suppose one wants to change from the α basis to the μ basis, namely

$$|\mu_m\rangle = \sum_i |\alpha_i\rangle \langle \alpha_i| \mu_m\rangle \tag{24.29}$$

which is found by inserting the completeness relation. Let creation operator $a^\dagger_{\alpha_i}$ create single particle state $|\alpha_i\rangle$ and antisymmetrize while creation operator $c^\dagger_{\mu_m}$

creates single particle state $|\mu_m\rangle$ and antisymmetrize. Then the correspondance between both sets of operators is clearly

$$c^\dagger_{\mu_m} = \sum_i a^\dagger_{\alpha_i} \langle \alpha_i | \mu_m \rangle \tag{24.30}$$

with the adjoint

$$c_{\mu_m} = \sum_i \langle \mu_m | \alpha_i \rangle a_{\alpha_i} \tag{24.31}$$

given as usual that $\langle \alpha_i | \mu_m \rangle = \langle \mu_m | \alpha_i \rangle^*$. Physically then, creating a particle in a state $|\mu_m\rangle$ is like creating it in a linear combination of states $|\alpha_i\rangle$. We can do the change of basis in the other direction as well.

If we define with $\langle \alpha_i | \mu_n \rangle$ a matrix for the change of basis, this matrix is unitary if $\langle \mu_m | \mu_n \rangle = \delta_{\mu_m,\mu_n}$. Indeed, inserting a complete set of states, we see that $\sum_i \langle \mu_m | \alpha_i \rangle \langle \alpha_i | \mu_n \rangle = \langle \mu_m | \mu_n \rangle = \delta_{\mu_m,\mu_n}$.

Since we have defined new creation- annihilation operators, it is quite natural to ask what are their commutation or anticommutation relations. It is easy to find using the change of basis formula and the completeness relation. Assuming that the creation-annihilation operators are for fermions, we find

$$\begin{aligned}
\left\{ c_{\mu_m}, c^\dagger_{\mu_n} \right\} &= \sum_i \sum_j \langle \mu_m | \alpha_i \rangle \left\{ a_{\alpha_i}, a^\dagger_{\alpha_j} \right\} \langle \alpha_j | \mu_n \rangle & (24.32)\\
&= \sum_i \sum_j \langle \mu_m | \alpha_i \rangle \delta_{i,j} \langle \alpha_j | \mu_n \rangle & (24.33)\\
&= \sum_i \langle \mu_m | \alpha_i \rangle \langle \alpha_i | \mu_n \rangle = \langle \mu_m | \mu_n \rangle . & (24.34)
\end{aligned}$$

Hence, if the transformation between basis is unitary, the new operators obey canonical anticommutation relations, namely

$$\left\{ c_{\mu_m}, c^\dagger_{\mu_n} \right\} = \delta_{m,n}. \tag{24.35}$$

When the change of basis is unitary, we say that we have made a canonical transformation. The same steps show that a unitary basis change also preserves the canonical commutation relations for bosons.

Remark 178 *The notation c_{μ_m}, a_{α_i} is rather clumsy. In practice, one uses, for example, f_i to label destruction operators for an f electron in a state i, d_i for d electrons, c_i for conduction electrons etc. In other words, the basis is identified by the choice of label for creation-annihilation operators, and the component by the index of that symbol.*

24.2.2 The position and momentum space basis

We recall this strange, but commonly used, basis that we have encountered in Sec.18.2.1. In this basis, we take continuum notation for space and discrete notation for momentum. Starting from $\langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')$ and $\langle \mathbf{k} | \mathbf{k}' \rangle = \delta_{\mathbf{k},\mathbf{k}'}$ it is easy to check by left or right multiplying that the following operators give the completeness relation

$$\sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| = 1 = \int d\mathbf{r} \, |\mathbf{r}\rangle \langle \mathbf{r}|$$

To go from one basis to the other, we use plane-waves that are normalized to unity in a volume $\mathcal{V}$, namely

$$\langle \mathbf{r} \, | \mathbf{k} \rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{24.36}$$

$$\langle \mathbf{k} \, | \mathbf{r} \rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{24.37}$$

We can check that $\langle \mathbf{r} \, | \mathbf{r}' \rangle$ is normalized in the continuum while $\langle \mathbf{k} \, | \mathbf{k}' \rangle$ is normalized as a discrete set of states

$$\langle \mathbf{r} \, | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} \, | \mathbf{k} \rangle \langle \mathbf{k} \, | \mathbf{r}' \rangle = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}') \tag{24.38}$$

$$\langle \mathbf{k} \, | \mathbf{k}' \rangle = \int d\mathbf{r} \langle \mathbf{k} \, | \mathbf{r} \rangle \langle \mathbf{r} \, | \mathbf{k}' \rangle = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')} = \delta_{\mathbf{k},\mathbf{k}'} \ . \tag{24.39}$$

To take the continuum limit of the discrete sum over $\mathbf{k}$, one uses eigenstates of momentum in a box where the separation between states is given by $\Delta k_x = 2\pi/L_x$, where L_x is the size of the box in the x direction, and similarly for the other directions.

Creation operators in eigenstates of position are usually denoted, $\psi^\dagger(\mathbf{r})$, while creation operators in eigenstates of momentum are denoted $c^\dagger_{\mathbf{k}}$. The basis change between them leads to

$$\psi^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} \langle \mathbf{k} \, | \mathbf{r} \rangle = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{24.40}$$

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} \langle \mathbf{r} \, | \mathbf{k} \rangle c_{\mathbf{k}} = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}}. \tag{24.41}$$

Given our above convention, the momentum operators obey the algebra of a discrete set of creation operators. Taking fermions as an example, we then have

$$\boxed{\left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = \delta_{\mathbf{k},\mathbf{k}'} \quad ; \quad \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = \left\{c^\dagger_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = 0} \tag{24.42}$$

while the position space creation-annihilation operators obey

$$\boxed{\left\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle \mathbf{r} \, | \mathbf{k} \rangle \left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} \langle \mathbf{k}' \, | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} \, | \mathbf{k} \rangle \langle \mathbf{k} \, | \mathbf{r}' \rangle = \langle \mathbf{r} \, | \mathbf{r}' \rangle = \delta(\mathbf{r}-\mathbf{r}')} \tag{24.43}$$

$$\boxed{\{\psi(\mathbf{r}), \psi(\mathbf{r}')\} = \left\{\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = 0} \tag{24.44a}$$

24.3 Wave functions

With N-particles, the wave function is obtained by projection on a position basis. If we have a single many-body state, $|\Phi\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_N} |0\rangle$ then the correspondance between first and second quantized description is in a sense contained in the following expression

$$\langle \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N | \ \Phi \rangle = \langle \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N | \ \alpha_1 \alpha_2 ... \alpha_N \rangle = \langle 0 | \psi(\mathbf{r}_N) \ldots \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_N} |0\rangle$$

which is proportional to a so-called Slater determinant if we have fermions. Indeed, using our change of basis formula,

$$\psi(\mathbf{r}) = \sum_i \langle \mathbf{r} | \alpha_i \rangle a_{\alpha_i} = \sum_i \phi_{\alpha_i}(\mathbf{r}) a_{\alpha_i} \tag{24.45}$$

any of the positions $\mathbf{r}$ can be in a state α_i, or vice versa the position $\mathbf{r}$ has amplitudes on all states, so you can check that the (unnormalized) wave function is equal to

$$\sum_p \varepsilon_p \phi_{\alpha_{p(1)}}(\mathbf{r}_1) \phi_{\alpha_{p(2)}}(\mathbf{r}_2) ... \phi_{\alpha_{p(N)}}(\mathbf{r}_N) = \text{Det} \begin{bmatrix} \phi_{\alpha_1}(\mathbf{r}_1) & \phi_{\alpha_1}(\mathbf{r}_2) & ... & \phi_{\alpha_1}(\mathbf{r}_N) \\ \phi_{\alpha_2}(\mathbf{r}_1) & \phi_{\alpha_2}(\mathbf{r}_2) & ... & \phi_{\alpha_2}(\mathbf{r}_N) \\ ... & ... & ... & \\ \phi_{\alpha_N}(\mathbf{r}_1) & \phi_{\alpha_N}(\mathbf{r}_2) & & \phi_{\alpha_N}(\mathbf{r}_N) \end{bmatrix} \tag{24.46}$$

where the sum is over all permutations $p(i)$ of the set i and ε_p is the signature of the permutation, given by $+1$ if the number of transpositions (interchanges) of pairs of creation operators to get back to the original order is even and -1 if the number of transpositions is odd.

Remark 179 *Closure relation and normalization:*

$$\boxed{\frac{1}{N!} \int d\mathbf{r}_1 d\mathbf{r}_2 ... d\mathbf{r}_N |\mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N\rangle \langle \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N|} \tag{24.47}$$

This closure relation implies that if we want to recover the usual expression for normalized wave functions, $\langle \Phi | \Phi \rangle = 1$, the determinant above should be multiplied by $1/\sqrt{N!}$. We recover our example with two particles where the normalization is $1/\sqrt{2}$.

Remark 180 *Many-Body wave function and basis states: It is very important to note that the most general state must be written as a linear combination of the states $a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_i} \dots a^\dagger_{\alpha_N} |0\rangle$ or of the above Slater determinants. In other words, a general many body state $|\Phi\rangle$ must be expanded as*

$$|\Phi\rangle = \sum_{i,j,...\ell,...} C^{i,j,...\ell,...} \left(a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} \dots a^\dagger_{\alpha_\ell} \dots |0\rangle \right) \tag{24.48}$$

where $C^{i,j,...\ell,...}$ are expansion coefficients. In a way, the Feynman diagrams that we will encounter are a way to write the various components of a general state.

Remark 181 *Wave functions live in Hilbert space: It is important to note that the (unnormalized) wave function*

$$\psi_{\alpha_1 \alpha_2 ... \alpha_N}(\mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N) = \langle \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N | \, \alpha_1 \alpha_2 ... \alpha_N \rangle$$

propagates, so to speak, in Hilbert space, not in ordinary space. The waves that we are familiar with in the classical world are functions of only the three spatial coordinates. Not so for the Schrödinger wave, unless there is a single particle to describe.

Remark 182 *One-particle wave function: The quantity $\psi_{\alpha_1 \alpha_2 ... \alpha_N}(\mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N)$ is often-called a one-particle wave function in the sense that it is just one member of a complete set of states where all particles are independent. The most general state $|\Phi\rangle$ above contains correlations, in addition to those induced by symmetrization or antisymmetrization.*

Remark 183 *Particles and waves: In $\psi_{\alpha_1 \alpha_2 ... \alpha_N}(\mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N)$ we see the wave, but we also see that there are N particles. And we need all this information to describe the system. The continuous and discrete aspects are present all at once.*

Remark 184 *For bosons, the expression is similar, but we compute the determinant without the signs coming from the permutations. This is called a permanent. The normalization will also have the* $1/\sqrt{N!}$ *coming from the closure relation in addition to the prefactor* $1/\sqrt{\prod_i n_{\alpha_i}!}$ *that we found in Eq. (24.28).*

24.4 One-body operators

The matrix elements of an arbitrary one-body operator $\widehat{U}$ (in the $N-$particle case) may be computed in the many-body basis made of one-body states where $\widehat{U}$ is diagonal. As an example of one-body operator, the operator $\widehat{U}$ could be an external potential so that the diagonal basis is position space. In the diagonal basis,

$$\widehat{U}\left|\alpha_i\right\rangle = U_{\alpha_i}\left|\alpha_i\right\rangle = \left\langle\alpha_i\right|\widehat{U}\left|\alpha_i\right\rangle\left|\alpha_i\right\rangle \tag{24.49}$$

where U_{α_i} is the eigenvalue. In this basis, one sees that the effect of the one-body operator is to produce the same eigenvalue, whatever the particular order of the states on which the first-quantized operator acts. For example, suppose we have three particles in an external potential, then the potential-energy operator is

$$V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right) \tag{24.50}$$

where $\mathbf{R}_i$ is an operator thatracts on the i^{th} position of the many body state. If this state is not symmetrized or antisymmetrized, then for example

$$\left(V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right)\right)\left|\mathbf{r}'\right\rangle\otimes\left|\mathbf{r}\right\rangle\otimes\left|\mathbf{r}''\right\rangle = \left(V\left(\mathbf{r}'\right) + V\left(\mathbf{r}\right) + V\left(\mathbf{r}''\right)\right)\left|\mathbf{r}'\right\rangle\otimes\left|\mathbf{r}\right\rangle\otimes\left|\mathbf{r}''\right\rangle \tag{24.51}$$

where $\mathbf{r}$ are labels, not operators. If that operator $V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right)$ had acted on another ordering such as $\left|\mathbf{r}\right\rangle \otimes \left|\mathbf{r}''\right\rangle \otimes \left|\mathbf{r}'\right\rangle$, the eigenvalue would have been identical, $V\left(\mathbf{r}\right) + V\left(\mathbf{r}''\right) + V\left(\mathbf{r}'\right)$. This means that if we act on a symmetrized or antisymmetrized version of that state, then

$$\left(V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right)\right)\left|\mathbf{r}', \mathbf{r}, \mathbf{r}''\right\rangle = \left(V\left(\mathbf{r}'\right) + V\left(\mathbf{r}\right) + V\left(\mathbf{r}''\right)\right)\left|\mathbf{r}', \mathbf{r}, \mathbf{r}''\right\rangle \tag{24.52}$$

In general then when we have N particles in a many-body state, the action of the one-body operator is

$$\sum_{\mu=1}^{N}\widehat{U}_\mu\left|\alpha_i, \alpha_j, \alpha_k \ldots\right\rangle = \left(U_{\alpha_i} + U_{\alpha_j} + U_{\alpha_k} + \ldots\right)\left|\alpha_i, \alpha_j, \alpha_k \ldots\right\rangle \tag{24.53}$$

Knowing the action of the number operator, we can write the same result differently

$$\sum_{\mu=1}^{N}\widehat{U}_\mu\left|\alpha_i, \alpha_j, \alpha_k \ldots\right\rangle = \sum_{m=1}^{\infty} U_{\alpha_m}\widehat{n}_{\alpha_m}\left|\alpha_i, \alpha_j, \alpha_k \ldots\right\rangle \tag{24.54}$$

in other words, there will be a contribution as long as α_i appears in the state. And if α_i occurs more than once, the corresponding eigenvalue U_{α_i} will appear more than once. Note also that I have assumed that there there is an infinite number of basis states $\left|\alpha_m\right\rangle$.

We hold a very elegant result. The one-body operator $\sum_m U_{\alpha_m}\widehat{n}_{\alpha_m}$ in second quantized notation makes no reference to the total number of particles nor to whether we are dealing with bosons or fermions. Note that in first quantization

the sum extends over all particle coordinates whereas in second quantization the sum over m extends over all *states*.

Using the change of basis formula explained above, we have that

$$\sum_i \langle \alpha_i | \widehat{U} | \alpha_i \rangle a^\dagger_{\alpha_i} a_{\alpha_i} = \sum_i \sum_m \sum_n c^\dagger_{\mu_m} \langle \mu_m | \alpha_i \rangle \langle \alpha_i | \widehat{U} | \alpha_i \rangle \langle \alpha_i | \mu_n \rangle c_{\mu_n}. \quad (24.55)$$

Since U is diagonal, we can add a sum over α_j and use the closure relation to arrive at the final result

$$\boxed{\sum_i U_{\alpha_i} \widehat{n}_{\alpha_i} = \sum_m \sum_n c^\dagger_{\mu_m} \langle \mu_m | \widehat{U} | \mu_n \rangle c_{\mu_n}.} \quad (24.56)$$

Let us give examples in the position and momentum representation. A one-body scattering potential in the continuum would be represented in second quantized version[1] by

$$\boxed{\widehat{U} = \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})} \quad (24.57)$$

which looks similar to the usual Schrödinger average. Similarly, the kinetic energy operator in the momentum representation is diagonal and it can be rewritten in the position basis using the change of variables of the previous section.

$$\widehat{T} = \sum_{\mathbf{k}} \langle \mathbf{k} | \frac{k^2}{2m} | \mathbf{k} \rangle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} = \sum_{\mathbf{k}} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \frac{k^2}{2m} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle \psi(\mathbf{r}') \quad (24.58)$$

$$= \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \frac{k^2}{2m} \psi(\mathbf{r}') \quad (24.59)$$

$$= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \left(-\frac{1}{2m} \nabla^2_{\mathbf{r}'} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \right) \psi(\mathbf{r}') \quad (24.60)$$

$$= \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \left(-\frac{1}{2m} \nabla^2_{\mathbf{r}'} \delta(\mathbf{r}-\mathbf{r}') \right) \psi(\mathbf{r}') \quad (24.61)$$

Using partial integration and assuming that everything vanishes at infinity or is periodic, we obtain,

$$\boxed{\widehat{T} = \left(-\tfrac{1}{2m}\right) \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \left(\nabla^2 \psi(\mathbf{r})\right) = \tfrac{1}{2m} \int d\mathbf{r} \boldsymbol{\nabla} \psi^\dagger(\mathbf{r}) \cdot \nabla \psi(\mathbf{r})}. \quad (24.62)$$

Again notice that second-quantized operators look like simple Schrödinger averages over wave functions.

24.5 Number operator and the nature of states in second quantization

This section is nothing new compared with what we already know, but it gives a different perspective on the whole formalism. Once an operator (the "single-particle" Hamiltonian for example) is in the diagonal form $\sum_i H_{\alpha_i} \widehat{n}_{\alpha_i}$, the theorem on commutators of ladder operators (24.1.3) can be used to find its eigenstates.

[1] We have denoted by $\widehat{U}$ the operator in both first and second quantization. Strictly speaking the operators are different. One needs to specify which representation one is working in.

Indeed, this theorem tells that if $|n\rangle$ is an eigenstate of $\widehat{n}_{\alpha_i}$, then $a^\dagger_{\alpha_i}|n\rangle$ is an eigenstate with eigenvalue $n+1$. If a ground state exists, this means that there is a state (the vacuum) which is such that $a_{\alpha_i}|0\rangle = 0$, in other words we cannot decrease the eigenvalue indefinitely if U_{α_i} for example is the Hamiltonian. Hence, the eigentates are of the form $a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_N}|0\rangle$ for N particles. This is analogous to what we have discussed for the harmonic oscillator.

It is important to note that these states form a complete set of many-body states. The most general eigenstate will be a linear combination of such states.

Remark 185 *The need to diagonalize: Note that to find the eigenstates of* $\sum_m \sum_n c^\dagger_{\mu_m} \langle \mu_m | \widehat{H} | \mu_n \rangle c_{\mu_n}$, *we need to diagonalize the matrix* $\langle \mu_m | \widehat{H} | \mu_n \rangle$. *The rules have not changed!*

24.6 Going backwards from second to first quantization

To convince ourselves that the field operators become wave functions in the special case of a single particle, consider the operator $\hat{U}$ of the previous section that is diagonal in the position basis. Then, the expectation value of that operator in a general N particle many-body state is $\langle \Phi | \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) | \Phi \rangle$. Inserting a complete set of states between the two field operators, only the states with $N-1$ particles survive so that

$$\begin{aligned} & \langle \Phi | \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) | \Phi \rangle \\ = & \frac{1}{(N-1)!} \int d\mathbf{r}_1 \ldots \int d\mathbf{r}_{N-1} \langle \Phi | \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) | \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} \rangle \langle \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} | \psi(\mathbf{r}) | \Phi \rangle \\ = & \frac{1}{(N-1)!} \int d\mathbf{r}_1 \ldots \int d\mathbf{r}_{N-1} \int d\mathbf{r} U(\mathbf{r}) \langle \Phi | \mathbf{r}, \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} \rangle \langle \mathbf{r}, \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} | \Phi \rangle . \end{aligned} \quad (24.63)$$

This last expression can be written in several suggestive ways. First, consider the form

$$\frac{1}{(N-1)!} \int d\mathbf{r} U(\mathbf{r}) \left(\int d\mathbf{r}_1 \ldots \int d\mathbf{r}_{N-1} \langle \mathbf{r}, \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} | \Phi \rangle \langle \Phi | \mathbf{r}, \mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_{N-1} \rangle \right), \quad (24.64)$$

which shows that the one-particle density matrix is obtained by tracing out the degrees of freedom that are not observed in the full density matrix $|\Phi\rangle\langle\Phi|$. In the case where $\langle\Phi|$ contains only one particle, the above expression reduces to what we expect from the one-particle Schrödinger equation, namely

$$\int d\mathbf{r} U(\mathbf{r}) \langle \mathbf{r} | \Phi \rangle \langle \Phi | \mathbf{r} \rangle = \int d\mathbf{r} U(\mathbf{r}) |\Phi(\mathbf{r})|^2 , \quad (24.65)$$

which suggests why the transformation from single-particle wave functions into field operators made sense. In the N-particle case, using the symmetry or anti-symmetry of the wave function, we can also rewrite the above expression for the average of a one-body operator Eq.(24.64) as a symmetric expression containing the most general many-body wave-function

$$\int d\mathbf{r}_1 \ldots \int d\mathbf{r}_N \sum_{i=1}^{N} U(\mathbf{r}_i) |\Phi(\mathbf{r}_1 \mathbf{r}_2 ... \mathbf{r}_N)|^2 . \quad (24.66)$$

24.7 Two-body operators.

A two-body operator involves the coordinates of two particles. An example is the Coulomb potential with position basis where $\widehat{V}_{1,2} = \widehat{V}(\mathbf{R}_1, \mathbf{R}_2)$ which is diagonal in position space, namely $\widehat{V}(\mathbf{R}_1, \mathbf{R}_2) |\mathbf{r}'\rangle \otimes |\mathbf{r}\rangle = V(\mathbf{r}', \mathbf{r}) |\mathbf{r}'\rangle \otimes |\mathbf{r}\rangle$.

Let us return to the general discussion. If we let the indices in $\widehat{V}_{1,2}$ refer to the potential energy between the first and second particles in the direct product, and if we are in the diagonal basis, we have in first quantization that

$$\widehat{V}_{1,2} |\alpha_i\rangle \otimes |\alpha_j\rangle = V_{\alpha_i\alpha_j} |\alpha_i\rangle \otimes |\alpha_j\rangle \tag{24.67}$$

$$\widehat{V}_{1,3} |\alpha_i\rangle \otimes |\alpha_j\rangle \otimes |\alpha_k\rangle = V_{\alpha_i\alpha_k} |\alpha_i\rangle \otimes |\alpha_j\rangle \otimes |\alpha_k\rangle \tag{24.68}$$

The abreviation $\widehat{V}_{1,3}$ in the position basis means $\widehat{V}(\mathbf{R}_1, \mathbf{R}_3)$ where $\mathbf{R}_1$ acts on the first one-particle Hilbert space and $\mathbf{R}_3$ acts on the third. In this basis, one sees that again the eigenvalue does not depend on the order in which the states are when the first-quantized operator acts. This means that

$$\frac{1}{2} \sum_{\mu=1}^{N} \sum_{\substack{\nu=1 \\ \nu\neq\mu}}^{N} \widehat{V}_{\mu,\nu} |\alpha_i, \alpha_j, \alpha_k \ldots\rangle = \left(V_{\alpha_i\alpha_j} + V_{\alpha_i\alpha_k} + V_{\alpha_j\alpha_k} + \ldots\right) |\alpha_i, \alpha_j, \alpha_k \ldots\rangle \tag{24.69}$$

where now on the right-hand side every interaction is counted only once. As above, $\widehat{V}_{\mu,\nu}$ refers to the potential energy between the μ and ν particles. If $|\alpha_i\rangle \neq |\alpha_j\rangle$, then the number of times that $V_{\alpha_i\alpha_j}$ occurs in the double sum is equal to $n_{\alpha_i} n_{\alpha_j}$. However, when $|\alpha_i\rangle = |\alpha_j\rangle$, then the number of times that $V_{\alpha_i\alpha_j}$ occurs is equal to $n_{\alpha_i}(n_{\alpha_i} - 1)$ because we are not counting the interaction of the particle with itself, as specified by $\nu \neq \mu$ in the sum. In general then,

$$\frac{1}{2} \sum_{\mu=1}^{N} \sum_{\substack{\nu=1 \\ \nu\neq\mu}}^{N} \widehat{V}_{\mu,\nu} |\alpha_i, \alpha_j, \alpha_k \ldots\rangle = \frac{1}{2} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} V_{\alpha_m\alpha_n} \left(\widehat{n}_{\alpha_m} \widehat{n}_{\alpha_n} - \delta_{m,n} \widehat{n}_{\alpha_n}\right) |\alpha_i, \alpha_j, \alpha_k \ldots\rangle . \tag{24.70}$$

Again the expression for the operator to the right is independent of the state it acts on. It is valid in general. I assumed that the basis α has an infinite number of states.

We can simplify the expression further. Defining

$$\boxed{\zeta = -1 \quad \text{for} \quad \text{fermions}} \tag{24.71}$$

$$\boxed{\zeta = 1 \quad \text{for} \quad \text{bosons}} \tag{24.72}$$

we can rewrite $\widehat{n}_{\alpha_i} \widehat{n}_{\alpha_j} - \delta_{i,j} \widehat{n}_{\alpha_i}$ in terms of creation and annihilation operators in such a way that the form is valid for both fermions and bosons

$$\widehat{n}_{\alpha_i} \widehat{n}_{\alpha_j} - \delta_{i,j} \widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_j} - \delta_{i,j} a^\dagger_{\alpha_i} a_{\alpha_i} = a^\dagger_{\alpha_i} \zeta a^\dagger_{\alpha_j} a_{\alpha_i} a_{\alpha_j} = a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_j} a_{\alpha_i}. \tag{24.73}$$

Second quantized operators are thus written in the simple form

$$\boxed{\tfrac{1}{2} \textstyle\sum_i \sum_j V_{\alpha_i\alpha_j} \left(\widehat{n}_{\alpha_i} \widehat{n}_{\alpha_j} - \delta_{i,j} \widehat{n}_{\alpha_i}\right) \equiv \tfrac{1}{2} \sum_i \sum_j (\alpha_i\alpha_j| \, V \, |\alpha_i\alpha_j) \, a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_j} a_{\alpha_i}} \tag{24.74}$$

where

$$|\alpha_i\alpha_j) \equiv |\alpha_i\rangle \otimes |\alpha_j\rangle . \tag{24.75}$$

Under unitary transformation to an arbitrary basis we have

$$\boxed{\widehat{V}=\frac{1}{2}\sum_m\sum_n\sum_p\sum_q\left(\mu_m\mu_n\right|V\left|\mu_p\mu_q\right)c_{\mu_m}^{\dagger}c_{\mu_n}^{\dagger}c_{\mu_q}c_{\mu_p}}. \tag{24.76}$$

Definition 15 *When a series of creation and annihilation operators are placed in such an order where all destruction operators are to the right, one calls this "normal order".*

Remark 186 *Note the inversion in the order of μ_p and μ_q in the annihilation operators compared with the order in the matrix elements (This could have been for the creation operator instead).*

Remark 187 *Note that the first state $(\alpha_i\alpha_j|V|\alpha_i\alpha_j)$ in both the bra and the ket is associated with the first coordinate in V, and the second state with the second label in V. This means that the notation $\left(\mu_m\mu_n\right|V\left|\mu_p\mu_q\right)$ for the two-body matrix element stands for, in the coordinate representation for example,*

$$\int d\mathbf{r}_1 d\mathbf{r}_2\phi_{\mu_m}^{*}\left(\mathbf{r}_1\right)\phi_{\mu_n}^{*}\left(\mathbf{r}_2\right)V\left(\mathbf{r}_1-\mathbf{r}_2\right)\phi_{\mu_p}\left(\mathbf{r}_1\right)\phi_{\mu_q}\left(\mathbf{r}_2\right). \tag{24.77}$$

Example 16 *In the case of a potential, such as the Coulomb potential, which acts on the densities, we have*

$$\boxed{\widehat{V}=\frac{1}{2}\int d\mathbf{x}\int d\mathbf{y}v\left(\mathbf{x}-\mathbf{y}\right)\psi^{\dagger}\left(\mathbf{x}\right)\psi^{\dagger}\left(\mathbf{y}\right)\psi\left(\mathbf{y}\right)\psi\left(\mathbf{x}\right)}. \tag{24.78}$$

24.8 Getting familiar with second quantized operators in the Heisenberg picture, commutator identities

In the previous section, we showed how to translate one- and two-body operators in the Schrödinger picture into the language of second quantization. The Heisenberg picture is defined as usual. In this section, we derive a few useful identities and study the case of quadratic Hamiltonians as an example.

In the Heisenberg picture

$$\boxed{c_{\mathbf{k}}\left(t\right)=e^{i\widehat{H}t}c_{\mathbf{k}}e^{-i\widehat{H}t}\quad;\quad c_{\mathbf{k}}^{\dagger}\left(t\right)=e^{i\widehat{H}t}c_{\mathbf{k}}^{\dagger}e^{-i\widehat{H}t}.} \tag{24.79}$$

It is easy to compute the time evolution in the case where the Hamiltonian is quadratic in creation and annihilation operators. Take for example

$$\widehat{H}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}} \tag{24.80}$$

The time evolution may be found from the Heisenberg equation of motion, which follows from differentiating the definition of the Heisenberg operators

$$i\frac{\partial c_{\mathbf{k}}\left(t\right)}{\partial t}=\left[c_{\mathbf{k}}\left(t\right),\widehat{H}\right]. \tag{24.81}$$

To evaluate the commutator, we note that since $\widehat{H}$ commutes with itself is is time independent and

$$\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c_{\mathbf{k}}^{\dagger}\left(t\right)c_{\mathbf{k}}\left(t\right). \tag{24.82}$$

To compute the commutator, we only need the equal-time commutator of the number operator $c_{\mathbf{k}}^{\dagger}(t) c_{\mathbf{k}}(t)$ with $c_{\mathbf{k}}(t)$, which is given by Eq.(24.24) and leads, for both fermions and bosons, to

$$i\frac{\partial c_{\mathbf{k}}(t)}{\partial t} = \left[c_{\mathbf{k}}(t), \widehat{H}\right] = \sum_{\mathbf{k}'} \epsilon_{\mathbf{k}'} \left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)\right] = \epsilon_{\mathbf{k}} c_{\mathbf{k}}(t) \tag{24.83}$$

whose solution is

$$\boxed{c_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}} t} c_{\mathbf{k}}} \tag{24.84}$$

Taking the adjoint,

$$\boxed{c_{\mathbf{k}}^{\dagger}(t) = c_{\mathbf{k}}^{\dagger} e^{i\epsilon_{\mathbf{k}} t}}. \tag{24.85}$$

If we had been working in a basis where $\widehat{H}$ was not diagonal, then repeating the steps above,

$$i\frac{\partial a_{\alpha}(t)}{\partial t} = \left[a_{\alpha}(t), \widehat{H}\right] = \sum_{\beta,\gamma} \langle\beta| \widehat{H} |\gamma\rangle \left[a_{\alpha}(t), a_{\beta}^{\dagger}(t) a_{\gamma}(t)\right] = \sum_{\gamma} \langle\alpha| \widehat{H} |\gamma\rangle a_{\gamma}(t) \tag{24.86}$$

Commutator identities: The following are very useful identities to get equations of motions, and in general equal-time commutators.

$$[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA \tag{24.87}$$

$$\boxed{[A, BC] = [A, B] C + B [A, C]} \tag{24.88}$$

$$\boxed{[A, BC] = \{A, B\} C - B \{A, C\}} \tag{24.89}$$

The first commutator identity is familiar from elementary quantum mechanics. The last one can be memorized by noting that it behaves as if the B had anticommuted with the A. It is always easier to remember the commutator of the number operator with creation or annihilation operators, but if you need to prove it again for yourself, the above identities can be used to evaluate the needed commutator either for fermions

$$\left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)\right] = \left\{c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\right\} c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}}(t) \tag{24.90}$$

or for bosons

$$\left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)\right] = \left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\right] c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}}(t) \tag{24.91}$$

Remark 188 *Commuting with a $c_{\mathbf{k}}(t)$ looks like taking a derivative with respect to $c_{\mathbf{k}'}^{\dagger}(t)$. This is important to remember.*

Remark 189 *The theorem on commutators of ladder operators Eq. (24.1.3) is useful to find the eigenstates of one-body Hamiltonians. Indeed, consider the Hamiltonian at the beginning of this section Eq. (24.80). Then, given that*

$$\left[H, c_{\mathbf{k}}^{\dagger}\right] = \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger}, \tag{24.92}$$

our theorem tells us that if $H|0\rangle = 0$, then $c_{\mathbf{k}}^{\dagger}|0\rangle$ is an eigenstate with energy $\varepsilon_{\mathbf{k}}$, while $c_{\mathbf{k}'}^{\dagger} c_{\mathbf{k}}^{\dagger}|0\rangle$ is an eigenstate with energy $\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'}$ etc.

25. *FORMAL DERIVATION OF SECOND QUANTIZATION

Planck's constant h is the same for all possible types of particles or waves. Fundamentally it is the size of the action of a physical process, measured in units of h that will determine whether that process behaves quantum mechanically or if the classical limit is appropriate. This was very clear in Feynman's path-integral formulation. In this section, I will write Planck's constant explicitly since it plays such a central role.

First quantization refers to the usual way one does quantum mechanics in introductory classes. One starts with particles whose position and momentum become operators that obey commutation relations. However, we know that one cannot entirely describe matter by particles. Particles behave sometimes like waves. And vice-versa. To paraphrase Feynman, *Quantum mechanics is strange, but it is strange in the same way for all forms of matter*. For example, the natural description of electromagnetism is based on waves, but these waves can show up as particles, namely photons. And vice-versa. So we should be able to have a description of quantum mechanics that starts purely from wave equations. We should be able to quantize waves. According to Coleman, [55] in 1927, Pascual Jordan and Oskar Klein [109] suggested that creation and annihilation operators are a convenient way to deal with many particles, as we did above. Jordan and Klein in 1928 proposed that the particle field and its complex conjugate are conjugate variables, as I will discuss here.

Whether we start from first or second quantization, the final description of nature that we have must be the same since the wave and the particle descriptions of matter are complementary, each by itself being insufficient.

In the preceding chapter, I introduced second quantization in a more pedestrian way that illustrates straighforwardly that first and second quantization are equivalent. In practice, when there are many particles, second quantization is most of the time the best way to formulate and attack the problem.

25.1 *A quantization recipe

Dirac [68] proposed a general recipe to quantize a theory: Replace classical coordinates and their conjugate momentum by operators and replace Poisson brackets by commutators. This is, in a way, the correspondance principle between classical and quantum mechanics. The classical and quantum versions of Lagrangians and Hamiltonians are the same, except that in the classical case we have numbers while we have operators in the quantum case.[1] It is useful to review the procedure in a way that does not require you to know what Poisson brackes are. This procedure

[1] There are rare instances (anomalies) where there are quantum corrections to the action that cannot be guessed from the classical version of the theory. These corrections are usually topological in nature.

works in almost all cases [2] that I know of. If you want to quantize an electrical circuit for example, that is the way to proceed.

- Find the classical Lagrangian L of the system, namely the Lagrangian whose Euler-Lagrange equations give back the equations of motion.
- For each coordinate q, identify the corresponding conjugate momentum $p = \partial L/\partial \dot{q}$ where $\dot{q}$ means dq/dt.
- Elevate q and p to the level of operators acting in Hilbert space.
- Declare that $[q, p] = i\hbar$ and that all other commutators vanish, including the commutators between coordinates belonging to the same particle but in different directions. In other words, $[q_i, p_j] = i\hbar\delta_{ij}$, where i and j stand for different coordinates of the same particle or for different particles.
- The equations of motion in the Hamiltonian formalism are given by the Heisenberg equations of motion

$$\frac{dq}{dt} = \frac{i}{\hbar}[H, q] \tag{25.1}$$
$$\frac{dp}{dt} = \frac{i}{\hbar}[H, p] \tag{25.2}$$

A few comments are in order.

- The center of mass of a particle obeys the same commutation relations with its conjugate momentum as the canonical ones. For example

$$\left[\frac{q_1 + q_2}{2}, p_1 + p_2\right] = \frac{1}{2}[q_1, p_1] + \frac{1}{2}[q_2, p_{21}] = i\hbar. \tag{25.3}$$

This is an extremely nice property which leads to the fact that collective coordinates behave just the same way as the constituents, or, if you want, collective coordinates are as quantum mechanical, or strange, as their elementary constituents. Quantum mechanics in its standard form applies also to large systems. We do not need to know what is most elementary. That takes us back to the remark on the notion of smallness 168.

Remark 190 *A remarkable proof of all this is that you can take at C_{60} molecule and check that its center of mass and total momentum obey standard commutation relations, which has as a consequence that one can observe Youg fringes for these big molecules [170] in a true quantum mechanical way, one at a time!*

- The classical Hamilton equations of motion are recovered as follows. Using $[A, BC] = [A, B]C + C[A, B]$,we have that $\left[q, p^2\right] = 2p[q, p]$,and by induction, $[q, p^n] = np^{n-1}[q, p]$, or for a general function of p, we can formally write $[q, f(p)] = \frac{\partial f}{\partial p}[q, p]$ .Conversely, we find $[g(q), p] = \frac{\partial g}{\partial q}[q, p]$. Using these results in the Heisenberg equations of motion with a time-independent Hamiltonian, we recover Hamilton's equations for the classical variable

$$\frac{dq}{dt} = \frac{i}{\hbar}[H, q] = \frac{i}{\hbar}\frac{\partial H}{\partial p}[p, q] = \frac{\partial H}{\partial p} \tag{25.4}$$
$$\frac{dp}{dt} = \frac{i}{\hbar}[H, p] = \frac{i}{\hbar}\frac{\partial H}{\partial q}[q, p] = -\frac{\partial H}{\partial q}. \tag{25.5}$$

[2] There are rare instances (anomalies) where there are quantum corrections to the action that cannot be guessed from the classical version of the theory. These corrections are usually topological in nature.

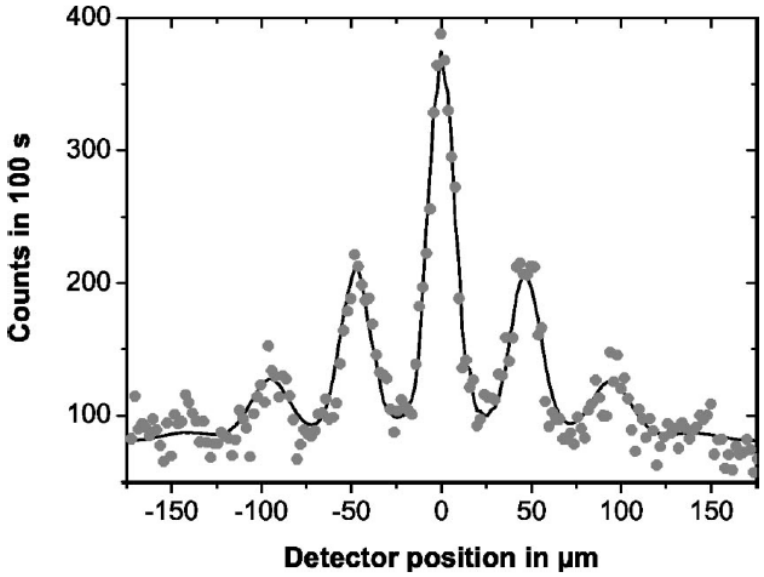


Figure 25-1 Interference pattern for C_{60} molecules passing one at a time through a double slit. This is the analog of Young's experiment with photons, but this time with large molecules. Quantum mechanics is bizarre, but it is always bizarre in the same way. For details, see Olaf Nairz, Markus Arndt, and Anton Zeilinger, American Journal of Physics 71, 319 (2003); doi: 10.1119/1.1531580.

25.2 *Applying the quantization recipe to wave equations

The electromagnetic field is the prime example of a classical field that must be quantized using the above principles. But since bosons can condense, their wave function can have a non-zero expectation value and that quantity comes close to being a classical variable. There are all sorts of caveats associated with that, but assume it makes sense. Then the Lagrangian for that classical variable is

$$L(t) = \int d^3\mathbf{r}\, \psi^*(\mathbf{r},t) \left(i\hbar \frac{d}{dt} + \frac{\hbar^2}{2m}\nabla^2 - V(\mathbf{r}) \right) \psi(\mathbf{r},t), \tag{25.6}$$

where $V(\mathbf{r})$, for simplicity, is taken as a one-body potential. It is important to keep in mind that in this expression the position $\mathbf{r}$ is not a dynamical variable, it is only a label for the field ψ. The filed ψ is an independent variable at each position, just as for the electromagnetic field. The total time derivative does not act on position, in other words, $d\mathbf{r}/d\mathbf{t}$ would not make any sense here.

This Lagrangian is chosen because the corresponding Euler-Lagrange equations reproduce Schrödinger's equation, as I proceed to show. Note that since ψ is a complex variable, ψ and ψ^* can be taken as independent variables. Since we work in the continuum, partial derivatives needed to obtain the Euler-Lagrange equations are replaced by functional derivatives, namely

$$\frac{\delta\psi(\mathbf{r},t)}{\delta\psi(\mathbf{r}',t)} = \delta(\mathbf{r}-\mathbf{r}').$$

We will make heavy use of functional derivatives in later chapters. The Euler-Lagrange equations for $\psi^*(\mathbf{r},t)$ are

$$\frac{d}{dt}\left(\frac{\delta L(t)}{\delta\left(\frac{d\psi^*(\mathbf{r},t)}{dt}\right)}\right)-\frac{\delta L(t)}{\delta\psi^*(\mathbf{r},t)} \tag{25.7}$$

$$=\left(i\hbar\frac{d}{dt}+\frac{\hbar^2}{2m}\nabla^2-V(\mathbf{r})\right)\psi(\mathbf{r},t)=0. \tag{25.8}$$

which is indeed Schrödinger equation. Integrating by parts with vanishing (or periodic) boundary conditions at infinity so as to have ∇^2 act on $\psi^*(\mathbf{r},t)$, the Euler-Lagrange equations for $\psi(\mathbf{r},t)$ give Schrödinger's equation for $\psi^*(\mathbf{r},t)$.

Continuing to follow the rules for quantization, we need the variable conjugate to the $\psi(\mathbf{r},t)$. It is given by

$$\frac{\delta L(t)}{\delta\left(\frac{d\psi(\mathbf{r},t)}{dt}\right)}=i\hbar\psi^*(\mathbf{r},t). \tag{25.9}$$

Hence, the theory can be quantized by declaring that $i\hbar\psi^*(\mathbf{r},t)$ and $\psi(\mathbf{r},t)$ are conjugate operators $i\hbar\psi^\dagger(\mathbf{r},t)$ and $\psi(\mathbf{r},t)$ that obey canonical equal-time commutation relations

$$\left[\psi(\mathbf{r},t),i\hbar\psi^\dagger(\mathbf{r},t)\right]=i\hbar\delta(\mathbf{r}-\mathbf{r}') \tag{25.10}$$

$$\left[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r},t)\right]=\delta(\mathbf{r}-\mathbf{r}'). \tag{25.11}$$

It turns out that taking anticommutation relations instead of commutation relations does not lead to any inconsistency. But then it becomes perfectly legitimate to doubt the starting point since fermions do not have a classical limit. Nevertheless, the derivation of the preceeding chapter is foolproof.

With the above commutation or anticommutation relations, in other words for either bosons or fermions, you can verify that

$$\left[\int d^3\mathbf{r}'\ \psi^\dagger(\mathbf{r}',t)\ \psi(\mathbf{r}',t),\psi^\dagger(\mathbf{r},t)\right]=\psi^\dagger(\mathbf{r},t) \tag{25.12}$$

$$\left[\int d^3\mathbf{r}'\ \psi^\dagger(\mathbf{r}',t)\ \psi(\mathbf{r}',t),\psi(\mathbf{r},t)\right]=-\psi(\mathbf{r},t) \tag{25.13}$$

Using our theorem on commutators of ladder operators (24.1.3) and proceeding as in the section on number operators and states,24.5 we have that for N particles, we can build a complete set of states with the basis states

$$\psi^\dagger(\mathbf{r}_1,t)\,\psi^\dagger(\mathbf{r}_2,t)\ldots\psi^\dagger(\mathbf{r}_N,t)\,|0\rangle. \tag{25.14}$$

There is a vacuum state and the operator

$$\int d^3\mathbf{r}'\ \psi^\dagger(\mathbf{r}',t)\ \psi(\mathbf{r}',t) \tag{25.15}$$

has integer eigenvalues that count the number of particles.

Remark 191 *Particles as excitations of the vacuum: As in the harmonic oscillator where phonons are elementary excitations added to the vacuum of the oscillator, here particles are excitations of the vacuum of the Schrödinger field. They are added in discrete countable amounts.*

A tentalizing, although not rigorous, connection to first quantization, can be obtained as follows. Let us define the position X and conjugate momentum P_x operators by declaring that the variables $\psi(\mathbf{r},t)$ and $\psi^*(\mathbf{r},t)$ entering the following usual expressions

$$\int d^3\mathbf{r}\ \psi^*(\mathbf{r},t)\ \mathbf{r}_x\ \psi(\mathbf{r},t) = X(t) \tag{25.16}$$

$$\int d^3\mathbf{r}\ \psi^*(\mathbf{r},t)\ \frac{i}{\hbar}\nabla_x\ \psi(\mathbf{r},t) = P_x(t) \tag{25.17}$$

are operators instead of classical fields. Then, the above commutation relations Eq.(25.10) (or anticommutation relations) yield the following result

$$[X(t), P_x(t)] = i\hbar \int d^3\mathbf{r}\ \psi^\dagger(\mathbf{r},t)\ \psi(\mathbf{r},t). \tag{25.18}$$

The right-hand side is the total number of particles. We thus recover the commutation relation we developed in the preceeding section for the center of mass coordinate in first quantization.

26. MOTIVATION FOR THE DEFINITION OF THE SECOND QUANTIZED GREEN'S FUNCTION G^R

Just as we showed that scattering and transport experiments measure correlation functions such as the density-density or current-current correlation function, we begin this chapter by showing that photoemission directly probes a one-particle correlation function. The last section will introduce and motivate further the definition of the second quantized Green's function.

26.1 Measuring a two-point correlation function (ARPES)

In a photoemission experiment, a photon ejects an electron from a solid. This is nothing but the old familiar photoelectric effect. In the angle-resolved version of this experiment (ARPES), the energy and the direction of the outgoing electron are measured. This is illustrated in Fig.(26-1). The outgoing electron energy can be measured. Because it is a free electron, this measurement gives the value of the wave vector through $k^2/2m$. Using energy conservation, the energy of the outgoing electron is equal to the energy of the incident photon E_{ph}, minus the work function W plus the energy of the electron in the system, ω, measured relative to the Fermi level.

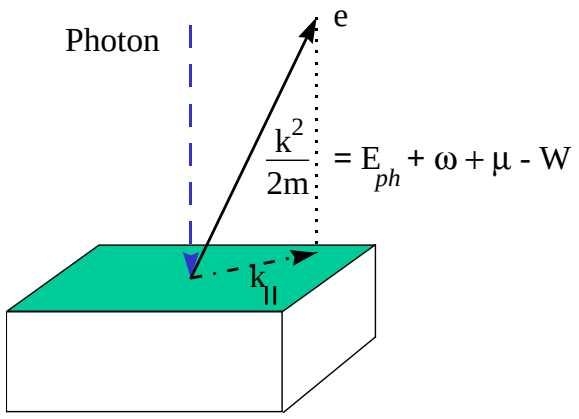


Figure 26-1 Schematic representation of an angle-resolved photoemission experiment. W is the work function.

The energy of the electron in the system ω will be mostly negative. The value of $\mathbf{k}_{||}$ may be extracted by simple geometric considerations from the value of k. Since in this experiment there is translational invariance only in the direction parallel to the plane, this means that in fact it is only the value of $\mathbf{k}_{||}$ that is

conserved. Hence, it is only for layered systems that we really have access to both energy ω and total momentum $\mathbf{k}_{||}$ of the electron when it was in the system.

We can give a sketchy derivation of the calculation of the cross-section as follows. The cross-section we will find below neglects, amongst other things, processes where energy is transferred from the outgoing electron to phonons or other excitations before it is detected (multiple scattering of outgoing electron). Such processes are referred to as "inelastic background". We start from Fermi's Golden rule. The initial state is a direct product $|m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em}$ of the state of the system $|m\rangle$, with the state $|0\rangle$ with no electron far away from the detector and with the state of the electromagnetic field that has one incoming photon $|1_{\mathbf{q}}\rangle_{em}$. The final state $|n\rangle \otimes |\mathbf{k}\rangle \otimes |0\rangle_{em}$ has the system in state $|n\rangle$ with one less electron, the detector with one electron in state $|\mathbf{k}\rangle$ and the electromagnetic field in state $|0\rangle_{em}$ with no photon. Strictly speaking, the electrons in the system should be antisymmetrized with the electrons in the detector, but when they are far enough apart and one electron is detected, we can assume that it is distinguishible from electrons in the piece of material. The coupling of matter with electromagnetic field that produces this transition from initial to final state is $-\mathbf{j}\cdot\mathbf{A}$ as we saw previously. Hence, the transition rate will be proportional to the square of the following matrix element

$$-\sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \otimes \langle 0|_{em} \mathbf{j}_{\mathbf{k}'} \cdot \mathbf{A}_{-\mathbf{k}'} |m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em} . \tag{26.1}$$

$$= -\sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \mathbf{j}_{\mathbf{k}'} |m\rangle \otimes |0\rangle \cdot \langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle_{em} \tag{26.2}$$

The vector potential is the analog of the position operator for harmonic vibration of the electromagnetic field. Hence, it is proportionnal to $a^{\dagger}_{-\mathbf{k}'} + a_{\mathbf{k}'}$, like for the harmonic oscillator excep that this time the particles involved are photons. The term with $\mathbf{k}' = \mathbf{q}$ with the destruction operator will lead to a non-zero value of $\langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle$. For the range of energies of interest, the wave vector of the photon $\mathbf{k}' = \mathbf{q}$ can be considered in the center of the Brillouin zone, $\mathbf{k}' \approx \mathbf{0}$. The current operator is a one-body operator. In the continuum, it is then given by

$$\mathbf{j}_{\mathbf{k}'=\mathbf{0}} = e \sum_{\mathbf{p}} \frac{\mathbf{p}}{m} c^{\dagger}_{\mathbf{p}} c_{\mathbf{p}}. \tag{26.3}$$

The value $\mathbf{p} = \mathbf{k}_{||}$ will lead to a non-zero matrix element. Overall then, the matrix element is

$$-\langle n| c_{\mathbf{k}_{||}} |m\rangle \left(\langle \mathbf{k}| c^{\dagger}_{\mathbf{k}_{||}} |0\rangle e \frac{\mathbf{k}_{||}}{m} \cdot \langle 0|_{em} \mathbf{A}_{\mathbf{k}'=\mathbf{q}\sim\mathbf{0}} |1_{\mathbf{q}}\rangle_{em} \right). \tag{26.4}$$

The term in large parenthesis is a matrix element that does not depend on the state of the system. Without going into more details of the assumptions going into the derivation then, Fermi's golden rule suggests, (see first section of Chapter 2) that the cross section for ejecting an electron of momentum $\mathbf{k}_{||}$ and energy ω (measured with respect to μ) is proportional to

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega + \mu - (E_m - E_n)\right) \tag{26.5}$$

$$\propto \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega - (K_m - K_n)\right) \tag{26.6}$$

$$\propto \int dt e^{i\omega t} \sum_{mn} e^{-\beta K_m} \langle m| c^{\dagger}_{\mathbf{k}_{||}} |n\rangle \langle n| e^{iK_n t} c_{\mathbf{k}_{||}} e^{-iK_m t} |m\rangle \tag{26.7}$$

$$\propto \int dt e^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle . \tag{26.8}$$

In the above equations, note that there is one more particle in state $|m\rangle$ than in state $|n\rangle$. This means that the minimum change in energy that we can have is $E_m - E_n = \mu$. With some extra energy, we can eject an electron that is farther away below the Fermi surface. Measuring energies with respect to the chemical potential, we define $K_m = E_m - N_m\mu$. For the last line, we have followed van Hove and used the same steps as in the corresponding derivation for the cross section for electron scattering in Sec. 7. We have achieved our goal of expressing the cross section in terms of a correlation function.

In the case of electron scattering that we related to density fluctuations, there was a relation between the correlation function and the spectral weight that could be established with the fluctuation-dissipation theorem. We will be able to achieve the same thing below in Sec. 31.2. More specifically, we will be able to rewrite this result in terms of the spectral weight $A\left(\mathbf{k}_{||},\omega\right)$ as follows,

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto f\left(\omega\right) A\left(\mathbf{k}_{||},\omega\right) \tag{26.9}$$

where $f\left(\omega\right)$ is the Fermi function.

Remark 192 *Time-evolution operator: It is very important to note that in the above expression for the cross section, Eq.(26.8), it is $K = H - \mu N$ that is the time evolution operator. This is what we will generally use, as soon as we go to the Matsubara formalism. The μN represents the effect of a particle reservoir. It comes in naturally above and represents the time evolution operator when we control the chemical potential instead of the number of particles. It makes the time-evolution operator in imaginary time more similar to the density matrix $e^{-\beta K_m}/Z$. More simply, this just corresponds to a choice of the zero of energy, namely ω is equal to zero for energies at the chemical potential. This can be seen from the above equations. Since we have by definition of K_n the equalities $e^{iK_nt}c_{\mathbf{k}_{||}}e^{-iK_mt} = e^{i(E_n-\mu N_n)t}c_{\mathbf{k}_{||}}e^{-i(E_m-\mu N_m)t}$ and $N_m - N_n = 1$, the phase factor $e^{i\mu t}$ can just be added to ω in the Fourier transform over time, illustrating why this choice of time evolution operator is related to the choice of zero of energy for ω.*

26.2 Definition of the many-body G^R and link with the previous one

When the Hamiltonian is quadratic in creation-annihilation operators, in other words when we have a one-body problem, the retarded single-particle Green's function we are about to define does reduce to the Green's function we studied in the one-body Schrödinger equation. Its actual definition is however better suited for many-body problems as we shall see in the present section. It is also important to note that while in the one-body Schrödinger equation, all the information is in G^R, in the Many-body case, it only gives information about propagation of a single particle, hence it does not contain all the information.

Consider the definition we had before

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right) = -i\left\langle\mathbf{r}\right| e^{-iH\left(t-t'\right)}\left|\mathbf{r}'\right\rangle\theta\left(t-t'\right). \tag{26.10}$$

We will reintroduce $-\mu N$ later by replacing H by $K = H - \mu N$. Since in second-quantization the operator $\psi^\dagger\left(\mathbf{r}\right)$ creates a particle at point $\mathbf{r}$, the following definition seems natural

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right) = -i\left\langle GS\right|\psi\left(\mathbf{r}\right)e^{-iH\left(t-t'\right)}\psi^\dagger\left(\mathbf{r}'\right)\left|GS\right\rangle\theta\left(t-t'\right) \tag{26.11}$$

In this expression, $|GS\rangle$ is a many-body vacuum (ground-state). Choosing appropriately the zero of energy, $H|GS\rangle = 0\,|GS\rangle = 0$ the above result could be written in an elegant way when we recall the definition of the operators in the Heisenberg representation

$$G^R(\mathbf{r},t;\mathbf{r}',t') = -i\langle GS|\,\psi(\mathbf{r},t)\,\psi^\dagger(\mathbf{r}',t')\,|GS\rangle\,\theta(t-t')\,. \tag{26.12}$$

This is not quite what we want except in the case where there is a single particle propagating. When there is a single particle propagating, anticommutation and the fact that $\psi(\mathbf{r},t)$ annihilates the vacuum means that we are left at time $t = t' + 0^+$ with

$$G^R\left(\mathbf{r},t+0^+;\mathbf{r}',t\right) = -i\delta(\mathbf{r}-\mathbf{r}') \tag{26.13}$$

reflecting the fact that the wave-function does not have the time to evolve in an infinitesimal time.

However, in the present case, the many-body vacuum $|GS\rangle$ is a linear combination of Slater determinants with many particles in each. This means that $\langle GS|\,\psi(\mathbf{r},t)\,\psi^\dagger(\mathbf{r}',t)\,|GS\rangle$ is not in general a delta function because $\psi(\mathbf{r},t)$ does not annihilate the ground state. This is a manifestation of the fact that we have a many-body problem and that particles are indistinguishable.

Nevertheless, we can recover the desired simple initial condition Eq.(26.13) even in the Many-Body case by adopting the following *definition,* which in a way takes into account the fact that not only electrons, but also holes can now propagate:

$$G^R(\mathbf{r},t;\mathbf{r}',t') = -i\langle GS|\left\{\psi(\mathbf{r},t)\,,\psi^\dagger(\mathbf{r}',t')\right\}|GS\rangle\,\theta(t-t') \quad ; \quad \text{for} \quad \text{fermions} \tag{26.14}$$

$$G^R(\mathbf{r},t;\mathbf{r}',t') = -i\langle GS|\left[\psi(\mathbf{r},t)\,,\psi^\dagger(\mathbf{r}',t')\right]|GS\rangle\,\theta(t-t') \quad ; \quad \text{for} \quad \text{bosons} \tag{26.15}$$

This is the zero-temperature definition. It is more general than in the one-body case, but it reduces to it when there is a single particle.

At finite temperature, the ground-state expectation value is replaced by a thermodynamic average. Hence we shall in general work with

Definition 17

$$\boxed{G^R(\mathbf{r},t;\mathbf{r}',t') = -i\left\langle\left\{\psi(\mathbf{r},t)\,,\psi^\dagger(\mathbf{r}',t')\right\}\right\rangle\theta(t-t') \quad ; \quad \textit{for} \quad \textit{fermions}} \tag{26.16}$$

$$\boxed{G^R(\mathbf{r},t;\mathbf{r}',t') = -i\left\langle\left[\psi(\mathbf{r},t)\,,\psi^\dagger(\mathbf{r}',t')\right]\right\rangle\theta(t-t') \quad ; \quad \textit{for} \quad \textit{bosons}} \tag{26.17}$$

These definitions have the desired property that at $t = t' + 0^+$, we have that $G^R(\mathbf{r},t+0^+;\mathbf{r}',t) = -i\delta(\mathbf{r}-\mathbf{r}')$ as follows from commutation or anti-commutation relations.

The expectation value $\left\langle c^\dagger_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle$ that we needed in the expression for the photoemission cross section is directly related to one of the terms in the anticommutator.

Remark 193 *Analogies: This definition is now analogous to* $\chi^R(t-t') = 2i\chi"(t-t')\,\theta(t-t')$ *which we had in linear response and in the harmonic oscillator example Eq. (3.14). The imaginary part of the Green's function will again be a commutator or an anticommutator and hence will obey sum-rules.*

Remark 194 *Green's function as a response function: Physically, this definition makes obvious that the Green's function is the response to an external probe that couples linearly to creation-annihilation operators. In the case of fermions, the external probe has to be an anticommuting number (a Grassmann variable, as we shall discuss later).*

26.3 Examples with quadratic Hamiltonians:

When the Hamiltonian is quadratic in creation-annihilation operators, the equation of motion obeyed by this Green's function is the same as in the one-body case. An example of quadratic Hamiltonian is that for free particles, in first quantized notation

$$\langle \mathbf{r}| \widehat{H} |\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m} \langle \mathbf{r} |\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m} \delta(\mathbf{r}-\mathbf{r}_1). \tag{26.18}$$

In the general second quantized case, we write

$$\widehat{H} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi^\dagger(\mathbf{r}_2,t) \langle \mathbf{r}_2| H |\mathbf{r}_1\rangle \psi(\mathbf{r}_1,t) \tag{26.19}$$

We give three calculations of the Green's function, two directly from the definition and one from the equations of motion (Schrödinger's equation). We do the calculation for fermions. The calculation for bosons is essentially the same.

***Calculation from the definition in the position basis:** For a *quadratic Hamiltonian*, one can also compute directly the Green's function from its definition since, if $|n\rangle$ is an eigenbasis, $\phi_n(\mathbf{r}) = \langle \mathbf{r}|n\rangle$, $\langle n'| H |n\rangle = E_n \delta_{n,n'}$

$$\psi(\mathbf{r},t) = \sum_n \langle \mathbf{r}|n\rangle a_n(t) = \sum_n e^{-iE_n t} \langle \mathbf{r}|n\rangle a_n = \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) a_n \tag{26.20}$$

$$\left\{\psi(\mathbf{r},t), \psi^\dagger(\mathbf{r}',0)\right\} = \sum_n \sum_m e^{-iE_n t} \phi_n(\mathbf{r}) \left\{a_n, a_m^\dagger\right\} \phi_m^*(\mathbf{r}') = \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \tag{26.21}$$

$$G^R(\mathbf{r},t;\mathbf{r}',0) = -i \left\langle \left\{\psi(\mathbf{r},t), \psi^\dagger(\mathbf{r}',0)\right\} \right\rangle \theta(t) = -i \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \theta(t) \tag{26.22}$$

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \int dt e^{i(\omega+i\eta)t} (-i) \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \theta(t) = \sum_n \frac{\phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} \tag{26.23}$$

Calculation from the definition in the diagonal basis: This is the simplest calculation. We already know from Sec.24.8 the evolution of the creation-annihilation operators in the Heisenberg representation. In the momentum basis, where H is diagonal, as in Eq.(24.80),

$$\widehat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \tag{26.24}$$

we have that

$$\begin{aligned} G^R(\mathbf{k};t) &= -i \left\langle \left\{c_{\mathbf{k}}(t), c_{\mathbf{k}}^\dagger\right\} \right\rangle \theta(t-t') \\ &= -ie^{-i\epsilon_{\mathbf{k}} t} \left\langle \left\{c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger\right\} \right\rangle \theta(t-t'). \end{aligned} \tag{26.25}$$

Using the fact that the equal-time anticommutator here will be simply unity, we find

$$G^R(\mathbf{k};t) = -ie^{-i\epsilon_{\mathbf{k}} t} \theta(t-t') \tag{26.26}$$

and Fourier transforming

$$G^R(\mathbf{k};\omega) = \frac{1}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \tag{26.27}$$

Calculation from the equations of motion: In general, the equation of motion can be obtained as follows

$$i\frac{\partial}{\partial t}G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)=i\frac{\partial}{\partial t}\left[-i\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^\dagger\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right)\right] \tag{26.28}$$

$$=\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^\dagger\left(\mathbf{r}',t'\right)\right\}\right\rangle\delta\left(t-t'\right)+i\left\langle\left\{\left[\widehat{H},\psi\left(\mathbf{r},t\right)\right],\psi^\dagger\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right) \tag{26.29}$$

Following the steps analogous to those in Eq.(24.90) above, using the anticommutation relations Eqs.(81.19)(81.18a), or more directly recalling the commutator of the number operator with a creation or an annihilation operator, it is clear that

$$\left[\widehat{H},\psi\left(\mathbf{r},t\right)\right]=-\int d\mathbf{r}_1\left\langle\mathbf{r}\right|\widehat{H}\left|\mathbf{r}_1\right\rangle\psi\left(\mathbf{r}_1,t\right) \tag{26.30}$$

so that

$$i\frac{\partial}{\partial t}G^R\left(\mathbf{r},t;\mathbf{r}',t'\right) \tag{26.31}$$

$$=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)-i\int d\mathbf{r}_1\left\langle\mathbf{r}\right|\widehat{H}\left|\mathbf{r}_1\right\rangle\left\langle\left\{\psi\left(\mathbf{r}_1,t\right),\psi^\dagger\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right)$$

$$=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)+\int d\mathbf{r}_1\left\langle\mathbf{r}\right|\widehat{H}\left|\mathbf{r}_1\right\rangle G^R\left(\mathbf{r}_1,t;\mathbf{r}',t'\right) \tag{26.32}$$

In the case under consideration, where there is no interaction, we recover the one-particle case we had before. Indeed, the last expression may be rewritten as

$$\int d\mathbf{r}_1\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_1\right\rangle G^R\left(\mathbf{r}_1,t;\mathbf{r}',t'\right)=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) \tag{26.33}$$

$$=\left\langle\mathbf{r}\left|\mathbf{r}'\right.\right\rangle\delta\left(t-t'\right) \tag{26.34}$$

where we recognize the equation (15.13) found in a previous Chapter. Formally then

$$\left\langle\mathbf{r}\right|\left(i\frac{\partial}{\partial t}-\widehat{H}\right)G^R\left(t-t'\right)\left|\mathbf{r}'\right\rangle=\left\langle\mathbf{r}\left|\mathbf{r}'\right.\right\rangle\delta\left(t-t'\right) \tag{26.35}$$

so that the operator form of the Green's function is the same as that found before, namely

$$\widehat{G}^R\left(t-t'\right)=\left(i\frac{\partial}{\partial t}-\widehat{H}\right)^{-1}\delta\left(t-t'\right) \tag{26.36}$$

It is convenient to rewrite the result for the equation of motion Eq.(26.33) in the following form that is more symmetrical in space and time.

$$\int d\mathbf{r}_1\int dt_1\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_1\right\rangle\delta\left(t-t_1\right)G^R\left(\mathbf{r}_1,t_1;\mathbf{r}',t'\right)=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) \tag{26.37}$$

We may as well let time play a more important role since in the many-body case it will be essential, as we have already argued in the context of the frequency dependence of the self-energy. The inverse of the Green's function in this notation is just like above,

$$G^R\left(\mathbf{r},t;\mathbf{r}_1,t_1\right)^{-1}=\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_1\right\rangle\delta\left(t-t_1\right). \tag{26.38}$$

Seen from this point of view, the integrals over time and space are the continuum generalization of matrix multiplication. The delta function is like the identity matrix. The above is *not* general. It applies only to this non-interacting case.

Remark 195 *Evidently, the last result can also be obtained simply by transforming from frequency to time and doing a change of basis from* $\mathbf{k}$ *to* $\mathbf{r}$ *in our diagonal-basis result* $G^R(\mathbf{k},\omega)^{-1} = \omega + i\eta - \varepsilon_{\mathbf{k}}$.

Definition 18 *The following short-hand notation is often used*

$$\boxed{G^R(1,1') \equiv G^R(\mathbf{r},t;\mathbf{r}',t')} \tag{26.39}$$

$$\boxed{G^R\left(1,\bar{1}\right)^{-1} G^R\left(\bar{1},1'\right) = \delta(1-1')} \tag{26.40}$$

where the index with the overbar stands for an integral.

26.4 Spectral representation of G^R and analogy with susceptibility

By analogy with what we have done previously for response functions χ, it is useful to introduce the spectral representation for the retarded Green's function. We obtain explicitly $\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)$ by integration in the complex plane and find that it is trivially related to $G^R(\mathbf{r},\mathbf{r}';\omega)$.

As before, we have

$$G^R(\mathbf{r},\mathbf{r}';t) = -i\left\langle\left\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',0)\right\}\right\rangle\theta(t) \tag{26.41}$$

but this time, the evolution operator is defined to take into account the fact that we will work in the grand-canonical ensemble. By analogy with the definition of the Matsubara operators, we now have

$$K = H - \mu N$$

$$\psi(\mathbf{r},t) \equiv e^{itK}\psi_S(\mathbf{r})\,e^{-itK} \tag{26.42}$$

$$\psi^\dagger(\mathbf{r},t) \equiv e^{itK}\psi_S^+(\mathbf{r})\,e^{-itK} \tag{26.43}$$

We now proceed by analogy with the response functions. On the left we show the definitions for response functions, and on the right the analogous definitions for response functions. Let

$$G^R(\mathbf{r},\mathbf{r}';t) = -iA(\mathbf{r},\mathbf{r}';t)\,\theta(t) \quad ; \quad \chi_{ij}^R(t) = 2i\chi_{ij}''(t)\,\theta(t) \tag{26.44}$$

where the *spectral weight* is defined by

$$\boxed{A(\mathbf{r},\mathbf{r}';t) \equiv \left\langle\left\{\psi(\mathbf{r},t),\psi^+(\mathbf{r}',0)\right\}\right\rangle} \quad ; \quad \chi_{ij}''(t) = \frac{1}{2}\left\langle\left[A_i(\mathbf{r},t),A_j(\mathbf{r}',0)\right]\right\rangle \tag{26.45}$$

Then taking the Fourier transform, one obtains the spectral representation

$$\boxed{G^R(\mathbf{r},\mathbf{r}';\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'}} \quad ; \quad \chi_{ij}^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi_{ij}''(\omega')}{\omega'-(\omega+i\eta)}. \tag{26.46}$$

The spectral weight will obey sum-rules, like χ'' did. For example

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A(\mathbf{r},\mathbf{r}';\omega') = \left\langle\left\{\psi(\mathbf{r},0),\psi^+(\mathbf{r}',0)\right\}\right\rangle = \delta(\mathbf{r}-\mathbf{r}')} \tag{26.47}$$

From such sum rules, a high-frequency expansion can easily be found as usual. But that is not our subject for now.

27. INTERACTION REPRESENTATION, WHEN TIME ORDER MATTERS

Perturbation theory in the many-body case is less trivial than in the one-body case. Whereas the Lippmann-Schwinger equation was written down for a single frequency, in the many-body case time and frequency dependence are unavoidable. To construct perturbation theory we will follow the same steps as those used in the derivation of linear response theory in Chapter 9. The only difference is that we will write a formally exact solution for the evolution operator in the interaction representation instead of using only the first order result. The important concept of time-ordered product comes out naturally from this exercise.

There is an important change of notation here. There will be no hat in general for operators, only for operators in the interaction picture, or interaction representation.

The plan is to recall the Heisenberg and Schrödinger pictures, and then to introduce the interaction representation in the case where the Hamiltonian can be written in the form

$$H = H_0 + V \tag{27.1}$$

where

$$[H_0, V] \neq 0 \tag{27.2}$$

Let us begin. We assume that H is time independent. Typical matrix elements we want to compute at finite temperature are of the form

$$\langle i| e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') |i\rangle \tag{27.3}$$

We do not write explicitly indices other than time to keep the notation simple. Recall the Heisenberg and Schrödinger picture

$$\psi_H(t) = e^{iHt} \psi_S e^{-iHt} \tag{27.4}$$

We define the time evolution operator

$$U(t,0) = e^{-iHt} \tag{27.5}$$

so that

$$\psi_H(t) = U(0,t) \psi_S U(t,0) \tag{27.6}$$

When we assume time-reversal symmetry, we can always make the replacement

$$U^\dagger(t,0) = U(0,t). \tag{27.7}$$

The differential equation for the time-evolution operator is

$$i\frac{\partial U(t,0)}{\partial t} = HU(t,0) \tag{27.8}$$

With the initial condition $U(0,0) = 1$ it has $U(t,0) = e^{-iHt}$ as its solution. It obeys the property

$$U(t,t') = U(t,0) U(0,t') = e^{-iH\left(t-t'\right)} \tag{27.9}$$

$$U^{-1}(t,0) = U(0,t) \tag{27.10}$$

$$U(t_0,t_0) = 1 \tag{27.11}$$

for arbitrary t_0

We are now ready to introduce the interaction representation. In this representation, the fields evolve with the unperturbed Hamiltonian

$$\boxed{\widehat{\psi}(t) = e^{iH_0 t}\psi_S e^{-iH_0 t}} \tag{27.12}$$

Note that we now use the caret (hat) to mean "interaction picture". We hope this change of notation causes no confusion. To introduce these interaction representation fields in a general matrix element,

$$\langle i|\, e^{-\beta H}\psi_H(t)\,\psi_H^\dagger(t')\,|i\rangle = \langle i|\, e^{-\beta H}U(0,t)\,\psi_S U(t,0)\,U(0,t')\,\psi_S^\dagger U(t',0)\,|i\rangle \tag{27.13}$$

it suffices to notice that it is easy to remove the extra $e^{iH_0 t}$ coming from the replacement of ψ_S by $e^{-iH_0 t}\widehat{\psi}(t)\,e^{iH_0 t}$ simply by including them in the definition of the evolution operator in the interaction representation

$$U_I(t,0) = e^{iH_0 t}U(t,0) \tag{27.14}$$

$$U_I(0,t) = U(0,t)\,e^{-iH_0 t} \tag{27.15}$$

$$U_I(t,0)\,U_I(0,t) = U_I(0,t)\,U_I(t,0) = 1 \tag{27.16}$$

With these definitions, we have that our general matrix element takes the form

$$\langle i|\, e^{-\beta H}\psi_H(t)\,\psi_H^\dagger(t')\,|i\rangle = \langle i|\, e^{-\beta H}U_I(0,t)\,\psi_I(t)\,U_I(t,0)\,U_I(0,t')\,\psi_I^\dagger(t')\,U_I(t',0)\,|i\rangle \tag{27.17}$$

The purpose of the exercise is evidently to find a perturbation expansion for the evolution operator in the interaction representation. It will be built starting from its equation of motion

$$i\frac{\partial U_I(t,0)}{\partial t} = e^{iH_0 t}(-H_0 + H)\,U(t,0) = e^{iH_0 t}V \quad \left(e^{-iH_0 t}e^{iH_0 t}\right) \quad U(t,0) \tag{27.18}$$

Since a general operator is a product of ψ fields, it will also evolve with time in the same way so it is natural to define the interaction representation for V as well. Our final result for the equation of motion for $U_I(t,0)$ is then

$$i\frac{\partial U_I(t,0)}{\partial t} = V_I(t)\,U_I(t,0)$$

Multiplying on the right by $U_I(0,t_0)$ we have a more general equation

$$\boxed{i\frac{\partial U_I(t,t_0)}{\partial t} = V_I(t)\,U_I(t,t_0)} \tag{27.19}$$

Remark 196 *$V_I(t)$ depends on time since by hypothesis it does not commute with H_0.*

Remark 197 *Difficulties associated with the fact that we have non-commuting operators: The solution of this equation is not $e^{-i\int V_I(t)dt}$. We will see momentarily how the real solution looks formally like an exponential while at the same time being very different from it. To write the solution as a simple exponential is wrong because it assumes that we can manipulate $U_I(t,t_0)$ as if it was a number. In reality it is an operator so that $\frac{\partial U_I(t,t_0)}{\partial t}U_I(t,t_0)^{-1} \neq \frac{\partial}{\partial t}\ln U_I(t,t_0)$. Indeed, note the ambiguity in writing the definition of this derivative: Should we write*

$$\frac{\partial}{\partial t}\ln U_I(t,t_0) = \lim_{\Delta t\to 0} U_I(t,t_0)^{-1}\left[U_I(t+\Delta t,t_0) - U_I(t,t_0)\right]/\Delta t$$

or

$$\lim_{\Delta t\to 0}\left[U_I\left(t+\Delta t,t_0\right)-U_I\left(t,t_0\right)\right]U_I\left(t,t_0\right)^{-1}/\Delta t\ ? \tag{27.20}$$

The two limits cannot be identical since in general

$$\lim_{\Delta t\to 0}\left[U_I\left(t+\Delta t,t_0\right),U_I\left(t,t_0\right)^{-1}\right]\neq 0. \tag{27.21}$$

because $U_I\left(t,t_0\right)$ is made up of operators such as V and e^{-iH_0t} that do not commute with each other.

To solve the equation for the evolution operator Eq.(27.19), it is more convenient to write the equivalent integral equation that is then solved by iteration. Integration on both sides of the equation and use of the initial condition Eq.(27.11) gives immediately

$$\int_{t_0}^{t}\frac{\partial U_I\left(t',t_0\right)}{\partial t'}dt'=-i\int_{t_0}^{t}dt'V_I\left(t'\right)U_I\left(t',t_0\right) \tag{27.22}$$

$$U_I\left(t,t_0\right)=1-i\int_{t_0}^{t}dt'V_I\left(t'\right)U_I\left(t',t_0\right) \tag{27.23}$$

Solving by iteration, we find

$$U_I\left(t,t_0\right)=1-i\int_{t_0}^{t}dt'V_I\left(t'\right)U_I\left(t',t_0\right)= \tag{27.24}$$

$$=\ 1-i\int_{t_0}^{t}dt'V_I\left(t'\right)+\left(-i\right)^2\int_{t_0}^{t}dt'V_I\left(t'\right)\int_{t_0}^{t'}dt''V_I\left(t''\right) \tag{27.25}$$

$$+\left(-i\right)^3\int_{t_0}^{t}dt'V_I\left(t'\right)\int_{t_0}^{t'}dt''V_I\left(t''\right)\int_{t_0}^{t"}dt'''V_I\left(t'''\right)+... \tag{27.26}$$

Suppose $t>t_0$ and consider a typical term in this series. By suitably defining a contour C and time-ordering operator along this contour T_c, it can be rearranged as follows

$$\left(-i\right)^3\int_{t_0}^{t}dt'V_I\left(t'\right)\int_{t_0}^{t'}dt''V_I\left(t''\right)\int_{t_0}^{t"}dt'''V_I\left(t'''\right) \tag{27.27}$$

$$=\left(-i\right)^3\frac{1}{3!}T_c\left[\int_C dt_1V_I\left(t_1\right)\int_C dt_2V_I\left(t_2\right)\int_C dt_3V_I\left(t_3\right)\right] \tag{27.28}$$

where

- C is a contour that is here just a real line segment going from t_0 to t.
- T_c is the "time-ordering operator" that acts on "time-ordered products". Assuming $t>t_0$, T_c *places the operator which appear later on the contour C to the left.* For the time being, T_c orders operators that are bosonic in nature. A generalization will appear soon with fermionic Green's functions.
- The integral on the lef-hand side of the last equation covers all possible times such that the operators with the time that is largest (latest) are to the left. The $\frac{1}{3!}$ comes from the fact that for a general $V_I\left(t_1\right)V_I\left(t_2\right)V_I\left(t_3\right)$ there are 3! ways of ordering the operators. All these possible orders appear in the integrals on the right-hand side of the last equation. The operator T_c always orders them in the order corresponding to the left-hand side, but this means that the integral on the left-hand side appears 3! times on the right-hand side, hence the overall factor of $\frac{1}{3!}$.

- A product of operators on which T_c acts is called a time-ordered product.

One also needs $U_I(0,t)$. In this case, with $t>0$, the operators at the earliest time are on the left. This means that the contour on which the T_c is defined is ordered along the opposite direction.

A general term of the series may thus be written as

$$U_I(t,t_0)=\sum_{k=0}^{\infty}(-i)^k\frac{1}{k!}T_c\left[\left(\int_C dt_1 V_I(t_1)\right)^k\right] \tag{27.29}$$

which we can in turn write in the convenient notation

$$\boxed{U_I(t,t_0)=T_c\left[\exp\left(-i\int_C dt_1 V_I(t_1)\right)\right]} \tag{27.30}$$

where the contour is as defined above. In other words, operators are ordered right to left from t_0 to t whether t, as a real number, is larger or smaller than t_0.

Remark 198 *Derivatives of time-ordered products: A very important property of time-ordered products in general and time-ordered exponentials in general, is that they behave as ordinary exponentials when we take derivatives, as can be seen from Eq. (27.19). This remains valid as long as every operator is acted upon by the time-ordering operator.*

We can check the limiting case $[H_0,V]=0$. Then V_I is independent of time and we recover the expected exponential expression for the time evolution operator.

The definition of the time-ordering operator is extremely useful in practice not only as a formal device that allows the time evolution to still look like an exponential operator (which is explicitly unitary) but also because in many instances it will allow us to treat operators on which it acts as if they were ordinary numbers.

In the zero-temperature formalism, the analog of $U_I(t,t_0)$ is the so-called S matrix. The time-ordering concept is due to Feynman and Dyson.

Remark 199 *Non-quadratic unperturbed Hamiltonians: It is important to notice that in everything above, H_0 does not need to be quadratic in creation-annihilation operators. With very few exceptions however,[36] it is quadratic since we want the "unperturbed" Hamiltonian to be easily solvable. Note that the case where H_0 is time dependent can also be treated but in this case we would have an evolution operator $U_0(t,0)$ instead of e^{-iH_0t}. The only property of the exponential that we really use in the above derivation is the composition law obeyed by time-evolution operators in general, namely $U_0(t,t')U_0(t',t'')=U_0(t,t'')$.*

Remark 200 *The general case of time-dependent Hamiltonians: The problem we just solved for the time evolution in the interaction picture Eq.(27.19) is a much more general problem that poses itself whenever the Hamiltonian is time-dependent.*

28. *KADANOFF-BAYM AND KELDYSH-SCHWINGER CONTOURS

While we have discussed only the time evolution of the operators in the interaction representation, it is clear that we should also take into account the fact that the density matrix $e^{-\beta H}$ should also be calculated with perturbative methods. The results of the previous section can trivially be extended to the density matrix by a simple analytic continuation $t \to -i\tau$. In doing so in the present section, we will discover the many advantages of imaginary time for statistical mechanics.

Let us define evolution operators and the interaction representation for the density matrix in basically the same way as before

$$e^{-\beta H} = U(-i\beta, 0) = e^{-iH_0(-i\beta)} U_I(-i\beta, 0) = e^{-\beta H_0} U_I(-i\beta, 0) \tag{28.1}$$

The solution of the imaginary time evolution equation

$$i\frac{\partial U_I(it'', 0)}{\partial(it'')} = V_I(it'') U_I(it'', 0)$$

is then

$$U_I(-i\beta, 0) = T_c\left[\exp\left(-i\int_C d(it'') V_I(it'')\right)\right] \tag{28.2}$$

where

$$\boxed{t'' \equiv \mathrm{Im}(t)} \tag{28.3}$$

$$V_I(it'') = e^{-t''H_0} V e^{t''H_0} \tag{28.4}$$

and the contour C now proceeds from $t'' = 0$ to $t'' = -\beta$.

Overall now, the matrix elements that we need to evaluate can be expressed in such a way that the trace will be performed over the unperturbed density matrix. Indeed, using our above results, we find

$$\langle i| e^{-\beta H} \psi_H(t) \psi_H^+(t') |i\rangle = \langle i| e^{-\beta H_0} U_I(-i\beta, 0) U_I(0, t) \psi_I(t) U_I(t, 0) U_I(0, t') \psi_I^+(t') U_I(t', 0) |i\rangle \tag{28.5}$$

We want to take initial states at a time t_0 so that in practical calculations where the system is *out of equilibrium* we can choose $t_0 = -\infty$ where we can assume that the system is in equilibrium at this initial time. Hence, we are here considering a more general case than we really need but that is not more difficult so let us continue. Since we are evaluating a trace, we are free to take

$$|i\rangle = U_I(0, t_0) |i(t_0)\rangle \tag{28.6}$$

then we have

$$\langle i| e^{-\beta H} = \langle i(t_0)| U_I(t_0, 0) e^{-\beta H} = \langle i(t_0)| \left(e^{-\beta H_0} e^{\beta H_0}\right) \left(e^{iH_0 t_0} e^{-iHt_0}\right) e^{-\beta H} \tag{28.7}$$

$$= \langle i(t_0)| e^{-\beta H_0} e^{iH_0(t_0 - i\beta)} e^{-iH(t_0 - i\beta)} = \langle i(t_0)| e^{-\beta H_0} U_I(t_0 - i\beta, 0) \tag{28.8}$$

This allows us to write an arbitrary matrix element entering the thermodynamic trace as the evolution along a contour in complex time

$$\langle i| e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') |i\rangle = \langle i(t_0)| e^{-\beta H_0} U_I(t_0 - i\beta, 0) U_I(0, t) \psi_I(t) U_I(t, 0) U_I(0, t') \psi_I^\dagger(t') U_I(t', 0) |i\rangle$$

$$= \langle i(t_0)| e^{-\beta H_0} U_I(t_0 - i\beta, t_0) U_I(t_0, t) \psi_I(t) U_I(t, t') \psi_I^\dagger(t') U_I(t', t_0) |i(t_0)\rangle \tag{28.9}$$

How would we evaluate the retarded Green's function in practice using this approach? Take the case of fermions. It is convenient to define $G^>(t-t')$ and $G^<(t-t')$ by

$$\boxed{G^>(t-t') = -i\left\langle \psi_H(t)\, \psi_H^\dagger(t') \right\rangle} \tag{28.10}$$

$$\boxed{G^<(t-t') = i\left\langle \psi_H^\dagger(t')\, \psi_H(t) \right\rangle} \tag{28.11}$$

in such a way that

$$G^R(t-t') = -i\left\langle \left\{ \psi_H(t), \psi_H^\dagger(t') \right\} \right\rangle \theta(t-t') \equiv \left[G^>(t-t') - G^<(t-t') \right] \theta(t-t') \tag{28.12}$$

To evaluate $G^>(t-t')$ for example, we would expand the evolution operators such as $U_I(t', t_0)$ as a power series in V_I, each power of V_I being associated with an integral of a time ordered product that would start from t_0 to go to the creation operator $\psi_I^\dagger(t')$, then go to the destruction operator $\psi_I(t)$ until it returns to $t_0 - i\beta$. This contour is illustrated in Fig.(28-1). It is this contour that determines the order of the operators, so that even if t' is a larger number than t, as illustrated on the right panel of this figure, the operator $\psi_I(t)$ always occur after $\psi_I^\dagger(t')$ on the contour, *i.e.* $\psi_I(t)$ is on the left of $\psi_I^\dagger(t')$ in the algebraic expression. The parts of the contour that follow the real axis are displaced slightly along the imaginary direction for clarity.

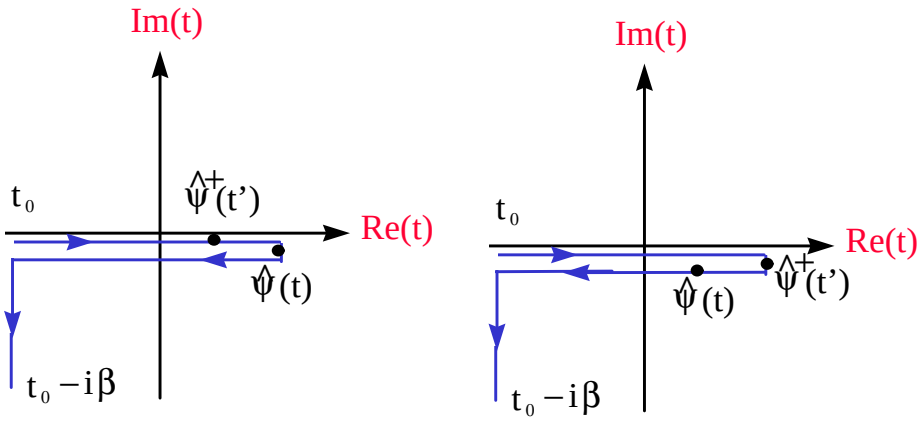


Figure 28-1 Kadanoff-Baym contour to compute $G^>(t-t')$.

We will see momentarily that it is possible to avoid this complicated contour to make calculations of equilibrium quantities. However, in non-equilibrium situations, such contours are unavoidable. In practice however, what is used by most authors is the Keldysh-Schwinger contour that is obtained by inserting $U_I(t', \infty) U_I(\infty, t') = 1$ to the left of $\psi_I^\dagger(t')$ in the algebraic expression Eq.(28.9). In practice this greatly simplifies the calculations since the contour, illustrated in Fig.(28-2), is such that integrals always go from $-\infty$ to ∞. To specify if a given creation or annihilation operator is on the upper or the lower contour, a simple 2×2 matrix suffices since there are only four possibilities..

In equilibrium, the analog of the fluctuation dissipation theorem in the form of Eq.(10.87) for correlation functions, allows us to relate $G^>$ and $G^<$, which means that we can simplify matters greatly and work with a single Green function.

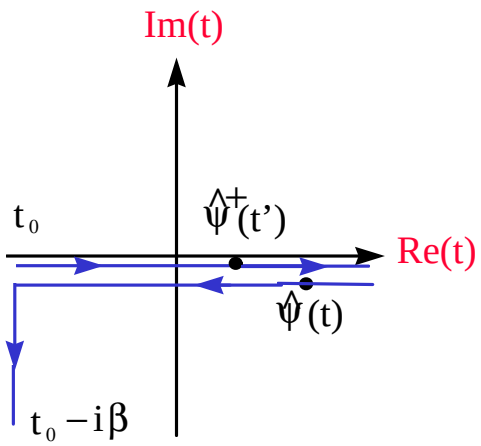


Figure 28-2 Keldysh-Schwinger contour.

Fundamentally, this is what allows us to introduce in the next section a simpler contour that is extremely more convenient for systems in equilibrium, and hence for linear response.

29. MATSUBARA GREEN'S FUNCTION AND ITS RELATION TO USUAL GREEN'S FUNCTIONS. (THE CASE OF FERMIONS)

In thermodynamic equilibrium the time evolution operator as well as the density matrix are exponentials of H times a complex number. To evaluate these operators perturbatively, one needs to calculate time-ordered products along a contour in the complex time domain that is relatively complicated, as we saw in the previous section. In the present section, we introduce a Green's function that is itself a time-ordered product but along the imaginary time axis only, as illustrated in Fig.(29-1) below. This slight generalization of the Green's function is a mathematical device that is simple, elegant and extremely convenient since the integration contour is now simple. In a sense, we take advantage of the fact that we are free to define Green's functions as we wish, as long as we connect them to observable quantities in at the end of the calculation. This is similar to what we did for correlation function. All the information about the system was in $\chi''(\mathbf{k},\omega)$, now it is all in the spectral weight $A(\mathbf{k},\omega)$, so that as long as we can extract the single-particle spectral weight we do not lose information.

What makes this Green function extremely useful for calculations is the fact that a) Perturbation theory tells us that time-ordered products are important. b) When evaluating time-ordered products that occur in the perturbation series, a theorem (Wick's theorem) tells us that all correlation functions are related to products of time-ordered Green's functions. So we might as well focus on this quantity from the start. c) For thermodynamic quantities, since only equal-time correlation functions are needed, it is clear that evaluation in imaginary time or in real time should be equivalent since only $t = 0$ is relevant. d) More generally, for time-dependent correlation functions we will see that in frequency space the analytic continuation to the physically relevant object, namely the retarded function, is trivial (only when the calculation is done analytically). We have already seen this with the Matsubara representation for correlation functions in Eq.(30.1) The same tricks apply not only to Green's functions but also to these correlation function.

After introducing the so-called Matsubara Green's function itself, we will study its properties. First, using essentially the same trick as for the fluctuation-dissipation theorem for correlation functions, we prove that for fermions these functions are antiperiodic in imaginary time. This allows us to expand them in a Fourier series. The spectral representation and the Lehmann representation, that we already discussed in the case of the harmonic oscillator, then allow us to make a clear connection between the Matsubara Green's function and the retarded function through analytic continuation. As usual, the spectral representation also allows us to do high-frequency expansions. We give specific examples of Matsubara Green's functions for non-interacting particles and show in general how to treat their Fourier series expansions, *i.e.* how to do sums over Matsubara frequencies.

29.1 Definition for fermions

As I just mentioned, it is natural to define the Green's function as we will do below for two reasons. First, perturbation theory shows clearly that imaginary-time ordered quantities come in naturally. Second, to compute physical orbservables such as the density-density correlation function $\left\langle T_\tau \psi^\dagger(\mathbf{r},\tau)\,\psi(\mathbf{r},\tau)\,\psi^\dagger(\mathbf{r}',\tau')\,\psi(\mathbf{r}',\tau')\right\rangle$,we need to take into account that the electron destroyed at $\mathbf{r}',\tau'$ by $\psi(\mathbf{r}',\tau')$ for example, can be then be created either by $\psi^\dagger(\mathbf{r},\tau)$ or by $\psi^\dagger(\mathbf{r}',\tau')$ since we must allow for all possible paths taken by the electron. This is the content of Wick's theorem. In other words, interference phenomena need to be taken into account. Since we need to know about all these possible electron propagations, the following quantity will be useful.

Definition 19 *The Matsubara Green's function is defined by*

$$\boxed{\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') = -\left\langle T_\tau \psi(\mathbf{r},\tau)\,\psi^\dagger(\mathbf{r}',\tau')\right\rangle} \tag{29.1}$$

$$= -\left\langle \psi(\mathbf{r},\tau)\,\psi^\dagger(\mathbf{r}',\tau')\right\rangle \theta(\tau-\tau') + \left\langle \psi^\dagger(\mathbf{r}',\tau')\,\psi(\mathbf{r},\tau)\right\rangle \theta(\tau'-\tau) \tag{29.2}$$

The definition of Ref.([141]) has an overall minus sign difference with the definition given here.

Remark 201 *The last equation then above defines the time ordering operator for fermions. It is very important to notice the minus sign associated with interchanging two fermion operators. This time-ordering operator is thus a slight generalization of the time-ordering operator we encountered before with the susceptibilities. There was no minus sign in this case associated with the interchange of operators. The time-ordering operator for bosonic quantities, such as V that appeared in the perturbation expansion, will never have a minus sign associated with the exchange of bosonic operators.*

We still need to specify a few things. First, the thermodynamic average is in the grand-canonical ensemble

$$\langle \mathcal{O}\rangle \equiv \frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]} \tag{29.3}$$

with μ the chemical potential and N is the total number of particle operator, while the time evolution of the operators is defined by

$$\boxed{\psi(\mathbf{r},\tau) \equiv e^{\tau(H-\mu N)}\psi_S(\mathbf{r})\,e^{-\tau(H-\mu N)}} \tag{29.4}$$

$$\boxed{\psi^\dagger(\mathbf{r},\tau) \equiv e^{\tau(H-\mu N)}\psi_S^+(\mathbf{r})\,e^{-\tau(H-\mu N)}} \tag{29.5}$$

For convenience, it is useful to define

$$\boxed{K \equiv H-\mu N} \tag{29.6}$$

Several points should attract our attention:

- The correspondence with the real-time evolution operators e^{-iHt} is done by noting that
$$\tau = -\operatorname{Im}(t) \tag{29.7}$$
or, in general for complex time
$$\boxed{\tau = it} \tag{29.8}$$

- In particular, evolution of the density matrix, or in general of an operator in imaginary time is easily deduced by doing the above replacement in our previous results. For example,

$$e^{-\beta K} = U(-i\beta, 0) = e^{-iK_0(-i\beta)} U_I(-i\beta, 0) = e^{-\beta K_0} U_I(-i\beta, 0) \quad (29.9)$$

- Strictly speaking, we should use $\psi(\mathbf{r}, -i\tau)$ if we want the symbol $\psi(\mathbf{r},t)$ for t complex to mean the same thing as before. That is why several authors write $\psi_I(\mathbf{r},\tau)$ for the Matsubara field operator. We will stick with $\psi(\mathbf{r},\tau)$ since this lack of rigor does not usually lead to confusion. We have already given enough different meanings to $\widehat{\ }$ in previous sections! Furthermore, this type of change of "confusion" in the notation is very common in Physics. For example, we should never write $f(\mathbf{k})$ to denote the Fourier transform of $f(\mathbf{r})$.

- $\psi^\dagger(\mathbf{r},\tau)$ is *not* the adjoint of $\psi(\mathbf{r},\tau)$. However, its analytic continuation $\tau \to it$ is the adjoint of $\psi(\mathbf{r},t)$.

- Using as usual the cyclic property of the trace, it is clear that $\mathcal{G}$ depends only on $\tau - \tau'$ and not on τ or τ' separately.

- It suffices to define the Matsubara Green's function $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau)$ in the interval $-\beta \leq \tau \leq \beta$. We do not need it outside of this interval. The perturbation expansion of $U_I(-i\beta, 0) = T_c\left[\exp\left(-\int_C d\tau V_I(\tau)\right)\right]$ evidently necessitates that we study at least the interval $0 \leq \tau \leq \beta$ but the other part of the interval, namely $-\beta \leq \tau \leq 0$ is also necessary if we want the time ordering operator to lead to both of the possible orders of ψ and $\psi^\dagger$: namely $\psi^\dagger$ to the left of ψ and $\psi^\dagger$ to the right of ψ. Both possibilities appear in G^R. If we had only $\tau > 0$, only one possibility would appear in the Matsubara Green's function. We will see however in the next section that, in practice, antiperiodicity allows us to trivially take into account what happens in the interval $-\beta \leq \tau \leq 0$ if we know what happens in the interval $0 \leq \tau \leq \beta$.

- To evaluate $U_I(-i\beta, 0) = T_c\left[\exp\left(-\int_C d\tau V_I(\tau)\right)\right]$ the time-ordering operator T_τ orders along the contour $(\mathrm{Im}(t) = -\beta) > (\mathrm{Im}(t') = \beta)$ which corresponds to $(\tau = \beta) > (\tau' = -\beta)$. The present contour is illustrated in Fig.(29-1). $U_I(-i\beta, 0)$ was also encountered in the previous section.

Remark 202 *Role of extra chemical potential in time evolution: The extra chemical potential in the evolution operator $e^{\tau(H-\mu N)}$ is convenient to make all operators, including the density matrix, evolve in the same way. We saw that the chemical potential came in naturally in the evaluation of the ARPES cross section. It was because we measured energy with respect to the chemical potential. The extra $e^{-\tau\mu N}$ disappears for equal-time quantities (thermodynamics) and in the calculation of expectation values $\langle \mathcal{O}^+(t)\mathcal{O}(t')\rangle$ for operators $\mathcal{O}$ which are bilinear in fermions of the form $(\psi^+\psi)$ at equal time. Indeed $\psi^+\psi$ commutes with the number operator so that in that case $\mathcal{O}^+(t) = e^{iHt}\mathcal{O}^+e^{-iHt} = e^{i(H-\mu N)t}\mathcal{O}^+e^{-i(H-\mu N)t}$. When Wick's theorem is used to compute expectation values, the creation and annihilation operators evolve then as above. In any case, as we just said, the addition of the chemical potential in the evolution operator just amounts to measuring the energy of single-particle excitations with respect to the chemical potential. To show this, first note that we work with Hamiltonians that conserve the number of particles, i.e. $[H, N] = 0$, which allows us to write $e^{it(H-\mu N)} = e^{itH}e^{-it\mu N}$. Then we have that $e^{it(H-\mu N)}\psi_S(\mathbf{r})\, e^{-it(H-\mu N)} = e^{it\mu}\left(e^{itH}\psi_S(\mathbf{r})\, e^{-itH}\right)$ because there is always one less particle in the new state once $\psi_S(\mathbf{r})$ has acted (You can also count the necessary commutators explicitly). Going to Fourier space, $\int dt e^{i(\omega+i\eta)t}$*

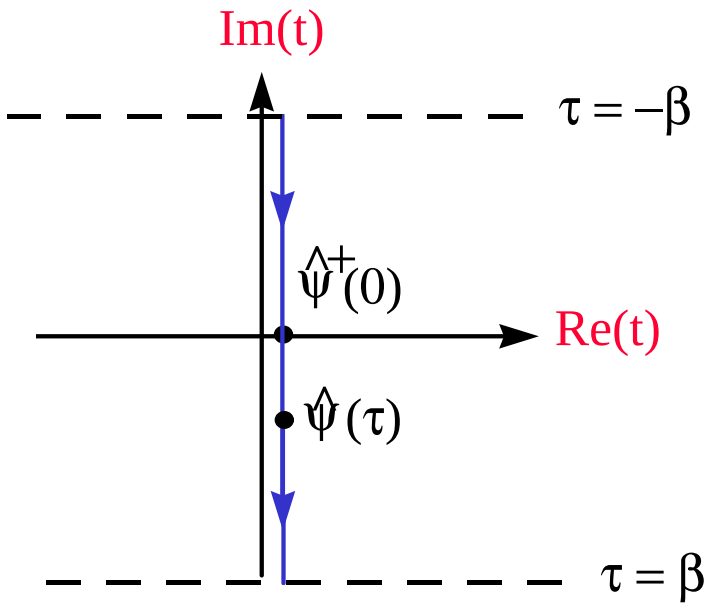


Figure 29-1 Contour for time ordering in imaginary time. Only the time difference is important. The contour is translated slightly along the real-time axis for clarity.

becomes $\int dt e^{i(\omega+i\eta+\mu)t}$ *so that indeed the difference between the Fourier transform of the Green's function where the evolution operator is* K *instead of* H *is equivalent to a change from* ω *to* $\omega+\mu$ *. With the latter definition,* $\omega=0$ *corresponds to single-particle excitations that are at the Fermi level. All of this will also be clarified by the Lehmann representation introduced later.*

29.2 Time ordered product in practice

Suppose I want to compute the following quantity for fermions:

$$\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau_3)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle. \tag{29.10}$$

We drop space indices to unclutter the equations. The time ordered product for fermions keeps tract of permutations, so if I exchange the first two operators for example, I find

$$\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau_3)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle = -\left\langle T_\tau \psi^\dagger(\tau_3)\psi(\tau_1)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle \tag{29.11}$$

I need not worry about delta functions at equal time or anything but the number of fermion exchanges. Indeed, whichever of the above two expressions I start with, if $\tau_1<\tau_2<\tau_3<\tau_4$, I will find at the end that

$$\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau_3)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle = -\left\langle \psi^\dagger(\tau_4)\psi^\dagger(\tau_3)\psi(\tau_2)\psi(\tau_1)\right\rangle. \tag{29.12}$$

We cannot, however, have two of the times equal for a ψ and a $\psi^\dagger$. We have to specify that one is infinitesimally larger or smaller than the other to know in which order to place the operators since they do not commute or anticommute.

Another interesting property of the time-ordered product is that we can differentiate exponentials with respect to parameters appearing in the argument as if it was an ordinary exponential. For example note how the derivative below is done

$$\begin{aligned} & \frac{\partial}{\partial\alpha}\left\langle T_\tau e^{\alpha\left(\psi(\tau_5)\psi^\dagger(\tau_6)\right)}\psi\left(\tau_1\right)\psi^\dagger\left(\tau_3\right)\psi\left(\tau_2\right)\psi^\dagger\left(\tau_4\right)\right\rangle \\ = & \left\langle T_\tau e^{\alpha\left(\psi(\tau_5)\psi^\dagger(\tau_6)\right)}\psi\left(\tau_5\right)\psi^\dagger\left(\tau_6\right)\psi\left(\tau_1\right)\psi^\dagger\left(\tau_3\right)\psi\left(\tau_2\right)\psi^\dagger\left(\tau_4\right)\right\rangle \end{aligned} \tag{29.13}$$

This can be understood as follows. The exponential is defined by its power series. One can thus do the expansion, differentiate term by term and re-exponentiate without worrying about the imaginary times appearing in the argument since the time-ordering operator will take care of that when the correlation function needs to be evaluated for a particular set of imaginary times.

29.3 Antiperiodicity and Fourier expansion (Matsubara frequencies)

Suppose $\tau < 0$. Then the definition Eq.(29.1) tells us that

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = \left\langle \psi^+\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},\tau\right)\right\rangle \tag{29.14}$$

Using the cyclic property of the trace twice, as in the demonstration of the fluctuation-dissipation theorem it is easy to show that

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = -\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right) \quad ; \quad -\beta < \tau < 0} \tag{29.15}$$

This boundary condition is sometimes known as the Kubo-Martin-Schwinger (KMS) boundary condition. [151]

Proof: Let

$$e^{-\beta\Omega} \equiv \mathrm{Tr}\left[e^{-\beta K}\right] \tag{29.16}$$

then because $\tau < 0$, it follows from the definition that

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = e^{\beta\Omega}\,\mathrm{Tr}\left[e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\psi\left(\mathbf{r},\tau\right)\right] \tag{29.17}$$

The cyclic property of the trace then tells us that

$$\begin{aligned} \mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) &= e^{\beta\Omega}\,\mathrm{Tr}\left[\psi\left(\mathbf{r},\tau\right)e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\right] && (29.18)\\ &= e^{\beta\Omega}\,\mathrm{Tr}\left[\left(e^{-\beta K}e^{\beta K}\right)\left(e^{K\tau}\psi\left(\mathbf{r}\right)e^{-K\tau}\right)e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\right] \\ &= \left\langle\psi\left(\mathbf{r},\tau+\beta\right)\psi^+\left(\mathbf{r}',0\right)\right\rangle \\ &= -\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right) && (29.19)\end{aligned}$$

The last line follows because given that $-\beta < \tau$, we necessarily have $\tau+\beta > 0$ so that the other θ function must be used in the definition Eq.(29.1) of the Matsubara Green's function and an extra sign appears.

If $\tau > 0$, the above arguments can be repeated to yield

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\beta\right) = -\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) \quad ; \quad \beta > \tau > 0} \tag{29.20}$$

Remark 203 *However, for $\tau > 0$ note that*

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) \neq -\mathcal{G}(\mathbf{r},\mathbf{r}';\tau+\beta) \quad ; \quad \tau > 0 \tag{29.21}$$

While $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau+\beta)$ for $\tau > 0$ is well defined, we never need this function. So we restrict ourselves to the interval $-\beta \leq \tau \leq \beta$ described in the previous section.

One can take advantage of the antiperiodicity property of the Green's function in the interval $-\beta \leq \tau \leq \beta$ to expand it in a Fourier series that will automatically guaranty that the crucial antiperiodicity property is satisfied. More specifically, we write

$$\boxed{\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)} \tag{29.22}$$

where the so-called Matsubara frequencies for fermions are odd, namely

$$\boxed{k_n = (2n+1)\pi T = \frac{(2n+1)\pi}{\beta}} \quad ; \quad n \quad \text{integer} \tag{29.23}$$

The antiperiodicity property will be automatically fulfilled because $e^{-ik_n\beta} = e^{-i(2n+1)\pi} = -1$.

Choice of units Here and from now on, we have taken Boltzmann's constant k_B to be equal to unity.

The expansion coefficients are obtained as usual for Fourier series of antiperiodic functions from

$$\boxed{\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)} \tag{29.24}$$

Note that only the $\tau > 0$ region of the domain of definition is needed, as promised. The case of bosons is left as an exercise.

Remark 204 *Domain of definition of the Matsubara Green's function: The value of $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)$ given by the Fourier series (29.22) for τ outside the interval $-\beta < \tau < \beta$, is in general different from the actual value of Eq.(29.1) $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') = -\left\langle T_\tau \psi(\mathbf{r},\tau)\psi^+(\mathbf{r}',\tau')\right\rangle$. Indeed, to define a Fourier series one extends the function defined in the interval $-\beta < \tau < \beta$ so that it is periodic in τ outside this interval with a period 2β. The true function $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') = -\left\langle T_\tau \psi(\mathbf{r},\tau)\psi^+(\mathbf{r}',\tau')\right\rangle$ has an envelope that is, instead, exponential outside the original interval. We will see an explicit example in the case of the free particles. In perturbation expansions, we never need $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)$ outside the interval where the series and the true definition give different answers. To avoid mathematical inconsistencies, it is nevertheless preferable in calculations to do Matsubara frequency sums before any other integral! It is possible to invert the order of integration and of summation in most of the cases, but we must beware.*

29.4 * G^R and $\mathcal{G}$ can be related using contour integration

To establish the relation between the Matsubara Green's function and the retarded one, and by the same token establish the spectral representation for $\mathcal{G}$, one usually proceeds with the Lehmann representation, as we did in section 30.1 for the

susceptibility. Even though this is a method that is never used in practice, it is instructive to use the method described below that shows explicitly the analytic continuation in the complex real plane. Begin with the definitions

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) = -\left\langle \psi(\mathbf{r},\tau)\,\psi^{+}(\mathbf{r}',0)\right\rangle \theta(\tau) + \left\langle \psi^{+}(\mathbf{r}',0)\,\psi(\mathbf{r},\tau)\right\rangle \theta(-\tau) \tag{29.25}$$

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = \int_0^{\beta} d\tau e^{ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) \tag{29.26}$$

$$= \int_0^{\beta} d\tau e^{ik_n\tau}\left[-\left\langle \psi(\mathbf{r},\tau)\,\psi^{+}(\mathbf{r}',0)\right\rangle\right]. \tag{29.27}$$

Assume that $k_n > 0$. Then, as illustrated in Fig.(29-2), we can deform the contour of integration within the domain of analyticity along $\mathrm{Re}(t) = \mathrm{Im}(\tau) > 0$. (The analyticity of $\left\langle \psi(\mathbf{r},\tau)\,\psi^{+}(\mathbf{r}',0)\right\rangle$ in that domain comes from $e^{-\beta H}$ in the trace. You will be able to prove this later by calculating $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)$ with the help of the spectral representation Eq.(29.34) and tricks for evaluating sums on Matsubara frequencies. For $\mathrm{Im}(\tau) = \infty$ there will be no contribution from the small segment since $e^{ik_n\tau}$ becomes a decaying exponential. The integral becomes

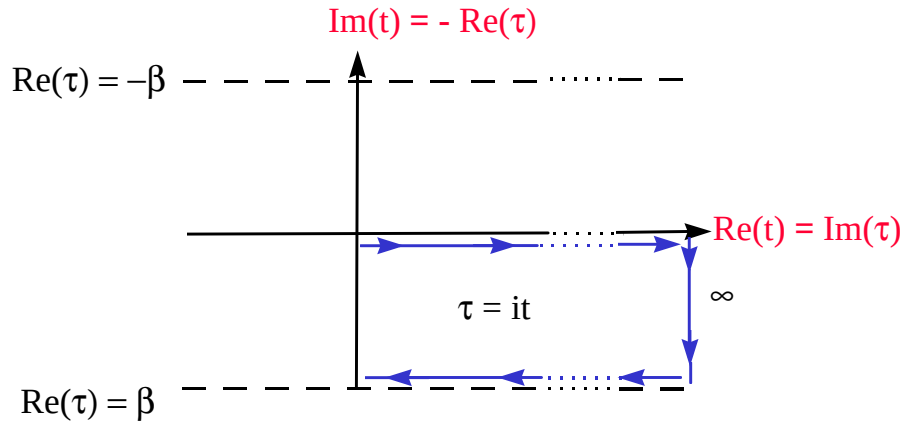


Figure 29-2 Deformed contour used to relate the Matsubara and the retarded Green's functions.

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = \tag{29.28}$$
$$\int_{t=0}^{t=\infty} d(it)\left[-\left\langle \psi(\mathbf{r},t)\,\psi^{+}(\mathbf{r}')\right\rangle\right] e^{ik_n(it)}$$
$$+\int_{t=\infty}^{t=0} d(it)\left[-\left\langle \psi(\mathbf{r},t-i\beta)\,\psi^{+}(\mathbf{r}')\right\rangle\right] e^{(ik_n)i(t-i\beta)}$$

In the last integral, we then use the results

$$e^{(ik_n)i(-i\beta)} = e^{(ik_n)\beta} = -1 \tag{29.29}$$

$$\int_{\infty}^{0} = -\int_{0}^{\infty} \tag{29.30}$$

$$\begin{aligned} -\left\langle \psi(\mathbf{r},t-i\beta)\,\psi^{+}(\mathbf{r}')\right\rangle &= \\ \left[-\left\langle e^{iK(t-i\beta)}\psi_S(\mathbf{r})\,e^{-iK(t-i\beta)}\psi_S^{\dagger}(\mathbf{r}')\right\rangle\right] &= \left[-\left\langle e^{\beta K}e^{iKt}\psi_S(\mathbf{r})\,e^{-iKt}e^{-\beta K}\psi_S^{\dagger}(\mathbf{r}')\right\rangle\right] \end{aligned} \tag{29.31}$$

It then suffices to cancel the left most $e^{\beta K}$ with the density matrix and to use the cyclic property of the trace to obtain for the integrand of the last integral,

$$= \left[- \left\langle \psi^{\dagger}\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},t\right)\right\rangle \right]. \tag{29.32}$$

Overall then, the integral in Eq.(29.28) is equal to

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = -i\int_0^{\infty} dt \left\langle \left\{ \psi\left(\mathbf{r},t\right), \psi^{\dagger}\left(\mathbf{r}',0\right)\right\}\right\rangle e^{i(ik_n)t} \tag{29.33}$$

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n - \omega'}.} \tag{29.34}$$

All that we assumed to deform the contour was that $k_n > 0$. Thus, $ik_n \rightarrow \omega + i\eta$ with $\eta > 0$ is consistent with the hypothesis and allows us to deform the contour as advertized. Comparing the formula for $\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)$ for $k_n > 0$ with the expression for the retarded Green's function(26.46), we see that analytic continuation is possible.

$$\boxed{G^R\left(\mathbf{r},\mathbf{r}';\omega\right) = \lim_{ik_n \rightarrow \omega + i\eta} \mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)} \tag{29.35}$$

If we had started with $k_n < 0$, analytic continuation $ik_n \rightarrow \omega - i\eta$ to the advanced Green's function would have been possible.

Remark 205 *Connectedness: For a general bosonic correlation function, similar spectral representations can also be defined for connected functions (see below). As an example of connected function, $\langle A(\tau) B\rangle - \langle A(\tau)\rangle \langle B\rangle$ is connected. The subtracted term allows the combination of correlation functions to behave as a response function and appears naturally in the functional derivative approach. If $\langle A(\tau)\rangle$ has a piece that is independent of τ, the subtraction allows the integral on the contour at infinity on the above figure to vanish even at zero Matsubara frequency. Otherwise, that would not be the case.*

29.5 The Lehmann representation tells us the physical meaning of the spectral weight and the relation between G^R and $\mathcal{G}$

For a general correlation function, not necessarily a Green's function, one establishes the connection between Matsubara functions and retarded functions by using the Lehmann representation. This representation is also extremely useful to extract the physical significance of the poles of correlation functions so this is why we introduce it at this point. We have already seen examples of Lehmann representation in the one-body case when we wrote in Eq.(26.23),

$$G^R\left(\mathbf{r},\mathbf{r}';\omega\right) = \sum_n \frac{\phi_n\left(\mathbf{r}\right)\phi_n^*\left(\mathbf{r}'\right)}{\omega + i\eta - E_n}$$

and also in Sec. 10.9 on correlation functions.

Let us consider the more general many-body case, starting from the Matsubara Green's function. It suffices to insert a complete set of energy eigenstates between each field operator in the expression for the spectral weight

$$\begin{aligned} A(\mathbf{r},\mathbf{r}';t) &\equiv \left\langle \left\{ \psi(\mathbf{r},t), \psi^{+}(\mathbf{r}',0) \right\} \right\rangle \qquad (29.36) \\ &= e^{\beta\Omega} \sum_{m,n} \Big[\langle n| e^{-\beta K} e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} |m\rangle \langle m| \psi_S^{\dagger}(\mathbf{r}') |n\rangle \\ &\quad + \langle n| e^{-\beta K} \psi_S^{\dagger}(\mathbf{r}') |m\rangle \langle m| e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} |n\rangle \Big] \end{aligned}$$

We now use $e^{-iKt}|n\rangle = e^{-iK_n t}|n\rangle$ with $K_n = E_n - \mu N_n$ if there are N_n particles in the initial state $|n\rangle$. In the first term above, $\langle n|$ has one less particle than $|m\rangle$ while the reverse is true in the second term so that $K_m - K_n = (E_m - \mu(N_n + 1) - E_n + \mu N_n)$ in the first term and $K_n - K_m = (E_n - \mu N_n - E_m + \mu(N_n - 1))$ in the second. Taking the Fourier transform $\int dt e^{i\omega' t}$ we have

$$\begin{aligned} A(\mathbf{r},\mathbf{r}';\omega') &= e^{\beta\Omega} \times \qquad (29.37) \\ &\sum_{mn} \Big[e^{-\beta K_n} \langle n| \psi_S(\mathbf{r}) |m\rangle \langle m| \psi_S^{\dagger}(\mathbf{r}') |n\rangle 2\pi\delta(\omega' - (E_m - \mu - E_n)) \\ &+ e^{-\beta K_n} \langle n| \psi_S^{\dagger}(\mathbf{r}') |m\rangle \langle m| \psi_S(\mathbf{r}) |n\rangle 2\pi\delta(\omega' - (E_n - \mu - E_m)) \Big] \end{aligned}$$

One can interpret physically the spectral weight as follows. It has two pieces, the first one for excited states with one more particle, and the second one for excited states with one more hole. Photoemission experiments (See Einstein's Nobel prize) access this last piece of the spectral weight, while Bremsstrahlung inverse spectroscopy (BIS) experiments measure the first piece.[1] Excited particle states contribute to positive frequencies ω' if their excitation energy is larger than the chemical potential, $E_m - E_n > \mu$ and to negative frequencies otherwise. Zero frequency means that the excitation energy is equal to the chemical potential. In other words, every excited single-particle or single-hole state corresponds to a delta function in the spectral weight whose weight depends on the overlap between initial states with one more particle at $\mathbf{r}'$ or one more hole at $\mathbf{r}$, and the true excited states.

Remark 206 *At zero temperature, we have*

$$\begin{aligned} A(\mathbf{r},\mathbf{r}';\omega') &= \sum_{m} \Big[\langle 0| \psi_S(\mathbf{r}) |m\rangle \langle m| \psi_S^{\dagger}(\mathbf{r}') |0\rangle 2\pi\delta(\omega' + \mu - (E_m - E_0)) \\ &+ \langle 0| \psi_S^{\dagger}(\mathbf{r}') |m\rangle \langle m| \psi_S(\mathbf{r}) |0\rangle 2\pi\delta(\omega' + \mu - (E_0 - E_m)) \Big] \end{aligned}$$

In the first term, E_m is the energy of an eigenstate with one more particle than the ground state. The minimal energy to add a particle is μ, hence, $E_m - E_0 \geq \mu$ and the delta function contributes to positive frequencies. In the second term however, E_m is the energy with one less particle so $0 \leq E_0 - E_m \leq \mu$ since we can remove a particle, or create a hole, below the Fermi surface. Hence the second term contributes to negative frequencies.

Remark 207 *By using $K = H - \mu N$ instead of H as time evolution operator, we have adopted, as mentioned above, a convention where the frequency ω represents the energy of single-particle excitations above or below the chemical potential. If we had used H as evolution operator, only ω instead of the combination $\omega + \mu$ would have appeared in the delta functions above.*

[1] To be more specific, these experiments add or remove particles in momentum, not position eigenstates. The only change that this implies in the discussion above is that $\psi_S^{(\dagger)}(\mathbf{r})$ should be replaced by $c_{\mathbf{p}}^{(\dagger)}$.

The spectral representation Eq.(29.34) immediately tells us that the poles of the single-particle Green's functions are at the same position as delta functions in the spectral weight, in other words they are at the excited single-particle or single-hole states. Doing changes of dummy summation indices we can arrange so that it is always $\langle n|$ that has one less particle. Then,

$$\boxed{A\left(\mathbf{r},\mathbf{r}';\omega'\right)=e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n}+e^{-\beta K_m}\right)\left\langle n\right|\psi_S\left(\mathbf{r}\right)\left|m\right\rangle\left\langle m\right|\psi_S^{\dagger}\left(\mathbf{r}'\right)\left|n\right\rangle 2\pi\delta\left(\omega'-\left(K_m-K_n\right)\right)} \tag{29.38}$$

Now I show that the spectral representation in Eq.(29.34) is valid for the Matsubara Green's function. By definition

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) &= \int_0^{\beta}d\tau e^{ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) &(29.39)\\ &= -\int_0^{\beta}d\tau e^{ik_n\tau}\left\langle\psi\left(\mathbf{r},\tau\right)\psi^{+}\left(\mathbf{r}',0\right)\right\rangle. &(29.40)\end{aligned}$$

Writing explicitly the trace, the density matrix and using complete sets of energy eigenstates, this can be rewritten as

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) &= -\int_0^{\beta}d\tau e^{ik_n\tau}e^{\beta\Omega}\sum_{mn}\left\langle n\right|e^{-\beta K}e^{K\tau}\psi_S\left(\mathbf{r}\right)e^{-K\tau}\left|m\right\rangle\left\langle m\right|\psi_S^{\dagger}\left(\mathbf{r}'\right)\left|n\right\rangle\\ &= -\int_0^{\beta}d\tau e^{(ik_n+K_n-K_m)\tau}e^{-\beta K_n}e^{\beta\Omega}\sum_{mn}\left\langle n\right|\psi_S\left(\mathbf{r}\right)\left|m\right\rangle\left\langle m\right|\psi_S^{\dagger}\left(\mathbf{r}'\right)\left|n\right\rangle.\end{aligned}$$

The integral of the exponential is easy to do. Using the equality $e^{ik_n\beta}=e^{i(2n+1)\pi}=-1$, which is valid given the definition of the Matsubara frequencies, we are left with

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n}+e^{-\beta K_m}\right)\frac{\langle n|\psi_S(\mathbf{r})|m\rangle\langle m|\psi_S^{\dagger}(\mathbf{r}')|n\rangle}{ik_n-(E_m-E_n-\mu)}}. \tag{29.41}$$

This is the Lehmann representation. It tells us how to interpret the poles of the analytically continued $\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)$, and importantly, it tells us that

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n-\omega'} \tag{29.42}$$

is a valid representation, with $A\left(\mathbf{r},\mathbf{r}';\omega'\right)$ exactly the same spectral weight Eq. (29.38) as the retarded Green's function.

Remark 208 *Standard way of proving analytical continuation formula: The standard way of proving that $G^R\left(\omega\right)=\lim_{ik_n\to\omega+i\eta}\mathcal{G}\left(ik_n\right)$ is to first find the Lehmann representation for both quantities, as we just did. The previous section does it in an unusual but instructive manner.*

29.6 Spectral weight and rules for analytical continuation

In this section, we summarize what we have learned for the analytic properties of the Matsubara Green's function and we clarify the rules for analytic continuation.[**?**]

The key result for understanding the analytical properties of $\mathcal{G}$ is the spectral representation Eq.(29.34). The spectral weight $A(\mathbf{r},\mathbf{r}';\omega')$ was discussed just in the previous subsection (See also Eq.(29.38) for the Lehmann representation).

The Matsubara Green's function and the retarded functions are special cases of a more general function defined in the complex frequency plane by

$$\boxed{G(\mathbf{r},\mathbf{r}';z)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{z-\omega'}} \tag{29.43}$$

This function is analytic everywhere except on the real axis. Physically interesting special cases are

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)=G(\mathbf{r},\mathbf{r}';ik_n)$$

$$G^R(\mathbf{r},\mathbf{r}';\omega)=\lim_{\eta\to 0}G(\mathbf{r},\mathbf{r}';\omega+i\eta) \tag{29.44}$$

$$G^A(\mathbf{r},\mathbf{r}';\omega)=\lim_{\eta\to 0}G(\mathbf{r},\mathbf{r}';\omega-i\eta) \tag{29.45}$$

The function $G(\mathbf{r},\mathbf{r}';z)$ has a jump on the real axis given by

$$\boxed{A(\mathbf{r},\mathbf{r}';\omega)=i\lim_{\eta\to 0}\left[G(\mathbf{r},\mathbf{r}';\omega+i\eta)-G(\mathbf{r},\mathbf{r}';\omega-i\eta)\right]} \tag{29.46}$$

$$A(\mathbf{r},\mathbf{r}';\omega)=i\left[G^R(\mathbf{r},\mathbf{r}';\omega)-G^A(\mathbf{r},\mathbf{r}';\omega)\right]$$

In the special case where $A(\mathbf{r},\mathbf{r}';\omega)$ is real (which is almost always the case in practice since we consider $\mathbf{r}=\mathbf{r}'$ or $\mathbf{k}=\mathbf{k}'$), we have

$$A(\omega)=-2\,\mathrm{Im}\,G^R(\omega) \tag{29.47}$$

like we have often used in the one-body case.

Remark 209 *$A(\mathbf{r},\mathbf{r}';\omega)$ can be complex in the presence of a spontaneously broken time-reversal symmetry or of a magnetic field since in those cases the wave functions can be complex. In this general case, since $G^R(\mathbf{r},\mathbf{r}';\omega)^*=G^A(\mathbf{r}',\mathbf{r};\omega)$, it follows from the above formulae that the spectral weight can be extracted from the anti-hermitian part of the Green function matrix, namely*

$$A(\mathbf{r},\mathbf{r}';\omega)=i\left[G^R(\mathbf{r},\mathbf{r}';\omega)-G^R(\mathbf{r}',\mathbf{r};\omega)^*\right]$$

as is further discussed in Eq.(32.20) below.

The previous results are summarized in Fig.(29-3) which displays the analytic structure of $G(\mathbf{r},\mathbf{r}';z)$. This function is analytical everywhere except on the real axis where it has a branch cut leading to a jump Eq.(29.46) in the value of the function as we approach the real axis from either the upper or lower complex half-plane. The limit as we come from the upper half-plane is equal to $G^R(\mathbf{r},\mathbf{r}';\omega)$ whereas from the lower half-plane it is equal to $G^A(\mathbf{r},\mathbf{r}';\omega)$. The Matsubara Green's function is defined only on a discrete but infinite set of points along the imaginary frequency axis.

The problem of finding $G^R(\mathbf{r},\mathbf{r}';\omega)$ along the real-time axis from the knowledge of the Matsubara Green's function is a problem of analytical continuation. Unfortunately, $G(z=ik_n)$ does not have a unique analytical continuation because there is an infinite number of analytical functions that have the same value along this discrete set of points. For example, suppose we know $G(z=ik_n)$, then $G(z)\left(1+\left(e^{\beta z}+1\right)\right)$ has the same value as $G(z)$ for all points $z=ik_n$ because $e^{ik_n\beta}+1=0$. Baym and Mermin[26], using results from the theory of complex functions, have obtained the following result.

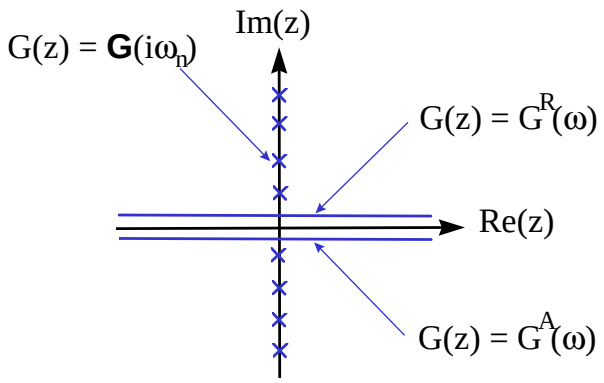


Figure 29-3 Analytical structure of $G(z)$ in the complex frequency plane. $G(z)$ reduces to either $G^R(\omega)$, $G^A(\omega)$ or $\mathcal{G}(i\omega_n)$ depending on the value of the complex frequency z. There is a branch cut along the real axis.

Theorem 20 *If*

1. $G(z)$ is analytic in the upper half-plane
2. $G(z) = \mathcal{G}(ik_n)$ for all Matsubara frequencies
3. $\lim_{z\to\infty} zG(z) = cst$

then the analytical continuation is unique and

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \lim_{ik_n\to\omega+i\eta} \mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) \tag{29.48}$$

The key point is the third one on the asymptotic behavior at high frequency. That this is the correct asymptotic behavior at high frequency follows trivially from the spectral representation Eq.(29.43) as long as we remember that the spectral weight is bounded in frequency. The non-trivial statement is that this asymptotic behavior suffices to make the analytical continuation unique. In practice this rarely poses a problem. The simple replacement $ik_n \to \omega + i\eta$ suffices. Nevertheless, the asymptotic behavior reflects a very fundamental property of the physical system, namely the anticommutation relations! It is thus crucial to check that it is satisfied. More on the meaning of the asymptotic behavior in subsection (32.1).

Remark 210 *Numerical calculations are often done in Matsubara frequency, or in imaginary time. This is much easir to handle than oscillating functions. The analytic continuation however is much more problematic. One can use Padé approximants if the data has very high precision, or Maximum Entropy analytic continuation[108] if it is less accurate. Software is available on the internet for these tasks. ([28])*

29.7 Matsubara Green's function for translationally invariant systems

We first present the definition of the Matsubara Green's function in momentum space since this is where, in translationally invariant systems, it will be diagonal.

Let us first show explicitly what we mean by Green's function in momentum space. We expect $\mathcal{G}(\mathbf{k};\tau-\tau') = -\left\langle T_\tau c_{\mathbf{k}}(\tau) c^\dagger_{\mathbf{k}}(\tau')\right\rangle$ but let us see this in detail.

With our definition of momentum and real space second quantized operators, and our normalization for momentum eigenstates Eq.(24.36) we have

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') = -\left\langle T_\tau \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\right\rangle = -\left\langle T_\tau \sum_{\mathbf{k}} \langle \mathbf{r}\,|\mathbf{k}\rangle c_{\mathbf{k}}(\tau) \sum_{\mathbf{k}'} c^\dagger_{\mathbf{k}'}(\tau')\langle \mathbf{k}'\,|\mathbf{r}'\rangle\right\rangle \tag{29.49}$$

$$\langle \mathbf{r}\,|\mathbf{k}\rangle\langle \mathbf{k}'\,|\mathbf{r}'\rangle = \frac{1}{\mathcal{V}} e^{i\mathbf{k}\cdot\mathbf{r}-i\mathbf{k}'\cdot\mathbf{r}'} = \frac{1}{\mathcal{V}} e^{i(\mathbf{k}-\mathbf{k}')\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)+i\left(\frac{\mathbf{k}+\mathbf{k}'}{2}\right)\cdot(\mathbf{r}-\mathbf{r}')}. \tag{29.50}$$

Assuming space translation invariance, we can integrate over the center of mass coordinate and divide by volume since $\frac{1}{\mathcal{V}}\int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) = 1$. Using

$$\frac{1}{\mathcal{V}}\int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) e^{i(\mathbf{k}-\mathbf{k}')\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)} = \frac{1}{\mathcal{V}}(2\pi)^3\delta(\mathbf{k}-\mathbf{k}') = \delta_{\mathbf{k},\mathbf{k}'} \tag{29.51}$$

we are left with

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') = -\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}(\tau) c^\dagger_{\mathbf{k}'}(\tau') e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}\right\rangle \tag{29.52}$$

$$\begin{aligned}
\mathcal{G}(\mathbf{k};\tau-\tau') &= \int d(\mathbf{r}-\mathbf{r}')\, e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') &(29.53)\\
&= \int d(\mathbf{r}-\mathbf{r}')\, e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\left[-\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}(\tau) c^\dagger_{\mathbf{k}'}(\tau') e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}\right\rangle\right]\\
&\boxed{\mathcal{G}(\mathbf{k};\tau-\tau') = -\left\langle T_\tau c_{\mathbf{k}}(\tau) c^\dagger_{\mathbf{k}}(\tau')\right\rangle} &(29.54)
\end{aligned}$$

which could have been guessed from the start! Our definitions of Fourier transforms just make this work.

Remark 211 *Momentum indices and translational invariance: Note that the conservation of total momentum corresponding to translational invariance corresponds to the sum of the momentum indices of the creation-annihilation operators being equal to zero. The sign of momentum is counted as negative when it appears on a creation operator.*

Remark 212 *Note that in the special case of non-interacting systems the easiest way to get the final result is to remember that we can use energy eigenstates to do the thermodynamic and quantum mechanical trace. Since eigenstates are of the form $c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2}\cdots|0\rangle$ and the time evolution can just be represented by $c_{\mathbf{k}'}(\tau) = \exp(-\zeta_{\mathbf{k}'})c_{\mathbf{k}'}$, as I show below. Then all the terms that do not have the same value of $\mathbf{k}$ for the creation and annihilation operators of the Green's function will vanish because they will create states that are orthogonal. Indeed, the set of states will then be different in the bra and the ket.*

29.8 Matsubara Green's function in the non-interacting case

In this section, we want to make the Matsubara Green's function our friend by looking at it in the non-interacting case from many different points of view. We

will see how it looks both in imaginary time and in Matsubara frequency, deriving the results in at least two very different ways: from the definition and from the equations of motion.

29.8.1 $\mathcal{G}_0(\mathbf{k}; ik_n)$ from the spectral representation

The above is a general result for a translationally invariant system. Let us specialize to non-interacting particles, namely to quadratic diagonal Hamiltonian

$$K_0 = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c^+_{\mathbf{k}} c_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c^+_{\mathbf{k}} c_{\mathbf{k}} \tag{29.55}$$

The result for the Green's function may be obtained either directly by calculating the spectral weight and integrating, or from the definition or by integrating the equations of motion. The three ways of obtaining the simple result

$$\boxed{\mathcal{G}_0(\mathbf{k}; ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}}}} \tag{29.56}$$

are instructive, so we will do all of them below. The simplest way to obtain the above result is to remember that

$$\boxed{G^R(\mathbf{k}; \omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}}} \tag{29.57}$$

which implies that $A(\mathbf{k},\omega) = 2\pi\delta(\omega - \zeta_{\mathbf{k}})$. Since the spectral weight is the same for $\mathcal{G}_0(\mathbf{k}; ik_n)$, the result follows. The only difference with the one-body case is in the presence of the chemical potential in $\zeta_{\mathbf{k}}$.

29.8.2 *$\mathcal{G}_0(\mathbf{k}; \tau)$ and $\mathcal{G}_0(\mathbf{k}; ik_n)$ from the definition

To evaluate the Green's function from its definition, we need $c_{\mathbf{k}}(\tau)$. That quantity may be obtained by solving the Heisenberg equations of motion,

$$\frac{\partial c_{\mathbf{k}}}{\partial \tau} = [K_0, c_{\mathbf{k}}] = -\zeta_{\mathbf{k}} c_{\mathbf{k}} \tag{29.58}$$

The commutator was easy to evaluate by recalling the theorem on number operators seen in Sec.24.1.3 $[n_{\mathbf{k}'}, c_{\mathbf{k}}] = -c_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}$ or by using our standard trick Eq.(24.89). The resulting differential equation is easy to integrate given the initial condition on Heisenberg operators. We obtain,

$$c_{\mathbf{k}}(\tau) = e^{-\zeta_{\mathbf{k}}\tau} c_{\mathbf{k}} \tag{29.59}$$

so that substituting in the definition,

$$\mathcal{G}_0(\mathbf{k}; \tau) = -\left\langle T_\tau c_{\mathbf{k}}(\tau) c^\dagger_{\mathbf{k}} \right\rangle = -e^{-\zeta_{\mathbf{k}}\tau} \left[\left\langle c_{\mathbf{k}} c^\dagger_{\mathbf{k}} \right\rangle \theta(\tau) - \left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle \theta(-\tau) \right] \tag{29.60}$$

using the standard result from elementary statistical mechanics,

$$\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle = f(\zeta_{\mathbf{k}}) = \frac{1}{e^{\beta\zeta_{\mathbf{k}}} + 1} \tag{29.61}$$

and $\left\langle c_{\mathbf{k}} c^\dagger_{\mathbf{k}} \right\rangle = 1 - \left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle$ we obtain

$$\boxed{\mathcal{G}_0(\mathbf{k}; \tau) = -e^{-\zeta_{\mathbf{k}}\tau} \left[(1 - f(\zeta_{\mathbf{k}})) \theta(\tau) - f(\zeta_{\mathbf{k}}) \theta(-\tau) \right]}. \tag{29.62}$$

Exercise 29.8.1 *Fermi-Dirac statistics: Show by explicit calculation in the grand-canonical ensemble that* $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = f(\zeta_{\mathbf{k}}) = \frac{1}{e^{\beta\zeta_{\mathbf{k}}}+1}$. *Hint: The grand partition function for non-interacting systems is equal to the product of the partition functions for each basis state* $\mathbf{k}$ *separately. And for each* $\mathbf{k}$*, the trace will be over states* $|0\rangle$ *and* $c_{\mathbf{k}}^{\dagger}|0\rangle$.

Remark 213 *Inadequacy of Matsubara representation outside the domain of definition: We see here clearly that if* $\tau < 0$ *the equality*

$$\mathcal{G}_0(\mathbf{k};\tau+\beta) = -\mathcal{G}_0(\mathbf{k};\tau) \tag{29.63}$$

is satisfied because $e^{-\zeta_{\mathbf{k}}\beta}(1-f(\zeta_{\mathbf{k}})) = f(\zeta_{\mathbf{k}})$. *On the other hand,*

$$\mathcal{G}_0(\mathbf{k};\tau+3\beta) \neq \mathcal{G}_0(\mathbf{k};\tau+\beta) \tag{29.64}$$

as we might have believed if we had trusted the expansion

$$\mathcal{G}_0(\mathbf{k};\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-ik_n\tau}\mathcal{G}_0(\mathbf{k};ik_n)$$

outside its domain of validity! The conclusion is that as long as the Matsubara frequency representation is used to compute functions inside the domain $-\beta < \tau < \beta$*, it is correct. The perturbation expansion of the interaction picture does not force us to use Green's functions outside this domain, so the Matsubara representation is safe!*

Remark 214 *Alternate evaluation of time evolution: We could have obtained the time evolution also by using the identity*

$$e^{A}Ce^{A} = C + [A,C] + \frac{1}{2!}[A,[A,C]] + \frac{1}{3!}[A,[A,[A,C]]] + \ldots \tag{29.65}$$

that follows from expanding the exponential operators. This is less direct.

Remark 215 *Appearance of* $\mathcal{G}_0(\mathbf{k};\tau)$ *: It is instructive to plot* $\mathcal{G}_0(\mathbf{k};\tau)$ *as a function of imaginary time. In some energy units, let us take* $\beta = 5$*, and then consider three possible values of* $\zeta_{\mathbf{k}}$*. First* $\zeta_{\mathbf{k}} = 0.2$*, i.e. for a value of momentum above the Fermi surface, then a value right at the Fermi surface,* $\zeta_{\mathbf{k}} = 0$ *and finally a value* $\zeta_{\mathbf{k}} = -0.2$ *corresponding to a momentum right below the Fermi surface. These cases are illustrated respectively in Figs.(29-4) to (29-6). Note that the jump at* $\tau = 0$ *is always unity, reflecting the anticommutation relations. What is meant by antiperiodicity also becomes clear. The extremal values near* $\pm\beta$ *and* ± 0 *are simply related to the occupation number, independently of interactions.*

Let us continue with the derivation of the Matsubara frequency result $\mathcal{G}_0(\mathbf{k};ik_n)$.

$$\mathcal{G}_0(\mathbf{k};ik_n) = \int_0^{\beta} d\tau e^{ik_n\tau}\mathcal{G}_0(\mathbf{k};\tau) = -(1-f(\zeta_{\mathbf{k}}))\int_0^{\beta} d\tau e^{ik_n\tau}e^{-\zeta_{\mathbf{k}}\tau} \tag{29.66}$$

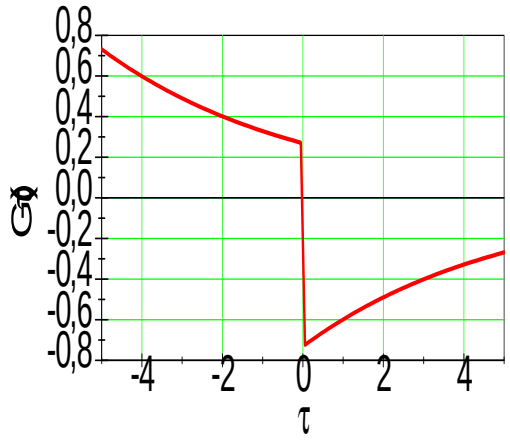
$$= -(1-f(\zeta_{\mathbf{k}}))\frac{e^{ik_n\beta}e^{-\zeta_{\mathbf{k}}\beta}-1}{ik_n-\zeta_{\mathbf{k}}} \tag{29.67}$$

$$= -(1-f(\zeta_{\mathbf{k}}))\frac{-e^{-\zeta_{\mathbf{k}}\beta}-1}{ik_n-\zeta_{\mathbf{k}}} = \frac{1}{ik_n-\zeta_{\mathbf{k}}} \tag{29.68}$$

The last equality follows because

$$(1-f(\zeta_{\mathbf{k}})) = \frac{e^{\zeta_{\mathbf{k}}\beta}}{e^{\zeta_{\mathbf{k}}\beta}+1} = \frac{1}{e^{-\zeta_{\mathbf{k}}\beta}+1} \tag{29.69}$$

We thus have our final result Eq.(29.56) for non-interacting particles.



Remark 216

Figure 29-4 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum above the Fermi surface.

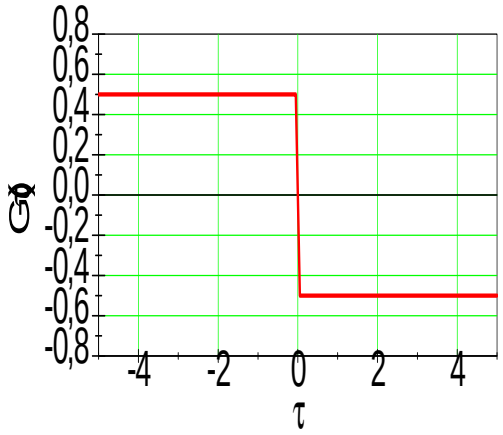


Figure 29-5 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum at the Fermi surface.

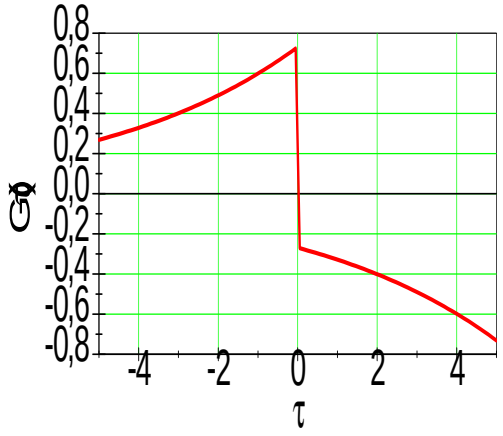


Figure 29-6 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum below the Fermi surface.

29.8.3 *$\mathcal{G}_0(\mathbf{k};\tau)$ and $\mathcal{G}_0(\mathbf{k};ik_n)$ from the equations of motion

In complete analogy with the derivation in subsection (26.3) we can obtain the equations of motion in the quadratic case.

$$\frac{\partial}{\partial\tau}\mathcal{G}_0(\mathbf{k};\tau) = -\frac{\partial}{\partial\tau}\left\langle T_\tau c_{\mathbf{k}}(\tau)\, c_{\mathbf{k}}^\dagger\right\rangle \tag{29.70}$$

$$= -\delta(\tau)\left\langle\left\{c_{\mathbf{k}}(\tau), c_{\mathbf{k}}^\dagger\right\}\right\rangle - \left\langle T_\tau\left(\frac{\partial}{\partial\tau}c_{\mathbf{k}}(\tau)\right)c_{\mathbf{k}}^\dagger\right\rangle \tag{29.71}$$

Using the equal-time anticommutation relations as well as the Heisenberg equations of motion for free particles Eq.(29.58) the above equation becomes,

$$\frac{\partial}{\partial\tau}\mathcal{G}_0(\mathbf{k};\tau) = -\delta(\tau) + \zeta_{\mathbf{k}}\left\langle T_\tau c_{\mathbf{k}}(\tau)\, c_{\mathbf{k}}^\dagger\right\rangle \tag{29.72}$$

so that the equation of motion for the Matsubara propagator is

$$\boxed{\left(\tfrac{\partial}{\partial\tau} + \zeta_{\mathbf{k}}\right)\mathcal{G}_0(\mathbf{k};\tau) = -\delta(\tau)} \tag{29.73}$$

To obtain the Matsubara-frequency result, we only need to integrate on both sides using the general expression to obtain Fourier coefficients Eq.(29.24)

$$\int_{0^-}^{\beta^-}\left[\left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}}\right)\mathcal{G}_0(\mathbf{k};\tau)\right]e^{ik_n\tau}d\tau = -1 \tag{29.74}$$

so that integrating by parts and including 0 in the domain of integration,

$$e^{ik_n\tau}\,\mathcal{G}_0(\mathbf{k};\tau)|_{0^-}^{\beta^-} - ik_n\mathcal{G}_0(\mathbf{k};ik_n) + \zeta_{\mathbf{k}}\mathcal{G}_0(\mathbf{k};ik_n) = -1. \tag{29.75}$$

The integrated term disappears because of the KMS boundary conditions (antiperiodicity) Eq.(29.15)

$$e^{ik_n\tau}\,\mathcal{G}_0(\mathbf{k};\tau)|_{0^-}^{\beta^-} = -\mathcal{G}_0\left(\mathbf{k};\beta^-\right) - \mathcal{G}_0\left(\mathbf{k};0^-\right) = 0. \tag{29.76}$$

Eq.(29.75) for the Matsubara Green's function then immediately gives us the desired result Eq.(29.56).

Exercise 29.8.2 *Non-interacting bosons: Recalling that for bosons we use even Matsubara frequencies, show from the equations of motion that the same result, Eq.(29.56), is valid also for conserved bosons.*

Alternatively, we can avoid $\tau = 0$ in the domain of integration. Then,

$$e^{ik_n\tau}\,\mathcal{G}_0(\mathbf{k};\tau)|_{0^+}^{\beta} - ik_n\mathcal{G}_0(\mathbf{k};ik_n) + \zeta_{\mathbf{k}}\mathcal{G}_0(\mathbf{k};ik_n) = 0 \tag{29.77}$$

and

$$e^{ik_n\tau}\,\mathcal{G}_0(\mathbf{k};\tau)|_{0^+}^{\beta} = -\mathcal{G}_0(\mathbf{k};\beta) - \mathcal{G}_0\left(\mathbf{k};0^+\right) = \left\langle\left\{c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger\right\}\right\rangle = 1 \tag{29.78}$$

since

$$-\mathcal{G}_0\left(\mathbf{k};0^+\right) = \left\langle c_{\mathbf{k}}c_{\mathbf{k}}^\dagger\right\rangle \tag{29.79}$$

$$-\mathcal{G}_0(\mathbf{k};\beta) = \frac{1}{Z}\mathrm{Tr}\left[c_{\mathbf{k}}e^{-\beta\hat{K}}c_{\mathbf{k}}^\dagger\right] = \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}\right\rangle. \tag{29.80}$$

This gives the same result, Eq.(29.56).

29.9 Sums over Matsubara frequencies

In the derivation above, we went from imaginary-time to Matsubara frequencies. We can also do the reverse, from Matsubara frequencies to imaginary time. So you need to learn about sums over Matsubara frequencies. This will be necessary in doing practical calculations even when we are not trying to go back to imaginary time. When we have products of Green's functions, we will use contour integration tricks that are the same as those in this section. Also, we may use partial fractions in such a way that the only sums to evaluate will basically look like

$$T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}}. \tag{29.81}$$

where $T = \beta^{-1}$. We have however to be careful since the result of this sum is ambiguous. Indeed, returning back to the motivation for these sums, recall that

$$\mathcal{G}(\mathbf{k};\tau) = T\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} \tag{29.82}$$

We already know that the Green's function has a jump at $\tau = 0$. In other words,

$$\left[\lim_{\tau\to 0^+} \mathcal{G}(\mathbf{k};\tau) = -\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \right\rangle\right] \neq \left[\lim_{\tau\to 0^-} \mathcal{G}(\mathbf{k};\tau) = \left\langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \right\rangle\right] \tag{29.83}$$

This inequality in turn means that

$$T\sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{29.84}$$

The sum does not converge uniformly in the interval including $\tau = 0$ because the $1/n$ decrease for $n \to \infty$ is too slow. Even if we can obtain a finite limit for the last sum by combining positive and negative Matsubara frequencies, what makes physical sense is only one or the other of the two limits $\tau \to 0^{\pm}$.

Remark 217 *The jump,* $\lim_{\tau\to 0^-} \mathcal{G}(\mathbf{k};\tau) - \lim_{\tau\to 0^+} \mathcal{G}(\mathbf{k};\tau)$ *is always equal to unity because of the anticommutation relations. The slow convergence in* $1/ik_n$ *is thus a reflection of the anticommutation relations and will remain true even in the interacting case. If the* $(ik_n)^{-1}$ *has a coefficient different from unity, the spectral weight is not normalized and the jump is not unity. This will be discussed shortly.*

Let us evaluate the Matsubara frequency sums. Considering again the case of fermions I will show as special cases that

$$\boxed{T\sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{e^{\beta\zeta_{\mathbf{k}}}+1} = f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k};0^-)} \tag{29.85}$$

$$\boxed{T\sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} = \frac{-1}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -1 + f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k};0^+)} \tag{29.86}$$

Obviously, the non-interacting Green's function has the correct jump $\mathcal{G}_0(\mathbf{k};0^-) - \mathcal{G}_0(\mathbf{k};0^+) = 1$.In addition, since $\mathcal{G}_0(\mathbf{k};0^-) = \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle$ and $\mathcal{G}_0(\mathbf{k};0^+) = -\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle$ the above results just tell us that $\left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle = f(\zeta_{\mathbf{k}})$ that we know from elementary statistical mechanics. The anticommutation relations immediately give $-\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle = -1 + f(\zeta_{\mathbf{k}})$. So these sums over Matsubara frequencies better behave as advertized.

Proof: [1] [2] To perform the sum over Matsubara frequencies, the standard trick is to go to the complex plane. The following function

$$-\beta\frac{1}{e^{\beta z}+1} \tag{29.87}$$

has poles for z equal to any fermionic Matsubara frequency: $z = ik_n$. Its residue at these poles is unity since for

$$z = ik_n + \delta z \tag{29.88}$$

we have

$$-\beta\frac{1}{e^{\beta z}+1} = -\beta\frac{1}{e^{ik_n\beta+\beta\delta z}+1} = -\beta\frac{1}{-1e^{\beta\delta z}+1} \tag{29.89}$$

$$\lim_{z-ik_n\to 0}\delta z\left[-\beta\frac{1}{e^{\beta z}+1}\right] = 1 \tag{29.90}$$

Similarly the following function has the same poles and residues:

$$\lim_{z-ik_n\to 0}\delta z\left[\beta\frac{1}{e^{-\beta z}+1}\right] = 1 \tag{29.91}$$

To evaluate the $\tau < 0$ case by contour integration, we use the residue theorem on the contour C_1, which is a sum of circles going counterclockwise around the points where z is equal to the Matsubara frequencies. Using Eq.(29.90), this allows us to establish the equality

$$-\frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{\beta z}+1}\frac{e^{-z\tau}}{z-\zeta_{\mathbf{k}}} = \frac{1}{\beta}\sum_n\frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}}. \tag{29.92}$$

This contour can then be deformed, as illustrated in Fig. (29-7), into C_1' and then into $C_2 + C_3$. There is no contribution from C_3 at $\mathrm{Re}\,(z) = \infty$ because the denominator of $\frac{e^{-z\tau}}{e^{\beta z}+1}$ makes the integrand converge exponentially since in $e^{-z(\tau+\beta)}$, $\tau+\beta$ is always positive ($\tau > -\beta$). Similarly, there is no contribution from C_2 at $\mathrm{Re}\,(z) = -\infty$ because in that case $\frac{e^{-z\tau}}{e^{\beta z}+1} \to e^{-z\tau}$ and $-z\tau < 0$. So finally, we have

$$\boxed{\frac{1}{\beta}\sum_n\frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = \frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{\beta\zeta_{\mathbf{k}}}+1} = e^{-\zeta_{\mathbf{k}}\tau}f\left(\zeta_{\mathbf{k}}\right)} \tag{29.93}$$

which agrees with the value of $\mathcal{G}_0\left(\mathbf{k};\tau\right)$ in Eq.(29.62) when $\tau < 0$. In particular, when $\tau = 0^-$ we have proven the identity (29.86) .

To evaluate the $\tau > 0$ case we use the same contour but with the other form of auxiliary function Eq.(29.91). We can again check that the integral over the circle at infinity vanishes because this time $e^{-z\tau}$ insures convergence when $\mathrm{Re}\,(z) = \infty$, $\tau > 0$ and $\frac{1}{e^{-\beta z}+1}$ ensures convergence when $\mathrm{Re}\,(z) = -\infty$ despite $e^{-z\tau}$ in the numerator. We then obtain,

$$\frac{1}{\beta}\sum_n\frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = \frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{-\beta z}+1}\frac{e^{-z\tau}}{z-\zeta_{\mathbf{k}}}. \tag{29.94}$$

Again, from $C_2 + C_3$, only the contribution from the pole in the clockwise directions survives so that we have,

$$\boxed{\frac{1}{\beta}\sum_n\frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}e^{\beta\zeta_{\mathbf{k}}}}{e^{\beta\zeta_{\mathbf{k}}}+1} = -e^{-\zeta_{\mathbf{k}}\tau}\left(1-f\left(\zeta_{\mathbf{k}}\right)\right).} \tag{29.95}$$

This agrees with the value of $\mathcal{G}_0\left(\mathbf{k};\tau\right)$ in Eq.(29.62) when $\tau > 0$. In particular, when $\tau = 0^+$ we have proven the identity (29.85).

[2] I thank Yan Wang, 2018, for this version of the proof.

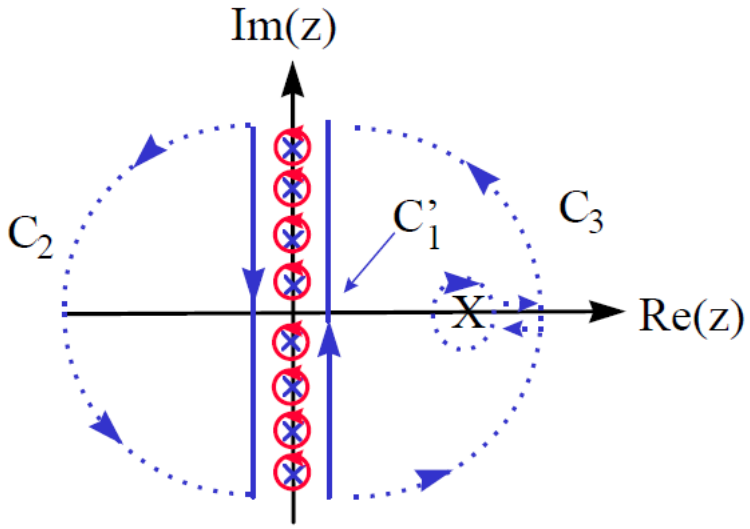


Figure 29-7 Evaluation of fermionic Matsubara frequency sums in the complex plane.

Remark 218 *Branch cut: When there is a branch cut all the way to infinity, the above proof is easy to generalize. For example, for a branch cut from* $\zeta_{\mathbf{k}}$ *to* ∞*, there are three integrals to do. Two of them extend from* ∞ *in two directions above and below the real axis and another one is an open circle around the end of the branch cut.*

Remark 219 *When there is a sum over Matsubara frequencies for a product of Green's function, the same trick as above applies. There are just more poles to go around when the contour is deformed.*

30. SUSCEPTIBILITY AND LINEAR RESPONSE IN MATSUBARA SPACE

Susceptibilities are also defined in Matsubara space. As in the fermionic case, analytic continuation suffices to obtain the retarded response. Knowing this, linear response takes a simple form in imaginary time that I will explain.

30.1 Matsubara frequencies for the susceptibility, as bosonic correlation function

Recall that all the information that we need for the susceptibility is in the spectral function χ''. To do actual calculations of correlation functions at finite temperature, whether by numerical or analytical means, it turns out that it is much easier to compute a function that is different from the retarded response function. By analogy with the fermionic case, that function is defined as follows

$$\chi_{A_i A_j}(\tau) = \frac{1}{\hbar}\langle A_i(\tau) A_j\rangle \theta(\tau) + \frac{1}{\hbar}\langle A_j A_i(\tau)\rangle \theta(-\tau) \tag{30.1}$$

where θ is the step function, an d where I have restored $\hbar$ to make the connection with previouys sections easier. By definition,

$$A_i(\tau) = e^{\tau K/\hbar} A_i e^{-\tau K/\hbar}. \tag{30.2}$$

In other words, if in this last equation we replace τ, a real number, by the purely imaginary number it, we recover that the operator evolves with the Heisenberg equations of motion. As above, this definition is motivated by the fact that the operator $e^{-\beta K}$ in the density matrix really looks like evolution $e^{-iKt/\hbar}$ in imaginary time. It is also customary to define the time ordering operator T_τ for bosonic correlation functions in such a way that operators are ordered from right to left by increasing order of time:

$$\chi_{A_i A_j}(\tau) = \frac{1}{\hbar}\langle T_\tau A_i(\tau) A_j\rangle . \tag{30.3}$$

That will be very useful in cunjunction with perturbation theory. As long as we can extract the spectral function χ'' from $\chi_{A_i A_j}(\tau)$ above, we are in good shape to obtain all we need.

I put back the $\hbar$ in this section so that we have at least one example with physical units.

To see how to do this, we first note that we can define $\chi_{A_i A_j}(\tau)$ on the interval $-\beta\hbar \le \tau \le \beta\hbar$, and that if we do that, this function *on this interval only* has some periodicity properties that can be put to use. More specifically, assume that

$-\beta\hbar < \tau < 0$,then from the definition of the function, we have that

$$\begin{aligned}
\chi_{A_iA_j}(\tau) &= \frac{1}{\hbar}\langle A_j A_i(\tau)\rangle = \frac{1}{\hbar}\mathrm{Tr}\left[e^{-\beta K}A_j A_i(\tau)\right]/Z \\
&= \frac{1}{\hbar}\mathrm{Tr}\left[A_i(\tau)\,e^{-\beta K}A_j\right]/Z \\
&= \frac{1}{\hbar}\mathrm{Tr}\left[e^{-\beta K}e^{\beta K}A_i(\tau)\,e^{-\beta K}A_j\right]/Z \\
&= \chi_{A_iA_j}(\tau+\beta\hbar) \qquad (30.4)
\end{aligned}$$

since now $\tau+\beta\hbar > 0$.We have a periodic function on a finite interval. Hence we can represent it by a Fourier series

$$\boxed{\chi_{A_iA_j}(\tau) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty} e^{-iq_n\tau}\chi_{A_iA_j}(iq_n)} \qquad (30.5)$$

where the so-called bosonic Matsubara frequencies are defined by

$$\boxed{q_n = \frac{2n\pi k_B T}{\hbar} = \frac{2n\pi}{\beta\hbar} \quad ; \quad n \quad \text{integer}} \qquad (30.6)$$

The periodicity property will be automatically fulfilled because $e^{-i\hbar q_n\beta} = e^{-i2n\pi} = 1$. The expansion coefficients are obtained as usual for Fourier series of periodic functions from

$$\boxed{\chi_{A_iA_j}(iq_n) = \int_0^{\beta\hbar} d\tau e^{iq_n\tau}\chi_{A_iA_j}(\tau)} \qquad (30.7)$$

By using the Lehmann representation, we can find a spectral representation for the latter function

$$\begin{aligned}
\chi_{A_iA_j}(iq_n) &= \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau e^{iq_n\tau}\langle A_i(\tau)A_j\rangle \\
&= \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau e^{iq_n\tau}\frac{1}{Z}\sum_{m,n} e^{-\beta K_n}\langle n|\,e^{K_n\tau/\hbar}A_i e^{-K_m\tau/\hbar}\,|m\rangle\langle m|A_j|n\rangle \\
&= \frac{1}{Z}\sum_{m,n}\frac{e^{-\beta K_n}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\left(e^{iq_n\beta\hbar+\beta K_n-\beta K_m}-1\right)}{i\hbar q_n-(E_m-E_n)} \qquad (30.8) \\
&= \frac{1}{Z}\sum_{m,n}\frac{e^{-\beta K_n}-e^{-\beta K_m}}{(E_m-E_n)-i\hbar q_n}\langle n|A_i|m\rangle\langle m|A_j|n\rangle \qquad (30.9)
\end{aligned}$$

where we used $e^{iq_n\beta\hbar} = 1$. Note that $K_m - K_n = E_m - E_n$ since the number operator commutes with A_i and A_j that are quadratic in fermions. Using the Lehmann representation for $\chi''_{A_iA_j}(\omega')$ Eq.(10.96) that we recopy here,

$$\begin{aligned}
\chi''_{A_iA_j}(\omega) &= \sum_{n,m}\frac{e^{-\beta K_n}-e^{-\beta Km}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\ \pi\,\delta(\hbar\omega-(K_m-K_n)) \\
&= \left(1-e^{-\beta\hbar\omega}\right)\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\times \qquad (30.10) \\
&\quad \langle n|A_i|m\rangle\langle m|A_j|n\rangle\ \pi\,\delta(\hbar\omega-(E_m-E_n)). \qquad (30.11)
\end{aligned}$$

we can write

$$\chi_{A_iA_j}(iq_n) = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-iq_n} \qquad (30.12)$$

which is clearly a special case of our general spectral representation Eq.(10.64). This is the response function in Matsubara frequency may be obtained from $\chi_{A_iA_j}(iq_n) = \chi_{A_iA_j}(z\to iq_n)$ whereas for the retarded function $\chi^R_{A_iA_j}(\omega) = \chi_{A_iA_j}(z\to\omega+i\eta)$.

Remark 220 *The Lehmann representation Eq. (30.10) gives another proof of the fluctuation-dissipation theorem.*

Remark 221 *Once we write the expansion in Matsubara frequencies, the function* $\chi_{A_iA_j}(\tau)$ *in Eq.(30.5) is defined by its periodic extension outside the interval of definition* $-\beta\hbar \leq \tau \leq \beta\hbar$. *That follows the standard procedure for Fourier series. Outside the interval of definition however, it does not coincide with the original* $\chi_{A_iA_j}(\tau)$ *Eq.(30.1). Indeed, take*

$$\chi_{A_iA_j}(\tau + 2\beta\hbar) = \mathrm{Tr}\left[e^{-\beta H}e^{2\beta H}A_i(\tau)\, e^{-2\beta H}A_j\right]/(Z\hbar).$$

There is no way this can become equal to $\chi_{A_iA_j}(\tau)$.

30.2 Linear response in imaginary time

Knowing that retarded responses can be obtained from analytical continuation it is clear that there is a formulation of linear response in imaginary time. I will do it with an example. Take as an external perturbation a scalar potential. We go to the interaction representation where the unperturbed Hamiltonian is that of the full system and the perturbation is a scalar potential $\phi(\mathbf{r}',\tau)$ in analogy with Eq. (11.37). Then, the perturbation is

$$\int d\mathbf{r}'\phi(\mathbf{r}',\tau)\,\rho(\mathbf{r}') \tag{30.13}$$

so that in the interaction representation, we have for the non-equilibrium current

$$\langle j_x(\mathbf{r},\tau)\rangle_{n.e.} = \left\langle T_\tau \exp\left[-\int_0^\beta d\tau' \int d\mathbf{r}'\phi(\mathbf{r}',\tau')\,\rho(\mathbf{r}',\tau')\right] j_x(\mathbf{r},\tau)\right\rangle. \tag{30.14}$$

The integral over τ' comes from perturbation theory. Given that in equilibrium the current vanishes, we are left, to linear order in the perturbation, with

$$\langle j_x(\mathbf{r},\tau)\rangle_{n.e.} = -\int_0^\beta d\tau' \int d\mathbf{r}'\,\langle T_\tau j_x(\mathbf{r},\tau)\,\rho(\mathbf{r}',\tau')\rangle\,\phi(\mathbf{r}',\tau'). \tag{30.15}$$

Fourier transforming in space and Matsubara frequency, we take advantage of the fact that the correlation function is a function of $\tau - \tau'$ and $\mathbf{r} - \mathbf{r}\prime$ so that we can use the convolution theorem and obtain,

$$\langle j_x(\mathbf{q},iq_n)\rangle_{n.e.} = -\chi_{j_x\rho}(\mathbf{q},iq_n)\,\phi(\mathbf{q},iq_n), \tag{30.16}$$

in complete analogy with what we found in the real-frequency formalism in Eq. (11.38). The susceptibility in Matsubara frequency is defined by

$$\chi_{j_x\rho}(\mathbf{q},iq_n) = \int_0^\beta d\tau \int d\mathbf{r}\; e^{iq_n(\tau-\tau')}e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\,\langle T_\tau j_x(\mathbf{r},\tau)\,\rho(\mathbf{r}',\tau')\rangle, \tag{30.17}$$

and the retarded response is obtained by simple analytic continuation.

31. PHYSICAL MEANING OF THE SPECTRAL WEIGHT: QUASIPARTICLES, EFFECTIVE MASS, WAVE FUNCTION RENORMALIZATION, MOMENTUM DISTRIBUTION.

To discuss the physical meaning of the spectral weight in the translationally invariant case, we first recall it in the non-interacting case, then write the Lehmann representation. That allows us to see its more general meaning. After our discussion of a photoemission experiment, we will be in a good position to understand the concepts of quasiparticles, wave-function renormalization, effective mass and momentum distribution. We will even have a first look at Fermi liquid theory, and see how it helps us to understand photoemission experiments.

31.1 Probabilistic interpretation of the spectral weight

The general result for the spectral weight in terms of the Green's function Eq.(29.46) gives us for non-interacting particles

$$A_0(\mathbf{k},\omega) = i\left[\frac{1}{\omega+i\eta-\zeta_{\mathbf{k}}}-\frac{1}{\omega-i\eta-\zeta_{\mathbf{k}}}\right] \tag{31.1}$$

$$= 2\pi\delta(\omega-\zeta_{\mathbf{k}}) \tag{31.2}$$

In physical terms, this tells us that for non-interacting particles in a translationally invariant system, a single excited particle or hole of momentum $\mathbf{k}$ added to an eigenstate is a true excited eigenstate located at anw energy $\omega=\zeta_{\mathbf{k}}$ above or below the Fermi level. In the interacting case, the Lehmann representation will show us clearly that what we just said is the correct interpretation.

For a different representation, for example for momentum, we can use [2] the definition in the translationally invariant case Eq. (29.54). The same change of basis on the spectral weight Eq.(29.38) gives us

$$\boxed{A(\mathbf{k},\omega')=e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n}+e^{-\beta K_m}\right)\left|\langle n|\,c_{\mathbf{k}}\,|m\rangle\right|^2 2\pi\delta\left(\omega'-(K_m-K_n)\right).} \tag{31.3}$$

The overlap matrix element $\left|\langle n|\,c_{\mathbf{k}}\,|m\rangle\right|^2$ that gives the magnitude of the delta function contribution to the spectral weight represents the overlap between the initial state with one more particle or hole in a momentum eigenstate and the true excited one-particle or one-hole state. The last equation clearly shows that $A(\mathbf{k},\omega')/(2\pi)$ is positive and we already know that it is normalized to unity,

$$\int\frac{d\omega'}{2\pi}A(\mathbf{k},\omega')=\left\langle\left\{c_{\mathbf{k}},c_{\mathbf{k}}^{\dagger}\right\}\right\rangle=1. \tag{31.4}$$

Hence it can be interpreted as the probability that a state formed from a true eigenstate $|n\rangle$ either by adding a particle in a single-particle state $\mathbf{k}$, namely $c_{\mathbf{k}}^{\dagger}|n\rangle$ (or adding a hole $c_{\mathbf{k}}|n\rangle$ in a single-particle state $\mathbf{k}$) is a true eigenstate whose energy is ω above or below the chemical potential. Clearly, adding a particle or a hole in a momentum eigenstate will lead to a true many-body eigenstate only if the momentum of each particle is individually conserved. This occurs only in the non-interacting case, so this is why the spectral weight is then a single delta function. In the more general case, many energy eigenstates will have a non-zero overlap with the state formed by simply adding a particle or a hole in a momentum eigenstate. While particle-like excitations will overlap mostly with eigenstates that are reached by adding positive ω, they can also overlap eigenstates that are reached by adding negative ω. In an analogous manner, hole-like eigenstates will be mostly at negative ω. Let us see how this manifests itself in a specific experiment.

Remark 222 *The high-frequency expansion of the Masubara Green's function leads to* $\int \frac{d\omega'}{2\pi} A(\mathbf{k},\omega')$ *as the coefficient of the first term* $1/ik_n$*. Hence, this one in the numerator is intimaterly related to anticommutation relations.*

Remark 223 *Energy vs momentum in an interacting system: It is clear that in an interacting system one must distinguish the momentum and the energy variables. The energy variable is* ω *the variable conjugate to time. Knowing the momentum of a single added electron or hole is not enough to know the added energy. This added energy would be* $k^2/2m$ *only in the case of non-interacting electrons.*

Remark 224 *Physical reason for high-frequency fall-off: The explicit expression for the spectral weight Eq.(31.3) suggests why the spectral weight falls off fast at large frequencies for a given* $\mathbf{k}$*, as we have discussed in Subsection (32.1). A state formed by adding one particle (or one hole) of momentum* $\mathbf{k}$ *should have exponentially small overlap with the true eigenstates of the system that have one more particle (or hole) but an arbitrarily large energy difference* ω *with the initial state.*

Remark 225 *Bohr's correpondence principle: In accord with Bohr's correpondence principle, absorption occurs at frequencies* ω' *that correspond to transitions between many-body states,* $K_m - K_n$*. These many-body states have a particle-number that differs by one. We have already mentioned this in Sec.(16.1) in the one-body context.*

31.2 Analog of the fluctuation dissipation theorem

We have seen in Eq.(G.13) the fluctuation dissipation theorem for correlation functions, (with $\hbar = 1$)

$$S_{A_i A_j}(\omega) = 2(1 + n_B(\omega))\chi''_{A_i A_j}(\omega) \tag{31.5}$$

where $n_B(\omega)$ is the Bose function. That can also be written in the form

$$\int dt e^{i\omega t} \langle A_i(t) A_j \rangle = (1 + n_B(\omega)) \int dt e^{i\omega t} \langle [A_i(t), A_j] \rangle . \tag{31.6}$$

It would be nice to find the analog for the Green's function because we saw, when we discussed ARPES in Sec. 26.1, that the cross section for angle-resolved

photoemission measures $\int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle$,which looks like one piece of the anticommutator.

The key is the real time version of the antiperiodicity that we discussed for Matsubara Green's functions in Sec. 26.4. I will demonstrate that

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle = f(\omega) A\left(\mathbf{k}_{||},\omega\right). \tag{31.7}$$

Proof: The most direct and simple proof is from the Lehmann representation for the spectral weight of basis states $\mathbf{k}$, Eq.(31.3). Note that we could do the same for the $\mathbf{r}$, $\mathbf{r\prime}$ states Eq.(29.38) or any other single-particle basis. The trick is to use $\delta(\omega' - (K_m - K_n))$ to rewrite $A(\mathbf{k},\omega)$ in terms of only the first or the second of the two terms entering the definition of $A(\mathbf{k},\omega)$ in terms of an anticomutator. More specifically, we can rewrite K_m in terms of K_n and ω'so that $A(\mathbf{k},\omega')$ is given only in terms of the first term entering the anticommutator

$$\begin{aligned} A(\mathbf{k},\omega') &= \left(1+e^{-\beta\omega'}\right) e^{\beta\Omega}\sum_{mn} e^{-\beta K_n}\langle n|c_{\mathbf{k}}|m\rangle\langle m|c^{\dagger}_{\mathbf{k}}|n\rangle 2\pi\delta(\omega' - (K_m - K_n)) \\ &= (1-f(\omega'))^{-1}\int dt e^{i\omega' t}\left\langle c_{\mathbf{k}}(t) c^{\dagger}_{\mathbf{k}}\right\rangle = (1-f(\omega'))^{-1} iG^{>}(\mathbf{k},\omega). \end{aligned} \tag{31.8}$$

Or we can also write K_n in terms of ω' and K_m so that only the second term of the anticommutator appears, namely

$$\begin{aligned} A(\mathbf{k},\omega') &= \left(e^{\beta\omega'}+1\right) e^{\beta\Omega}\sum_{mn} e^{-\beta K_m}\langle m|c^{\dagger}_{\mathbf{k}}|n\rangle\langle n|c_{\mathbf{k}}|m\rangle 2\pi\delta(\omega' - (K_m - K_n)) \\ &= f(\omega')^{-1}\int dt e^{i\omega' t}\left\langle c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}}(t)\right\rangle = f(\omega')^{-1}\left(-iG^{<}(\mathbf{k},\omega)\right). \end{aligned} \tag{31.9}$$

In general, one defines

$$\boxed{G^{<}\left(\mathbf{k}_{||},\omega\right) = i\int dt\, e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle ;\; G^{>}\left(\mathbf{k}_{||},\omega\right) = -i\int dt\, e^{i\omega t}\left\langle c_{\mathbf{k}_{||}}(t) c^{\dagger}_{\mathbf{k}_{||}}\right\rangle} \tag{31.10}$$

***Alternate proof:** To get a few more general results about $G^{<}\left(\mathbf{k}_{||},\omega\right)$ and $G^{>}\left(\mathbf{k}_{||},\omega\right)$ we present the following alternate proof. The cross section is proportional to the Fourier transform of $G^{<}\left(\mathbf{k}_{||},\omega\right)$ as defined in Eq.(28.11).

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle \equiv -iG^{<}\left(\mathbf{k}_{||},\omega\right) \tag{31.11}$$

One can relate $G^{<}$ and $G^{>}$ to the spectral weight in a very general way through the Fermi function. This is done using the usual cyclic property of the trace (fluctuation-dissipation theorem). From

$$\begin{aligned} \left\langle c_{\mathbf{k}_{||}}(t) c^{\dagger}_{\mathbf{k}_{||}}\right\rangle &= Z^{-1}\mathrm{Tr}\left[e^{-\beta K}\left(e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt}\right) c^{\dagger}_{\mathbf{k}_{||}}\right] \\ &= Z^{-1}\mathrm{Tr}\left[\left(e^{\beta K} e^{-\beta K}\right) c^{\dagger}_{\mathbf{k}_{||}} e^{-\beta K}\left(e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt}\right)\right] \\ &= \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t+i\beta)\right\rangle \end{aligned} \tag{31.12}$$

one finds by simple use of definitions and change of integration variables,

$$A\left(\mathbf{k}_{||},\omega\right) = \int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}\left(t\right) + c_{\mathbf{k}_{||}}\left(t\right) c^{\dagger}_{\mathbf{k}_{||}}\right\rangle \tag{31.13}$$

$$= \int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}\left(t\right)\right\rangle + \int dt e^{i\omega\left(t+i\beta-i\beta\right)}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}\left(t+i\beta\right)\right\rangle$$

$$= \left(1+e^{\beta\omega}\right)\int dt e^{i\omega t}\left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}\left(t\right)\right\rangle \tag{31.14}$$

$$= f\left(\omega\right)^{-1}\left(-iG^{<}\left(\mathbf{k}_{||},\omega\right)\right) \tag{31.15}$$

Substituting in Eq.(31.11) proves Eq.(31.7). Note that since from the definitions in Eqs.(28.10) and (28.11) the spectral weight is obtained from

$$A\left(\mathbf{k}_{||},\omega\right) = -i\left[G^{<}\left(\mathbf{k}_{||},\omega\right) - G^{>}\left(\mathbf{k}_{||},\omega\right)\right] \tag{31.16}$$

we also have the result

$$iG^{>}\left(\mathbf{k}_{||},\omega\right) = \left(1-f\left(\omega\right)\right)A\left(\mathbf{k}_{||},\omega\right) \tag{31.17}$$

31.3 Some experimental results from ARPES

The state of technology and historical coincidences have conspired so that the first class of layered (quasi-two-dimensional) compounds that became available for ARPES study around 1990 were high temperature superconductors. These materials have properties that make them non-conventional materials that are not yet understood using standard approaches of solid-state Physics. Hence, people started to look for two-dimensional materials that would behave as expected from standard models. Such a material, semimetallic $TiTe_2$ was finally found around 1992. For our purposes, quasi-two-dimensional just means here that the Fermi velocity perpendicular to the planes is much smaller than the Fermi velocity in the planes. The results of this experiment[6] appear in Fig.(31-1).

We have to remember that the incident photon energy is $21.2eV$ while the variation of ω is on a scale of $200meV$ so that, for all practical purposes, the momentum vector in Fig.(26-1) is a fixed length vector. Hence, the angle with respect to the incident photon suffices to define the value of $\mathbf{k}_{||}$. Each curve in Fig.(31-1) is for a given $\mathbf{k}_{||}$, in other words for a given angle measured from the direction of incidence of the photon. The intensity is plotted as a function of the energy of the outgoing electron. Hence these plots are often called EDC (energy distribution curves). The zero corresponds to an electron extracted from the Fermi level. Electrons with a smaller kinetic energy come from states with larger binding energy. In other words, each of the curves above is basically a plot of the hole-like part of $A\left(\mathbf{k}_{||},\omega\right)$, or if you want $f\left(\omega\right)A\left(\mathbf{k}_{||},\omega\right)$. From band structure calculations, one knows that the angle $\theta = 14.75^0$ corresponds to the Fermi level (marked k_F on the plot) of a $Ti-3d$ derived band. It is for this scattering angle that the agreement between experiment and Fermi liquid theory is best (see Sec.(31.5) below). The plots for angles $\theta < 14.75^0$ correspond to wave vectors above the Fermi level. There, the intensity is *much* smaller than for the other peaks. For $\theta = 13^0$, the experimental results are scaled up by a factor 16. The intensity observed for wave-vectors above $\omega = 0$ comes from the Fermi function and also from the non-zero projection of the state with a given $\mathbf{k}$ on several values of ω in the spectral weight.

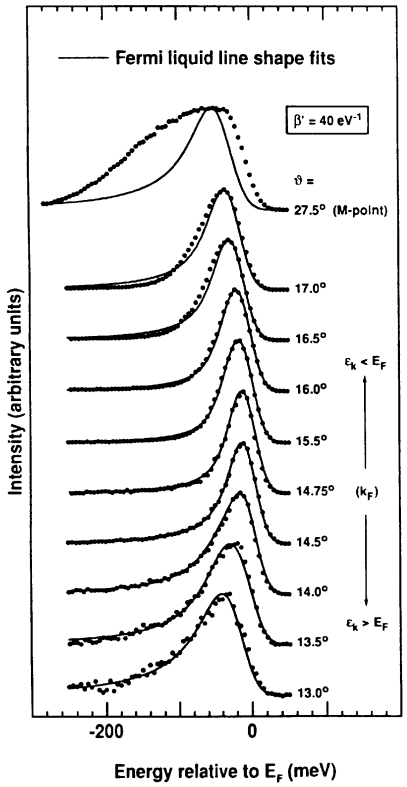


Figure 31-1 ARPES spectrum of $1-T-TiTe_2$, after R. Claessen, R.O. Anderson, J.W. Allen, C.G. Olson, C. Janowitz, W.P. Ellis, S. Harm, M. Kalning, R. Manzke, and M. Skibowski, Phys. Rev. Lett **69**, 808 (1992).

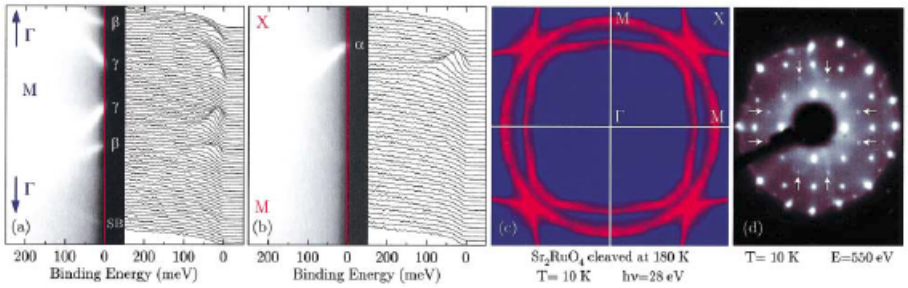


FIG. 4 (color). EDC's and intensity plot $I(\mathbf{k}, \omega)$ along Γ-M-Γ and M-X [panels (a) and (b), respectively]. Panel (c): E_F intensity map. Panel (d): LEED pattern recorded at the end of the FS mapping. All data were taken at 10 K on Sr_2RuO_4 cleaved at 180 K.

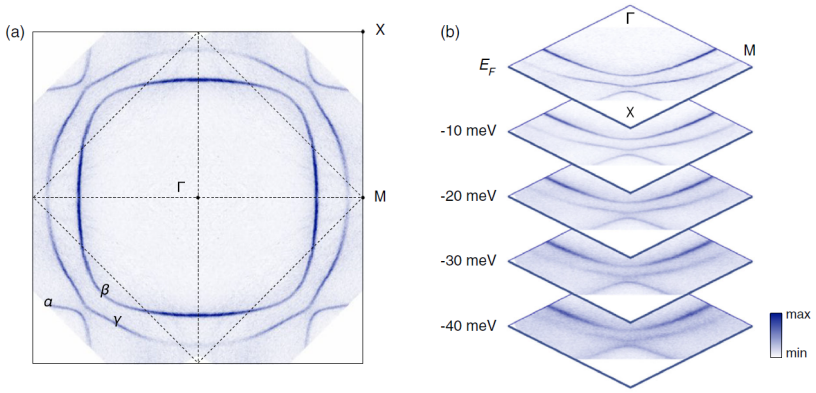


Figure 31-2 Momentum distribution curves. a) at the Fermi level, and b) at various energies below the Fermi surface. From Phys. Rev. X, **2**, 021048 (2019).

The energy resolution is $35meV$. Nevertheless, it is clear that the line shapes are larger than the energy resolution: Clearly the spectral weight is not a delta function and the electrons in the system are not free particles. Nevertheless, there is a definite maximum in the spectra whose position changes with $\mathbf{k}_{||}$. It is tempting to associate the width of the line to a lifetime. In other words, a natural explanation of these spectra is that the electrons inside the system are "quasiparticles" whose energy disperses with wave vector and that have a lifetime. We try to make these concepts more precise below.

One can also make plots of the probability of having a certain momentum at the Fermi level $\omega = 0$. This is usually represented by a color plot called MDC, momentum distribution curve. A spectacular case, shown in Fig. (31.3) is that of strontium ruthenate Sr_2RuO_4 [57], also interesting because it was proposed to be a topological superconductor, a proposal that is still subject of research at the time of writing:

Fig. (31-2) shows some beautiful experimental and theoretical recent work on this compound. [228] On the left is the Fermi surface and on the right various MDC's at energies below the Fermi surface. This should be contrasted with high-temperature superconductors in Fig. 31.3. The Fermi surface seems to vanish in thin air ([157]).Getting back to strontium ruthenate [228], Fig. (31-3) shows some detailed comparisons between experiment and theory. The theory is based on density-functional theory, augmented by dynamical mean-field calculations, topics we will address in subsequent chapters. The calculation shows that the effect of spin-orbit interactions is crucial. The red dots are the measurements and

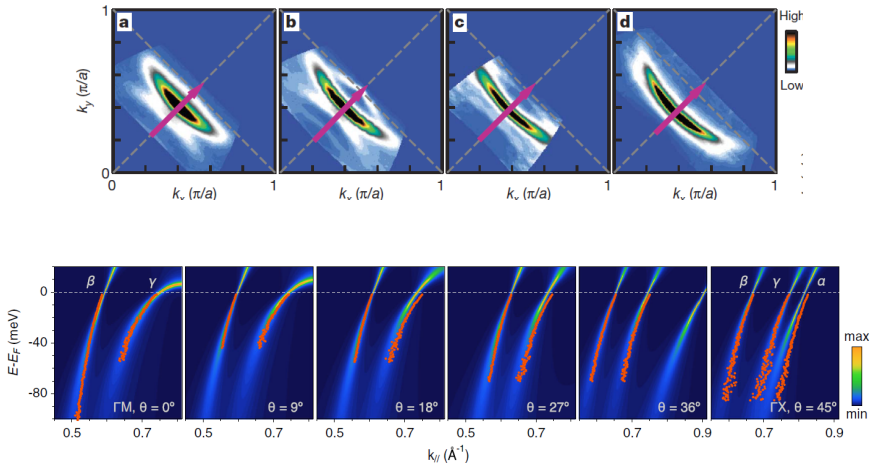


Figure 31-3 Comparison between theory and experiment for strontium ruthenate. The theory is from electronic structure including spin-orbit interactions and supplemented with the effect of interactions using Dynamical Mean-Field theory. From Phys. Rev. X, **2**, 021048 (2019).

the color curves the calculations.

31.4 Quasiparticles

The intuitive notions we may have about lifetime and effective mass of an electron caused by interactions in a solid can all be extracted from the self-energy, as I will show. As we discussed in Chapter 17, for a general interacting system, the one-particle Green's function takes the form,

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \sum^R(\mathbf{k},\omega)} \tag{31.18}$$

We can drop $i\eta$ since $\mathrm{Im}\sum^R(\mathbf{k},\omega)$ is negative to preserve causality and always larger than $i\eta$ that should anyway be taken to zero at the end.[1] The spectral weight corresponding to $G^R(\mathbf{k},\omega)$ then is,

$$\begin{aligned} A(\mathbf{k},\omega) &= -2\,\mathrm{Im}\,G^R(\mathbf{k},\omega) && (31.19)\\ &= \frac{-2\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{\left(\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\sum^R(\mathbf{k},\omega)\right)^2 + \left(\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2}. && (31.20)\end{aligned}$$

If the imaginary part of the self-energy, the scattering rate, is not too large and varies smoothly with frequency, conditions I will refine when I discuss Fermi liquids soon, the spectral weight will have a maximum whenever, at fixed **k,** there is a value of ω that satisfies

$$\boxed{\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega) = 0.} \tag{31.21}$$

We assume the solution of this equation exists. Let $E_{\mathbf{k}} - \mu$ be the value of ω for which this equation is satisfied. $E_{\mathbf{k}}$ is the so-called *quasiparticle energy* [4]. This energy is clearly in general different from the results of band structure calculations that are usually obtained by neglecting the frequency dependence of the self-energy. Expanding $\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$ around $\omega = E_{\mathbf{k}} - \mu = 0$ where $A(\mathbf{k},\omega)$ is a maximum, we find

$$\begin{aligned} \omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega) &\approx 0 + \frac{\partial}{\partial\omega}\left[\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\right]_{\omega=E_{\mathbf{k}}-\mu}(\omega - E_{\mathbf{k}} + \mu) + \ldots\\ &\approx \left(1 - \left.\frac{\partial\,\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)}{\partial\omega}\right|_{E_{\mathbf{k}}-\mu}\right)(\omega - E_{\mathbf{k}} + \mu) + \ldots \qquad (31.22)\end{aligned}$$

If we define the "quasiparticle weight" or square of the wave function renormalization by

$$\boxed{Z_{\mathbf{k}} = \frac{1}{1 - \frac{\partial}{\partial\omega}\,\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}}} \tag{31.23}$$

then in the vicinity of the maximum, the spectral weight takes the following simple form in the vicinity of the Fermi level, where the peak is sharpest

$$\begin{aligned} A(\mathbf{k},\omega) &\approx 2\pi Z_{\mathbf{k}}\frac{1}{\pi}\frac{-Z_{\mathbf{k}}\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + \left(Z_{\mathbf{k}}\,\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2} + inc && (31.24)\\ &= 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + (\Gamma_{\mathbf{k}}(\omega))^2}\right] + inc. && (31.25)\end{aligned}$$

[1] In exact diagonalizations where the self-energy is still represented by a set of delta functions, the $i\eta$ should be kept everywhere.

The last equation needs some explanation. First, it is clear that I have defined the scattering rate

$$\boxed{\Gamma_{\mathbf{k}}(\omega) = -Z_{\mathbf{k}} \operatorname{Im} \Sigma^R(\mathbf{k},\omega)} \tag{31.26}$$

Second, the quantity in square brackets looks, as a function of frequency. At least if we can neglect the frequency dependence of the scattering rate. The integral over frequency of the square bracket is unity. Since $A(\mathbf{k},\omega)/2\pi$ is normalized to unity, this means both that

$$Z_{\mathbf{k}} \leq 1 \tag{31.27}$$

and that there are additional contributions to the spectral weight that we have denoted *inc* in accord with the usual terminology of "incoherent background". The equality in the last equation holds only if the real part of the self-energy is frequency independent.

It is also natural to ask how the quasiparticle disperses, in other words, what is its effective Fermi velocity compared with that of the bare particle. Let us define the bare velocity by

$$v_{\mathbf{k}} = \nabla_{\mathbf{k}} \zeta_{\mathbf{k}} \tag{31.28}$$

and the renormalized velocity by

$$v^*_{\mathbf{k}} = \nabla_{\mathbf{k}} E_{\mathbf{k}} \tag{31.29}$$

Then the relation between both quantities is obtained by taking the gradient of the quasiparticle equation Eq.(31.21).

$$\nabla_{\mathbf{k}} \left[E_{\mathbf{k}} - \mu - \zeta_{\mathbf{k}} - \operatorname{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu) \right] = 0 \tag{31.30}$$

$$v^*_{\mathbf{k}} - v_{\mathbf{k}} - \nabla_{\mathbf{k}} \operatorname{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu) - \left. \frac{\partial \operatorname{Re} \Sigma^R(\mathbf{k},\omega)}{\partial \omega} \right|_{E_{\mathbf{k}} - \mu} v^*_{\mathbf{k}} = 0 \tag{31.31}$$

where $\nabla_{\mathbf{k}}$ in the last equation acts only on the first argument of $\operatorname{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)$. The last equation is easily solved if we can write that $\mathbf{k}$ dependence of Σ^R as a function of $\zeta_{\mathbf{k}}$ instead, something that is always possible for spherical Fermi surfaces. In such a case, $\nabla_{\mathbf{k}} \to (\nabla_{\mathbf{k}} \zeta_{\mathbf{k}}) \partial / \partial \zeta_{\mathbf{k}}$ as we can see for example when $\zeta_{\mathbf{k}} = \mathbf{k}^2/2m$ and we have

$$\boxed{v^*_{\mathbf{k}} = v_{\mathbf{k}} \frac{1 + \frac{\partial}{\partial \zeta_{\mathbf{k}}} \operatorname{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial \omega} \operatorname{Re} \Sigma^R(\mathbf{k},\omega)\big|_{\omega = E_{\mathbf{k}} - \mu = 0}}.} \tag{31.32}$$

In cases where the electronic (band) structure has correctly treated the $\mathbf{k}$ dependence of the self-energy, or when the latter is negligible, then the renormalized Fermi velocity differs from the bare one only through the famous quasiparticle renormalization factor. In other words, $v^*_{\mathbf{k}} = Z_{\mathbf{k}} v_{\mathbf{k}}$. The equation for the renormalized velocity is also often written in terms of a mass renormalization instead. Indeed, we will discuss later the fact that the Fermi wave vector k_F is unmodified by interactions for spherical Fermi surfaces (Luttinger's theorem). Defining then $m^* v^*_{k_F} = k_F = m v_{k_F}$ means that our equation for the renormalized velocity gives us

$$\boxed{\frac{m}{m^*} = \lim_{\mathbf{k} \to \mathbf{k}_F} \frac{1 + \frac{\partial}{\partial \zeta_{\mathbf{k}}} \operatorname{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial \omega} \operatorname{Re} \Sigma^R(\mathbf{k},\omega)\big|_{\omega = E_{\mathbf{k}} - \mu}}} \tag{31.33}$$

Remark 226 *In the jargon, the quasiparticle piece of the spectral weight Eq. (31.20) is called the "coherent" piece of the spectral weight, by contrast with the incoherent contribution that I mentionned above.*

31.5 Fermi liquid interpretation of ARPES

Let us see how to interpret the experiments of the previous subsection in light of the quasiparticle model just described. First of all, the wave vectors studied are all close to the Fermi surface as measured on the scale of k_F. Hence, every quantity appearing in the quasiparticle spectral weight Eq.(31.25) that depends on the self-energy is evaluated at the Fermi wave vector, which can however be angle dependent. The frequency dependence of the self-energy then is most important. The experiments were carried out at $T = 20K$ where the resistivity has a T^2 temperature dependence. This is the regime dominated by electron-electron interactions, where so-called Fermi liquid theory applies. What is Fermi liquid theory?[2]

It would require more than the few lines that we have to explain it, but roughly speaking, for our purposes, let us say that it uses the fact that phase space for electron-electron scattering vanishes at zero temperature and at the Fermi surface, to argue that the quasiparticle model applies to interacting electrons. Originally the model was developed by Landau for liquid ^3He which has fermionic properties, hence the name Fermi Liquid theory. It is a very deep theory that in a sense justifies all the successes of the almost-free electron picture of electrons in solids. I cannot do it justice here. A simple way to make its main ingredients plausible, [5] is to assume that near the Fermi surface in the limit of zero temperature, the self-energy is *i)* analytic and *ii)* has an imaginary part that vanishes at zero frequency. The latter result follows from general considerations on the Pauli exclusion principle and available phase space that are briefly summarized in Fig. (31-4). I will give an alternate derivation in the section on the electron-gas.

Let us define real and imaginary parts of the retarded self-energy by

$$\Sigma^R = \Sigma' + i\Sigma'' \tag{31.34}$$

Our two hypothesis imply that Σ'' has the Taylor expansion

$$\Sigma''(\mathbf{k}_F;\omega) = \alpha\omega - \gamma\omega^2 + \dots \tag{31.35}$$

The imaginary part of the retarded self-energy must be negative to insure that the retarded Green's function has poles in the lower half-plane, as is clear from the general relation between Green function and self-energy Eq. (31.18). This means that we must have $\alpha = 0$ and $\gamma > 0$. Fermi liquid theory keeps only the leading term

$$\Sigma'' = -\gamma\omega^2$$

We will verify for simple models that this quadratic frequency dependence is essentially correct in $d \geq 3$.

We know that the imaginary part of the self-energy must vanish at infinite frequency where free-particle behavior is expected, (Sec. 32.1) as in the harmonic oscillator case. Following Refs. [162] and [**?**], we take the following smooth cutoff model, neglecting impurity scattering and temperature

$$\Sigma''(\omega) = \begin{cases} -s\frac{\omega^2}{\omega^{*2}} & \text{for } \omega < \omega^* \\ -sF\left(\frac{\omega}{\omega^*}\right) & \text{for } \omega > \omega^* \end{cases}, \tag{31.36}$$

where ω^* is the frequency at which ω^2 behavior stops, $2s$ is the electron-electron scattering rate (in units $\hbar = 1$) without many-body effects, and the cutoff function

[2] A short summary on internet by Ross McKenzie
https://docs.google.com/viewer?a=v&pid=sites&srcid=ZGVmYXVsdGRvbWFpbnxjb25kZW5zZWRjb25jZXB0czN8Z

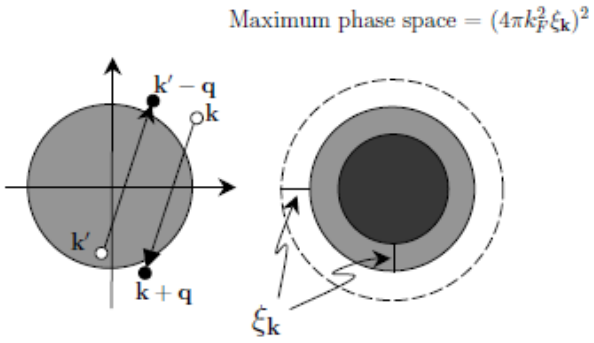


Figure 15.1: The two-particle scattering event that gives rise to a finite life time of the quasiparticles. Both momentum and energy have to be conserved. This together with the Pauli principle cause the phase space available for the scattering to be very limited, which is illustrated on the right hand figure. The dashed circle indicates the energy of the initial state. Since the particle can only loose energy, the other particle which is scattered out of state $\mathbf{k}'$ can only gain energy. Furthermore, because of the Pauli principle the final states of both particles have to lie outside the Fermi surface and therefore the phase space volume for the final state $\mathbf{k}+\mathbf{q}$ (white area) and for the initial state $\mathbf{k}'$ (gray area) both scale with $\xi_{\mathbf{k}}$ giving rise to a maximum total phase proportional to $\xi_{\mathbf{k}}^2$.

Figure 31-4 Taken from H. Bruus and K. Flensberg, "Introduction to Many-body theory in condensed matter physics".

$F(y)$ takes the value unity at $y = 1$ and then decreases monotonically to zero afterwards[3]. A more realistic model, as we will see, crosses over from ω^2 behavior while continuing to increase in absolute value before decreasing. But that does not modify the result that we are looking for, namely that the real-part of the self-energy obtained by Kramers-Kronig gives a value of Z consistent with quasiparticle behavior. So let us forge ahead.

The real part is then obtained from the Kramers-Kronig relation Eq.(19.1) that must be obeyed by the self-energy. We make the additional assumption that $\Sigma''(\omega)$ is even in frequency. Another way to state that is that we assume particle-hole symmetry. Following the same arguments as those used for damping of the harmonic oscillator, in Sec.2.3 (Sec. also Sec.32.2), the Kramers-Kronig relation give us for small ω

$$\left[\Sigma'(\mathbf{k}_F;\omega) - \Sigma'(\mathbf{k}_F;\infty)\right] = \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\Sigma''(\mathbf{k}_F;\omega')}{\omega'-\omega} \tag{31.37}$$

$$= -\frac{s}{(\omega^*)^2}\mathcal{P}\int_{-\omega^*}^{\omega^*}\frac{d\omega'}{\pi}\frac{\left(\omega'^2-\omega^2+\omega^2\right)}{\omega'-\omega} \tag{31.38}$$

$$-2s\mathcal{P}\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F\left(\frac{\omega}{\omega^*}\right)}{\omega'-\omega}$$

[3] Σ'' in this model has a discontinuous first derivative at $\omega = \omega^*$, which is why it is not a quite realistic model, even though it is better than a sharp cutoff model.

Let us focus on the first integral. It can be evaluated as follows

$$-\frac{s}{(\omega^*)^2}\mathcal{P}\int_{-\omega^*}^{\omega^*}\frac{d\omega'}{\pi}\frac{(\omega'-\omega)(\omega'+\omega)}{\omega'-\omega}-\frac{s}{(\omega^*)^2}\omega^2\mathcal{P}\int_{-\omega^*}^{\omega^*}\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega} \tag{31.39}$$

$$= -\frac{s}{\pi}-\frac{2s}{\pi}\left(\frac{\omega}{\omega^*}\right)-\frac{s}{\pi}\left(\frac{\omega}{\omega^*}\right)^2\ln\left|\frac{\omega^*-\omega}{\omega^*+\omega}\right|. \tag{31.40}$$

The constant term is added to $\Sigma'(\mathbf{k}_F;\infty)$ to give the total contribution to the zero-frequency limit of the real-part of the self-energy, which leads to the renormalization of the chemical potential. Since $\ln[(1-x)/(1+x)]\sim -2x$, in the limit $\omega \ll \omega^*$ there is no linear in ω contribution from the logarithm. The remaining term involving F can be expanded in a power series in ω/ω^*. So there is term linear in ω coming from that. We are finally left with

$$\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k}_F,\omega)\Big|_{\omega=0}=-\frac{2s\zeta}{\pi\omega^*} \tag{31.41}$$

where ζ is a number of less than 2 when estimated with the above model for the cutoff (as discussed in a remark below). Hence

$$\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k},\omega)\Big|_{\omega=0}<0 \tag{31.42}$$

This in turn means that the corresponding value of Z_{k_F} is less than unity, as we had concluded in Eqs.(31.23) and (31.27) above. In summary, the analyticity hypothesis along with the vanishing of $\Sigma''(0)$ implies the existence of quasiparticles.

Remark 227 *Warning: there are subtleties. The above results assume that there is a cutoff to $\Sigma''(\mathbf{k}_F;\omega')$. The argument just mentioned in Eq.(31.41) fails when the integral diverges. Then, the low frequency expansion for the self-energy in Eq.(31.38) cannot be done. Expanding under the integral sign is no longer valid. One must do the principal part integral first. In fact, even for a Fermi liquid at finite temperature, $\Sigma''(\mathbf{k}_F;\omega)\sim\omega^2+(\pi T)^2$ so that the $(\pi T)^2$ appears to lead to a divergent integral in Eq.(31.41). Returning to the original Kramers-Krönig expression for Σ' however, the principal part integral shows that the constant term $(\pi T)^2$ for $\Sigma''(\mathbf{k}_F;\omega)$ does not contribute at all to Σ' if the cutoff in Σ'' is symmetric at positive and negative frequencies. In practice one can encounter situations where $\partial\Sigma/\partial\omega>0$. In that case, we do not have a Fermi liquid since $Z>1$ is inconsistent with the normalization of the spectral weight. One can work out an explicit example in the renormalized classical regime of spin fluctuations in two dimensions. (Appendix D of [255]).*

Remark 228 *To estimate the contribution from the cutoff, note that the denominator can be expanded in powers of ω/ω' because by construction, $\omega<\omega^*$ and we assume that $F\left(\frac{\omega}{\omega^*}\right)$ decreases at least as a power law starting from unity, making the integral convergent. So, recalling that this all started with F an even function of its argument,*

$$-2s\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F\left(\frac{\omega}{\omega^*}\right)}{\omega'}\sum_{n=0}^{\infty}\left(\frac{\omega}{\omega'}\right)^{2n+1} \tag{31.43}$$

the linear in ω contribution from this term is

$$-2s\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F\left(\frac{\omega}{\omega^*}\right)}{\omega'}\left(\frac{\omega}{\omega'}\right)\leq-\frac{2s}{\pi}\frac{\omega}{\omega^*}\int_1^{\infty}dy\frac{1}{y^2}=-\frac{2s}{\pi}\frac{\omega}{\omega^*} \tag{31.44}$$

which must be added to the linear in ω contribution, leading to the above estimate for the value of ζ.

The solid lines in Fig.(31-1) are two-parameter fits that also take into account the wave vector and energy resolution of the experiment [6]. One parameter is $E_k - \mu$ while the other one is γ', a quantity defined by substituting the Fermi liquid approximation in the equation for damping Eq.(31.26)

$$\Gamma_{k_F}(\omega) = Z_{k_F}\gamma\omega^2 = \gamma'\omega^2. \tag{31.45}$$

Contrary to E_k, the damping parameter γ' is the same for all curves. The solid-line fits are obtained with $\gamma' = 40eV^{-1}$ (β' on the figure). The fits become increasingly worse as one moves away from the Fermi surface, as expected. It is important to notice, however, that even the small left-over weight for wave-vectors above the Fermi surface $\left(\theta < 14.75^0\right)$ can be fitted with the same value of γ. This weight is the tail of a quasiparticle that could be observed at positive frequencies in inverse photoemission experiments (so-called BIS). The authors compared the results of their fits to the theoretical estimate, [7] $\gamma = 0.067\omega_p/\varepsilon_F^2$. Using $\omega_p = 18.2eV$, $\varepsilon_F = 0.3eV$ and the extrapolated value of Z_{k_F} obtained by putting[4] $r_s = 10$ in electron gas results, [8] they find $\gamma' < 5\,(eV)^{-1}$ while their experimental results are consistent with $\gamma' = 40 \pm 5\,(eV)^{-1}$. The theoretical estimate is almost one order of magnitude smaller than the experimental result. This is not so bad given the crudeness of the theoretical model (electron gas with no lattice effect). In particular, this system is a semimetal so that there are other decay channels than just the one estimated from a single circular Fermi surface. Furthermore, electron gas calculations are formally correct only for small r_s while there we have $r_s = 10$.

More recent experiments have been performed by Grioni's group [14]. Results are shown in Fig. (31-5). In this work, authors allow for a constant damping $\Gamma_0 = 17\ meV$ coming from the temperature and from disorder and then they fit the rest with a Fermi velocity $\hbar v_F = 0.73 \pm 0.1eV\ \dot{A}$ close to band structure calculations, $\hbar v_F = 0.68\ eV\ \dot{A}$ and γ' that varies between 0.5 eV^{-1} (16^0) and 0.9 eV^{-1} (14.5^0). The Fermi liquid fit is just as good, but the interpretation of the origin of the broadening terms is different. This shows that it is not always easy to interpret ARPES data, even for Fermi liquids. But we saw in Fig. (31-3) that modern electronic structure calculations that include the effect of correlations can be quite successful.

Theoretical estimates for high-temperature superconductors are two orders of magnitude smaller than the observed result [6].

Remark 229 *What allows the existence of the Fermi liquid is the vanishing of the imaginary part of the self-energy at $\omega = 0$. Electrons at the Fermi energy have an infinite lifetime at zero temperature. In addition, their lifetime vanishes faster than their energy ω so that "quasiparticles" survive in the vicinity of the Fermi surface. I will show that at finite temperature and $\omega = 0$, their lifetime is proportional to T^2. As a consequence, their width is sufficiently small that it makes sense to populate the quasiparticle states following the Fermi function.*

Remark 230 *Asymmetry of the lineshape: The line shapes are asymmetrical, with a tail at energies far from the Fermi surface (large binding energies). This is consistent with the fact that the "inverse lifetime" $\Gamma_{k_F}(\omega) = Z_{k_F}\gamma\omega^2$ is not a constant, but is instead larger at larger binding energies.*

Remark 231 *Failure of Fermi liquid at high-frequency: Clearly the Fermi liquid expression for the self-energy fails at large frequencies since we know from its spectral representation that the real-part of the self-energy goes to a frequency-independent constant at large frequency, the first correction being proportional to $1/\omega$ as discussed below in subsection (32.1). Conversely, there is always a cutoff*

[4] r_s is the average electron spacing expressed in terms of the Bohr radius.

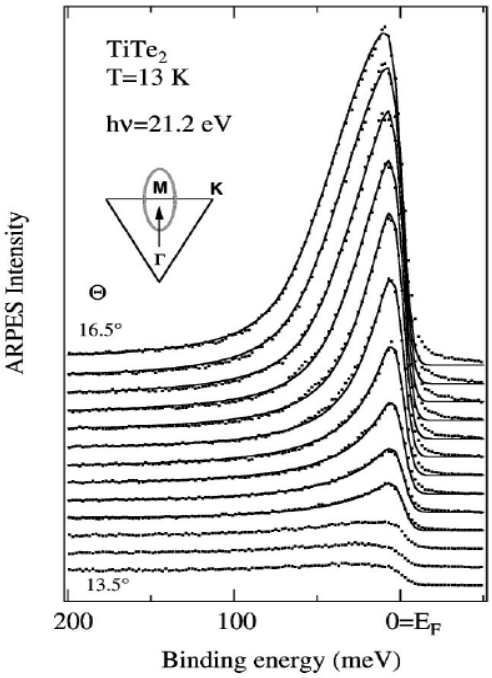


Figure 31-5 Figure 1 from Ref.[14] for the ARPES spectrum of 1*T*-$TiTe_2$ measured near the Fermi surface crossing along the high-symmetry ΓM direction ($\theta = 0$ is normal emission). The lines are results of Fermi liquid fits and the inset shows a portion of the Brillouin zone with the relevant ellipsoidal electron pocket.

in the imaginary part of the self-energy. This is not apparent in the Fermi liquid form above but we had to assume its existence for convergence. The cutoff on the imaginary part is analogous to the cutoff in χ''. Absorption cannot occur at arbitrary high frequency.

Remark 232 *Destruction of quasiparticles by critical fluctuations in two dimensions: Note that it is only if Σ'' vanishes fast enough at low frequency that it is correct to expand the Kramers-Kronig expression in powers of the frequency to obtain Eq.(31.41). When $\Sigma''(\omega)$ vanishes slower than ω^2, then Eq.(31.41) for the slope of the real part is not valid. The integral does not converge uniformly and it is not possible to interchange the order of differentiation and integration. In such a case it is possible to have the opposite inequality for the slope of the real part $\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k},\omega)\big|_{\omega=0} > 0$. This does not lead to any contradiction, such as $Z_{k_F} > 1$, because there is no quasiparticle solution at $\omega = 0$ in this case. This situation occurs for example in two dimensions when classical thermal fluctuations create a pseudogap in the normal state before a zero-temperature phase transition is reached [9].*

31.6 Momentum distribution in an interacting system

In an interacting system, momentum is not a good quantum number so $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ is *not* equal to the Fermi distribution. On the other hand, $n_{\mathbf{k}} = \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ can be computed from the spectral weight. By taking the Fourier transform of Eq.(31.7) $\int dt e^{i\omega t} \left\langle c_{\mathbf{k}_{||}}^{\dagger} c_{\mathbf{k}_{||}}(t) \right\rangle = f(\omega) A\left(\mathbf{k}_{||}, \omega\right)$ one finds

$$\boxed{\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega') A(\mathbf{k}, \omega')}. \tag{31.46}$$

Alternate derivation

$$\begin{aligned} \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle &= \lim_{\tau \to 0^-} \left[- \left\langle T_{\tau} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger} \right\rangle \right] \\ &= \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) \end{aligned} \tag{31.47}$$

To compute the latter quantity from the spectral weight, it suffices to use the spectral representation Eq.(29.34)

$$\begin{aligned} \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) &= T \lim_{\tau \to 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \\ &= T \lim_{\tau \to 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}, \omega')}{ik_n - \omega'} \end{aligned} \tag{31.48}$$

Using the result Eq.(29.85) found above for the sum over Matsubara frequencies, we are left with the desired result.

Our result means that the momentum distribution is a Fermi-Dirac distribution only if the spectral weight is a delta function. This occurs for free particles or, more generally if the real-part of the self-energy is frequency independent since, in this case, the Kramers-Kronig relations imply that the imaginary part of the self-energy vanishes so that Eq.(31.20) for the spectral weight gives us a delta function.

Remark 233 *Jump of the momentum distribution at the Fermi level: Even if* $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ *is no-longer a Fermi-Dirac distribution in an interacting system, nevertheless at zero-temperature in a system subject only to electron-electron interaction, there is a jump in* $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ *at the Fermi level. The existence of this jump can be seen as follows. At zero temperature, our last result gives us*

$$\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \int_{-\infty}^{0} \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega') \tag{31.49}$$

Let us take the quasiparticle form Eq.(31.25) of the spectral weight with the Fermi liquid expression Eq.(31.45) for the scattering rate. The incoherent background varies smoothly with $\mathbf{k}$ *and hence cannot lead to any jump in occupation number. The quasiparticle piece on the other hand behaves when* $k \to k_F$*, or in other words when* $E_{\mathbf{k}} - \mu \to 0$*, as* $Z_{k_F} \delta(\omega)$*. At least crudely speaking. When* $E_{\mathbf{k}} - \mu \to 0^-$*, this delta function is inside the integration domain hence it contributes to the integral,*

while when $E_{\mathbf{k}} - \mu \to 0^+$ *the delta function is outside and does not contribute to the integral. This means that there is a big difference between these two nearby wave vectors, namely*

$$\lim_{\mathbf{k}\to\mathbf{k}_f^-} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle - \lim_{\mathbf{k}\to\mathbf{k}_f^+} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle = Z_{k_F} \tag{31.50}$$

In the above argument, we have done as if $\Gamma_{\mathbf{k}}(\omega)$ *was frequency independent and infinitesimally small in Eq.(31.25). This is not the case so our argument is rather crude. Nevertheless, if one uses the actual frequency-dependent forms and does the frequency integral explicitly, one can check that the above conclusion about the jump is true (although less trivial).*

Remark 234 *Fermi surface and interactions: The conclusion of the previous remark is that even in an interacting system, at zero temperature there is a sharp Fermi surface as in the free electron model, except that the jump is less than unity. For simplicity we have discussed the spinless case. A qualitative sketch of the zero-temperature momentum distribution in an interacting system appears in Fig.(31-6). Since momentum of a single particle is not a good quantum number anymore, some states above the Fermi momentum are now occupied while others below are empty. Nevertheless, the notion of a Fermi surface is well defined by the sharp jump that I just discussed.*

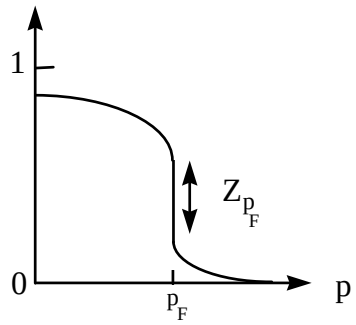


Figure 31-6 Qualitative sketch of the zero-temperature momentum distribution in an interacting system.

Remark 235 *It is possible to compute* $n_{\mathbf{k}}$ *from the Green's function directly by doing the sum over Matsubara frequencies. To avoid having to deal with sums that need convergence factor, it suffices to use the folloing trick [142]:*

$$n_{\mathbf{k}} = \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle \tag{31.51}$$

$$n_{\mathbf{k}} = 1 - \left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle \tag{31.52}$$

$$2n_{\mathbf{k}} - 1 = T \sum_{n=-\infty}^{\infty} \left(e^{-ik_n 0^-} + e^{-ik_n 0^+} \right) \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \tag{31.53}$$

$$= T \sum_{n=-\infty}^{\infty} e^{-ik_n 0^-} \left[\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) + \mathcal{G}(\mathbf{r}, \mathbf{r}'; -ik_n) \right] \tag{31.54}$$

$$= T \sum_{n=-\infty}^{\infty} 2 \operatorname{Re} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) . \tag{31.55}$$

In the last equation I removed the convergence factor because $\mathrm{Re}\,\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)$ *is proportional to* $1/\left(ik_n\right)^2$ *at infinity so the sum converges withou the need for* $e^{-ik_n 0^-}$.

Remark 236 *The "Marginal Fermi liquid" hypothesis was formulated for cuprates [241]. In this approach,* $\Sigma'' \sim -|\omega|$ *and* Z *vanishes logarithmically with* ω.

Remark 237 *Luttinger's theorem: More generally, in a Fermi liquid the volume of reciprocal space contained within the Fermi surface defined by the jump, is independent of interactions. This is Luttinger's theorem. In the case where the Fermi surface is spherical, this means that* k_F *is unaffected.*

32. *MORE FORMAL MATTERS : ASYMPTOTIC BEHAVIOR, CAUSALITY, GAUGE TRANSFORMATION

In designing approximations, we have to try to preserve as many as possible of the exact properties. Sum rules are such properties. They determine the structure of the high-frequency expansion and hence one can also check whether a given approximation preserves the sum rules by looking at its high-frequency expansion. This is the first topic we will discuss. The second topic concerns restrictions imposed by causality. This has become a very important topic in the context of Dynamical Mean-field theory or other approaches that describe the physics that occurs at strong coupling, such as the Mott transition. We will come back on this in later chapters.

32.1 *Asymptotic behavior of $\mathcal{G}\left(\mathbf{k};ik_n\right)$ and $\Sigma\left(\mathbf{k};ik_n\right)$

As usual, the high-frequency asymptotic properties of the Green's function are determined by sum rules. From the spectral representation(29.34), we obtain, for the general interacting case

$$\lim_{ik_n\to\infty}\mathcal{G}\left(\mathbf{k};ik_n\right)=\lim_{ik_n\to\infty}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{k};\omega'\right)}{ik_n-\omega'} \tag{32.1}$$

$$=\lim_{ik_n\to\infty}\frac{1}{ik_n}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)=\lim_{ik_n\to\infty}\frac{1}{ik_n}\left\langle\left\{c_{\mathbf{k}},c_{\mathbf{k}}^{+}\right\}\right\rangle=\lim_{ik_n\to\infty}\frac{1}{ik_n} \tag{32.2}$$

Defining the self-energy as usual

$$\mathcal{G}\left(\mathbf{k};ik_n\right)=\frac{1}{ik_n-\zeta_{\mathbf{k}}-\Sigma\left(\mathbf{k},ik_n\right)} \tag{32.3}$$

the correct asymptotic behavior for the Green's function implies that the self-energy at high frequency cannot diverge: It must go to a constant independent of frequency

$$\lim_{ik_n\to\infty}\Sigma\left(\mathbf{k},ik_n\right)=cst. \tag{32.4}$$

We will see later that the value of this constant is in fact given correctly by the Hartree-Fock approximation.

The converse of the above result [5] for the Green's function, is that if

$$\lim_{ik_n\to\infty}\mathcal{G}\left(\mathbf{k};ik_n\right)=\lim_{ik_n\to\infty}\frac{1}{ik_n}$$

then that is all that is needed to obtain an approximation for the Green's function which obeys the anticommutation relation:

$$\mathcal{G}\left(\mathbf{k};0^{-}\right)-\mathcal{G}\left(\mathbf{k};0^{+}\right)=\left\langle c_{\mathbf{k}}^{+}c_{\mathbf{k}}\right\rangle+\left\langle c_{\mathbf{k}}c_{\mathbf{k}}^{+}\right\rangle=1 \tag{32.5}$$

Proof :It suffices to notice that

$$\mathcal{G}\left(\mathbf{k};0^{-}\right)-\mathcal{G}\left(\mathbf{k};0^{+}\right)=\frac{1}{\beta}\sum_{n}\left[e^{-ik_{n}0^{-}}-e^{-ik_{n}0^{+}}\right]\mathcal{G}\left(\mathbf{k};ik_{n}\right) \tag{32.6}$$

We can add and subtract the asymptotic behavior to obtain,

$$\frac{1}{\beta}\sum_{n}\left[\left(e^{-ik_{n}0^{-}}-e^{-ik_{n}0^{+}}\right)\left(\mathcal{G}\left(\mathbf{k};ik_{n}\right)-\frac{1}{ik_{n}}\right)\right]+\frac{1}{\beta}\sum_{n}\left(e^{-ik_{n}0^{-}}-e^{-ik_{n}}\right)\frac{1}{ik_{n}} \tag{32.7}$$

In the first sum, $\mathcal{G}\left(\mathbf{k};ik_{n}\right)-\frac{1}{ik_{n}}$ decays faster than $\frac{1}{ik_{n}}$ so that the convergence factors are not needed for the sum to converge. This means that this first sum vanishes. The last sum gives unity, as we easily see from the previous section. This proves our assertion.

Remark 238 *High-frequency expansion for the Green's function and sum-rules: The coefficients of the high-frequency expansion of* $\mathcal{G}\left(\mathbf{k};ik_{n}\right)$ *in powers of* $1/ik_{n}$ *are obtained from sum rules on the spectral weight, in complete analogy with what we have found in previous chapters. The fact that* $A\left(\mathbf{k},\omega\right)$ *falls fast enough to allow us to expand under the integral sign follows from the fact that all frequency moments of* $A\left(\mathbf{k},\omega\right)$ *, namely* $\int d\omega\omega^{n}A\left(\mathbf{k},\omega\right)$ *, exist and are given by equal-time commutators. Explicit expressions for* $A\left(\mathbf{k},\omega\right)$ *in terms of matrix elements, as given in Subsection(31.1) above, show physically why* $A\left(\mathbf{k},\omega\right)$ *falls so fast at large frequencies. As an example, to show that the coefficient of the* $1/ik_{n}$ *term in the high frequency expansion is equal to* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)$ *it is sufficient that* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|\omega' A\left(\mathbf{k};\omega'\right)\right|$ *exists.[3] This can be seen as follows,*

$$\begin{aligned}
ik_{n}\mathcal{G}\left(\mathbf{k};ik_{n}\right)-\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)\left(\frac{ik_{n}}{ik_{n}-\omega'}-1\right) && (32.8)\\
&= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)\frac{\omega'}{ik_{n}-\omega'} && (32.9)\\
&\leq \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|A\left(\mathbf{k};\omega'\right)\frac{\omega'}{ik_{n}-\omega'}\right| && (32.10)\\
&\leq \left|\frac{1}{ik_{n}}\right|\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|A\left(\mathbf{k};\omega'\right)\omega'\right| && (32.11)
\end{aligned}$$

If the integral exists then, it is a rigorous result that

$$\lim_{ik_{n}\rightarrow\infty}ik_{n}\mathcal{G}\left(\mathbf{k};ik_{n}\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right) \tag{32.12}$$

This is an important result. It suggests that approximate theories that give 1 *as the coefficient of* $\left(ik_{n}\right)^{-1}$ *in the high frequency expansion have a normalized spectral weight. However[3] the above proof assumes that there is indeed a spectral representation for* $\mathcal{G}\left(\mathbf{k};ik_{n}\right)$ *. A Green's function for a theory that is not causal fails to have a spectral representation. If a spectral representation is possible, the analytically continued approximate* $G^{R}\left(\mathbf{k},\omega\right)$ *is necessarily causal. Approximate theories may not be causal. This failure of causality may reflect a phase transition, as we will see later, or may simply be a sign that the approximation is bad. As an example, suppose that we obtain* $\mathcal{G}\left(\mathbf{k};ik_{n}\right)=\left(ik_{n}-ia\right)^{-1}$ *. This has the correct high-frequency behavior but its analytical continuation does not satisfy causality. It has no spectral representation. On the other hand,* $\mathcal{G}\left(\mathbf{k};ik_{n}\right)=\left(ik_{n}+\left(k_{n}/\left|k_{n}\right|\right)ia\right)^{-1}$ *has a Lorentzian as a spectral weight and is causal. It may also occur that the approximate theory may have* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)=1$ *but* $A\left(\mathbf{k};\omega'\right)<0$ *for some range of* ω'*. This unphysical result may again signal that the approximate theory fails because of a phase transition or because it is a bad approximation.*

32.2 *Implications of causality for G^R and Σ^R

Consider the retarded Green function as a matrix in $\mathbf{r}, \mathbf{r}'$. We will show that the real and imaginary parts of G^R and of Σ^R are each Hermitian matrices. in addition, $\operatorname{Im} G^R$ and $\operatorname{Im} \Sigma^R$ are both negative definite (except in the special case of non-interacting particles where $\operatorname{Im} \Sigma^R = 0$). From our general considerations with the harmonic oscillator at the beginning, we know that the self-energy, that acts as a damping, has to be retarded as well. Nevertheless, we will see this explicitly in this section.

In analogy with the Matsubara Green function Eq.(29.41) G^R has the Lehmann representation

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = e^{\beta\Omega} \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \frac{\langle n| \psi_S(\mathbf{r}) |m\rangle \langle m| \psi_S^\dagger(\mathbf{r}') |n\rangle}{\omega + i\eta - (E_m - E_n - \mu)}. \quad (32.13)$$

In a basis where the matrix $\operatorname{Im} G^R(\mathbf{r}, \mathbf{r}'; \omega)$ is diagonal, say for quantum number α, then

$$\begin{aligned} \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega) &= -\pi \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \langle n| c_{\boldsymbol{\alpha}} |m\rangle \langle m| c_{\boldsymbol{\alpha}}^\dagger |n\rangle \delta(\omega - (E_m - E_n - \mu)) \\ &= -\pi \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) |\langle n| c_{\boldsymbol{\alpha}} |m\rangle|^2 \delta(\omega - (E_m - E_n - \mu)) \quad (32.14) \end{aligned}$$

which proves that the matrix for the imaginary part is negative definite. The negative sign comes from the $+i\eta$ in the original formula and is clearly a consequence of causality. In that same diagonal basis,

$$\operatorname{Re} G^R(\boldsymbol{\alpha}; \omega) = e^{\beta\Omega} \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \frac{|\langle n| c_{\boldsymbol{\alpha}} |m\rangle|^2}{\omega - (E_m - E_n - \mu)}. \quad (32.15)$$

When we change to an arbitrary basis (say $\mathbf{r}, \mathbf{r}'$ for definiteness) with the unitary transformation U, we find, using also $\operatorname{Im} G^R(\boldsymbol{\alpha}; \omega) = \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega)^*$ and $\operatorname{Re} G^R(\boldsymbol{\alpha}; \omega) = \operatorname{Re} G^R(\boldsymbol{\alpha}; \omega)^*$ that

$$\begin{aligned} G^R(\mathbf{r}, \mathbf{r}'; \omega) &= U(\mathbf{r}, \boldsymbol{\alpha}) G^R(\boldsymbol{\alpha}; \omega) U^\dagger(\boldsymbol{\alpha}, \mathbf{r}') & (32.16) \\ &= U(\mathbf{r}, \boldsymbol{\alpha}) \operatorname{Re} G^R(\boldsymbol{\alpha}; \omega) U^\dagger(\boldsymbol{\alpha}, \mathbf{r}') + iU(\mathbf{r}, \boldsymbol{\alpha}) \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega) U^\dagger(\boldsymbol{\alpha}, \mathbf{r}') \\ &\equiv X(\mathbf{r}, \mathbf{r}'; \omega) + iY(\mathbf{r}, \mathbf{r}'; \omega) & (32.17) \\ G^R(\mathbf{r}, \mathbf{r}'; \omega)^* &= X(\mathbf{r}, \mathbf{r}'; \omega)^* - iY(\mathbf{r}, \mathbf{r}'; \omega)^* & (32.18) \\ &= U^*(\mathbf{r}, \boldsymbol{\alpha}) \operatorname{Re} G^R(\boldsymbol{\alpha}; \omega) U(\mathbf{r}', \boldsymbol{\alpha}) - iU^*(\mathbf{r}, \boldsymbol{\alpha}) \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega) U(\mathbf{r}', \boldsymbol{\alpha}) \\ &= U(\mathbf{r}', \boldsymbol{\alpha}) \operatorname{Re} G^R(\boldsymbol{\alpha}; \omega) U^\dagger(\boldsymbol{\alpha}, \mathbf{r}) - iU(\mathbf{r}', \boldsymbol{\alpha}) \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega) U^\dagger(\boldsymbol{\alpha}, \mathbf{r}) \\ &= X(\mathbf{r}', \mathbf{r}; \omega) - iY(\mathbf{r}', \mathbf{r}; \omega) & (32.19) \end{aligned}$$

where there is an implicit sum over $\boldsymbol{\alpha}$. Comparing Eqs.(32.18) and (32.19), we see that in an arbitrary canonical basis, we can write $G^R = X - iY$ and $G^A = X + iY$ where both X and Y are hermitian matrices.

Remark 239 *Spectral weight as the anti-hermitian part of G^R : In the diagonal basis, the spectral weight is $-2 \operatorname{Im} G^R(\boldsymbol{\alpha}; \omega)$, which becomes simply $-2Y$ with Y hermitian in a general basis. In an arbitrary basis, it is better then to say that the spectral weight can be extracted from the anti-hermitian part of G^R, namely from*

$$\left(G^R(\mathbf{r}, \mathbf{r}'; \omega) - G^R(\mathbf{r}', \mathbf{r}; \omega)^*\right) = 2iY(\mathbf{r}, \mathbf{r}'; \omega). \quad (32.20)$$

The definition as the value of the cut along the real axis of $G(z)$ is also always valid.

Following Potthoff [195] we show that the retarded self-energy as a matrix has the same properties as G^R. First, we need to prove that

$$\frac{1}{A \pm iB} = X \mp iY \tag{32.21}$$

with X and Y both Hermitian and Y positive definite if A and B are both Hermitian with B positive definite. A positive definite matrix can always be written in the form $B = D^\dagger D$ where D is Hermitian, i.e. $D^\dagger = D = B^{1/2}$. Using this property, we have

$$\frac{1}{A \pm iB} = D^{-1} \frac{1}{D^{\dagger -1} A D^{-1} \pm iI} D^{\dagger -1}, \tag{32.22}$$

where we assumed that B is invertible (in particular, it cannot vanish). Since $D^{\dagger -1} A D^{-1}$ is Hermitian as well, we can diagonalize it by a unitary transformation $D^{\dagger -1} A D^{-1} = U c U^\dagger$ where c is a diagonal matrix. Thus,

$$\frac{1}{A \pm iB} = D^{-1} U \frac{1}{c \pm iI} U^\dagger D^{\dagger -1} = D^{-1} U \frac{c \mp iI}{c^2 + 1} U^\dagger D^{\dagger -1} = X \mp iY \tag{32.23}$$

with X and Y Hermitians since $\left(U^\dagger D^{\dagger -1}\right)^\dagger = D^{-1} U$. In addition, Y is positive definite since in the diagonal basis $Y \to \left(c^2 + 1\right)^{-1}$. Now, define $\left(G^R\right)^{-1} = (A - iB)^{-1} = X + iY$ and $\left(G_0^R\right)^{-1} = (A_0 - iB_0)^{-1} = X_0 + iY_0$ so that

$$\left(G^R\right)^{-1} = X + iY = \left(G_0^R\right)^{-1} - \Sigma^R = X_0 + iY_0 - \Sigma^{'R} - i\Sigma^{''R}. \tag{32.24}$$

Then, given that X, Y and X_0, Y_0 are Hermitians, we have that $\Sigma^{'R}$ and $\Sigma^{''R}$ are Hermitian matrices. In addition, $\Sigma^{''R}$ is negative definite since Y_0 is infinitesimal which implies that $Y - Y_0$ can only be positive (or vanish in the non-interacting case). In the special case where the matrices are real symmetric instead of Hermitian, $\Sigma^{''R}$ and $\Sigma^{'R}$ are respectively the imaginary and real parts of the self-energy.

32.3 Gauge transformation for the Green's function

We have seen that under a gauge transformation (11.1), the single particle wave function transforms as

$$\langle \mathbf{r}| \, \psi'(t) \rangle = e^{ie\Lambda(\mathbf{r},t)} \langle \mathbf{r}| \, \psi(t) \rangle \tag{32.25}$$

If we define a gauge transformation for the field operators (not the wave function) as follows

$$\psi^\dagger(\mathbf{r},\tau) \to e^{-ie\Lambda(\mathbf{r},\tau)} \psi^\dagger(\mathbf{r},\tau), \tag{32.26}$$

then

$$\left(\psi^\dagger(\mathbf{r},\tau)|0\rangle = e^{K\tau}|\mathbf{r}\rangle\right) \to e^{-ie\Lambda(\mathbf{r},\tau)} e^{K\tau}|\mathbf{r}\rangle \tag{32.27}$$

and any one-body state will transform correctly.

The Green's function is defined by a trace and the Boltzmann factor is gauge invariant, so that under a gauge transformation

$$\boxed{\mathcal{G}(1,2) = -\left\langle T_\tau \left(\psi(1)\psi^\dagger(2)\right)\right\rangle \to e^{ie\Lambda(1)} \mathcal{G}(1,2) e^{-ie\Lambda(2)}.} \tag{32.28}$$

To satisfy the boundary condition, we need that

$$\Lambda(\mathbf{r},\tau) = \Lambda(\mathbf{r},\tau+\beta) \tag{32.29}$$

33. THREE GENERAL THEOREMS

Risking to wear your patience out, we still have to go through three general theorems used repeatedly in Many-Body theory. Wick's theorem forms the basis ot the diagram technique in many-body theory. The linked-cluster theorems, or cumulant expansions, are much more general theorems that are also necessary to set up the machinery of diagrams. Finally, we prove a variational principle for the free energy that allows us to give a physical meaning to Hartree-Fock theory as the best one-body Hamiltonian for any given problem. This variational principle is useful for ordinary system, but also becomes indispensable when there is a broken symmetry.

33.1 Wick's theorem

Wick's theorem allows us to compute arbitrary correlation functions of any Hamiltonian that is quadratic in Fermion or Boson operators. That is clearly what we need to do perturbation theory, but let us look in a bit more details at how this comes about. We will need to compute in the interaction picture

$$\mathcal{G}(\tau) = -\frac{\mathrm{Tr}\left[e^{-\beta H_0} T_\tau \left(U_I(\beta,\tau)\,\psi_I(\tau)\,U_I(\tau,0)\,\psi_I^\dagger(0)\right)\right]}{\mathrm{Tr}\left[e^{-\beta H_0} T_\tau U_I(\beta,0)\right]} \tag{33.1}$$

Because $U_I(\tau,0)$ always contains an even number of fermions, it can be commuted with creation-annihilation operators without paying the price of minus signs so that

$$\boxed{\mathcal{G}(\tau) = -\frac{\mathrm{Tr}\left[e^{-\beta H_0} T_\tau \left(U_I(\beta,0)\psi_I(\tau)\psi_I^\dagger(0)\right)\right]}{\mathrm{Tr}\left[e^{-\beta H_0} T_\tau U_I(\beta,0)\right]}} \tag{33.2}$$

More specifically the evolution operator is,

$$\boxed{U_I(\beta,0) = T_\tau\left[\exp\left(-\int_0^\beta d\tau_1 V_I(\tau_1)\right)\right]} \tag{33.3}$$

Expanding this evolution operator to first order in the numerator of the Green's function one obtains

$$-\mathrm{Tr}\left[e^{-\beta H_0} T_\tau\left(\psi_I(\tau)\,\psi_I^\dagger(0)\right)\right] + \int_0^\beta d\tau_1 \mathrm{Tr}\left[e^{-\beta H_0} T_\tau\left(V_I(\tau_1)\,\psi_I(\tau)\,\psi_I^\dagger(0)\right)\right] \tag{33.4}$$

where in the case of a two-body interaction (Coulomb for example), $V_I(\tau_1)$ contains four field operators.

Wick's theorem allows us to evaluate expectation values such as those above. More generally, it allows us to compute expectation values of creation-annihilation operators such as,

$$\left\langle a_i(\tau_i)\,a_j(\tau_j)\,a_k^\dagger(\tau_k)\,a_l^\dagger(\tau_l)\right\rangle_0 \tag{33.5}$$

as long as the density matrix $e^{-\beta H_0}$ is that of a quadratic Hamiltonian.

Note that since quadratic Hamiltonians conserve the number of particles, expectation values vanish when the number of creation operators does not match the number of destruction operators.

Lemma 21 *If* $H_0 = \varepsilon_1 a_1^\dagger a_1 + \varepsilon_2 a_2^\dagger a_2$ *then* $\left\langle a_1 a_1^\dagger a_2 a_2^\dagger \right\rangle = \left\langle a_1 a_1^\dagger \right\rangle \left\langle a_2 a_2^\dagger \right\rangle$.

Proof: To understand what is going on, it is instructive to study first the problem where a single fermion state can be occupied. Then

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{\mathrm{Tr}\left[e^{-\beta H_0} a_1 a_1^\dagger\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} \tag{33.6}$$

$$= \frac{\langle 0| a_1 a_1^\dagger |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right) a_1 a_1^\dagger \left(a_1^\dagger |0\rangle\right)}{\langle 0| |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right)\left(a_1^\dagger |0\rangle\right)} = \frac{1}{1+e^{-\beta\epsilon_1}} \tag{33.7}$$

For two fermion states $1, 2$, then the complete set used to evaluate the trace is

$$|0\rangle |0\rangle, \quad a_1^\dagger |0\rangle |0\rangle, \quad |0\rangle a_2^\dagger |0\rangle, \quad a_1^\dagger |0\rangle a_2^\dagger |0\rangle \tag{33.8}$$

so that

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1+e^{-\beta\epsilon_2}}{1+e^{-\beta\epsilon_2}} = \frac{1}{1+e^{-\beta\epsilon_1}}. \tag{33.9}$$

The easiest way to understand the last result is to recall that $\left(1+a_1^\dagger\right)\left(1+a_2^\dagger\right)|0\rangle$ will generate the trace so that we can factor each subspace. The last result will remain true for an arbitrary number of fermion states, in other words

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}} = \frac{1}{1+e^{-\beta\epsilon_1}}. \tag{33.10}$$

Furthermore,

$$\left\langle a_1 a_1^\dagger a_2 a_2^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \frac{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}} \tag{33.11}$$

$$= \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \tag{33.12}$$

$$= \left\langle a_1 a_1^\dagger \right\rangle \left\langle a_2 a_2^\dagger \right\rangle \tag{33.13}$$

Theorem 22 *Any expectation value such as* $\left\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l)\right\rangle_0$ *calculated with a density matrix* $e^{-\beta K_0}$ *that is quadratic in field operators can be computed as the sum of all possible products of the type* $\left\langle a_j(\tau_j) a_k^\dagger(\tau_k)\right\rangle_0 \left\langle a_i(\tau_i) a_l^\dagger(\tau_l)\right\rangle_0$ *that can be formed by pairing creation and annihilation operators. For a given term on the right-hand side, there is a minus sign if the order of the operators is an odd permutation of the order of operators on the left-hand side.*

A simple case: We first prove a simple special case where we can see everything that happens. The trick to prove the theorem ([10]) is to transform the operators to the basis where H_0 is diagonal, to evaluate the expectation values, then to transform back to the original basis. Let Greek letters stand for the basis where H_0 is diagonal. Using the formula for basis changes, we have, (with an implicit sum over Greek indices)

$$\left\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l)\right\rangle_0 = \tag{33.14}$$

$$\langle i|\,\alpha\rangle \langle j|\,\beta\rangle \left\langle a_\alpha(\tau_i) a_\beta(\tau_j) a_\gamma^\dagger(\tau_k) a_\delta^\dagger(\tau_l)\right\rangle_0 \langle\gamma|\,k\rangle \langle\delta|\,l\rangle \tag{33.15}$$

We already know from Eq.(29.59) that

$$a_\alpha(\tau_i) = e^{-\zeta_\alpha \tau_i} a_\alpha \quad ; \quad a_\alpha^\dagger(\tau_i) = a_\alpha^\dagger e^{\zeta_\alpha \tau_i} \tag{33.16}$$

so that

$$\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0 \tag{33.17}$$

$$= \langle i|\ \alpha\rangle\, e^{-\zeta_\alpha \tau_i}\, \langle j|\ \beta\rangle\, e^{-\zeta_\beta \tau_j} \left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 e^{\zeta_\gamma \tau_k}\, \langle \gamma|\ k\rangle\, e^{\zeta_\delta \tau_l}\, \langle \delta|\ l\rangle \tag{33.18}$$

What we need to evaluate then are expectation values of the type

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 . \tag{33.19}$$

Evaluating the trace in the diagonal basis, we see that we will obtain a non-zero value only if indices of creation and annihilation operators match two by two or are all equal. Suppose $\beta = \gamma$, $\alpha = \delta$ and $\alpha \neq \beta$. Then, as in the lemma

$$\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger \right\rangle_0 = \left\langle a_\alpha a_\alpha^\dagger \right\rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0 \tag{33.20}$$

If instead, $\beta = \delta$, $\alpha = \gamma$ and $\alpha \neq \beta$, then

$$\left\langle a_\alpha a_\beta a_\alpha^\dagger a_\beta^\dagger \right\rangle_0 = -\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger \right\rangle_0 = -\left\langle a_\alpha a_\alpha^\dagger \right\rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0 . \tag{33.21}$$

The last case to consider is $\alpha = \beta$, $\beta = \delta$, $\alpha = \gamma$

$$\left\langle a_\alpha a_\alpha a_\alpha^\dagger a_\alpha^\dagger \right\rangle_0 = 0. \tag{33.22}$$

All these results, Eqs.(33.20)(33.21) and the last equation can be combined into one formula

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 = \left\langle a_\alpha a_\alpha^\dagger \right\rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0 (\delta_{\alpha,\delta}\delta_{\beta,\gamma} - \delta_{\alpha,\gamma}\delta_{\beta,\delta}) \tag{33.23}$$

$$= \left\langle a_\alpha a_\delta^\dagger \right\rangle_0 \left\langle a_\beta a_\gamma^\dagger \right\rangle_0 - \left\langle a_\alpha a_\gamma^\dagger \right\rangle_0 \left\langle a_\beta a_\delta^\dagger \right\rangle_0 \tag{33.24}$$

which is easiest to remember as follows,

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle = \left\langle \overset{\downarrow}{a_\alpha} a_\beta \overset{\downarrow}{a_\gamma^\dagger} a_\delta^\dagger \right\rangle + \left\langle \overset{\downarrow}{a_\alpha} a_\beta \overset{\downarrow}{a_\gamma^\dagger} a_\delta^\dagger \right\rangle \tag{33.25}$$

in other words, all possible pairs of creation and annihilation operators must be paired ("contracted") in all possible ways. There is a minus sign if an odd number of operator exchanges (transpositions) is necessary to bring the contracted operators next to each other on the right-hand side (In practice, just count one minus sign every time two operators are permuted). Substituting Eq.(33.24) back into the expression for the original average expressed in the diagonal basis Eq.(33.18) we have

$$\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0 \tag{33.26}$$

$$= \left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_j(\tau_j)\, a_k^\dagger(\tau_k) \right\rangle_0 - \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0$$

By induction (not done here) one can show that this result generalizes to the expectation value of an arbitrary number of creation-annihilation operators.

Definition 23 *Contraction: In the context of Wick's theorem, we call each factor* $\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0$ *on the right-hand side, a "contraction".*

Since Wick's theorem is valid for an arbitrary time ordering, it is also valid for time-ordered products so that, for example

$$\boxed{\left\langle T_\tau \left[a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 =} \tag{33.27}$$

$$\boxed{\left\langle T_\tau \left[a_i(\tau_i)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 - \left\langle T_\tau \left[a_i(\tau_i)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j)\, a_l^\dagger(\tau_l) \right] \right\rangle_0}. \tag{33.28}$$

The only simplification that occurs with time-ordered products is the following. Note that, given the definition of time-ordered product, we have

$$\left\langle T_\tau \left[a_i(\tau_i)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 = -\left\langle T_\tau \left[a_k^\dagger(\tau_k)\, a_i(\tau_i) \right] \right\rangle_0 \tag{33.29}$$

Indeed, the left-hand side and right-hand side of the above equation are, respectively

$$\left\langle T_\tau \left[a_i(\tau_i)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 = \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \theta(\tau_i - \tau_k) \tag{33.30}$$

$$- \left\langle a_k^\dagger(\tau_k)\, a_i(\tau_i) \right\rangle_0 \theta(\tau_k - \tau_i) \tag{33.31}$$

$$-\left\langle T_\tau \left[a_k^\dagger(\tau_k)\, a_i(\tau_i) \right] \right\rangle_0 = -\left\langle a_k^\dagger(\tau_k)\, a_i(\tau_i) \right\rangle_0 \theta(\tau_k - \tau_i) \tag{33.32}$$

$$+ \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \theta(\tau_i - \tau_k) \tag{33.33}$$

In other words, operators can be permuted at will inside a time-ordered product, in particular inside a contraction, as long as we take care of the minus-signs associated with permutations. This is true for time-ordered products of an arbitrary number of operators and for an arbitrary density matrix. The overall minus sign that comes in the permutations on the left hand side of Eq.(33.28) is the same as that which comes from the corresponding permutations on the right-hand side.

On the other hand, if we apply Wick's theorem to a product that is not time ordered, then we have to remember that

$$\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \neq -\left\langle a_k^\dagger(\tau_k)\, a_i(\tau_i) \right\rangle_0 \tag{33.34}$$

as we can easily verify by looking at the special case $\tau_k = \tau_i$ or by going to a diagonal basis. We can anticommute operators at will to do the "contractions" but they cannot be permuted *inside* a contraction $\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0$.

In practice, we will apply Wick's theorem to time-ordered products. In numerical calculations it is sometimes necessary to apply it to objects that are not time-ordered.

Example 24 *To make the example of Wick's theorem Eq.(33.28) more plausible, we give a few examples, Suppose first that the time order to the left of Eq.(33.28) is such that the destruction operators are inverted. Then,*

$$\left\langle T_\tau \left[a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 = -\left\langle a_j(\tau_j)\, a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0 \tag{33.35}$$

which means that since i and j have exchanged roles, in doing the contractions as above there is one more permutation to do, which gets rid of the extra minus sign and reproduces the right-hand side of Eq.(33.28). More explicitly, to do the contractions as above, we have to change i for j on both the right- and the left-hand side of Eq.(33.26). Doing this and substituting above, we obtain

$$\left\langle a_j(\tau_j)\, a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0 = \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 - \left\langle a_j(\tau_j)\, a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \right. \tag{33.36}$$

which we substitute in the previous equation to obtain exactly what the right-hand side of Eq.(33.28) would have predicted. To take another example, suppose that the time orders are such that

$$\left\langle T_\tau \left[a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 = -\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0 . \tag{33.37}$$

Then, to do the contractions we proceed as above, being careful not to permute creation and annihilation operators within an expectation value

$$\begin{aligned} & -\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0 \\ = & -\left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_k^\dagger(\tau_k)\, a_j(\tau_j) \right\rangle_0 - \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0 \end{aligned} \tag{33.38}$$

The right-hand side of Eq.(33.28) gives us

$$\begin{aligned} & \left\langle T_\tau \left[a_i(\tau_i)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 - \left\langle T_\tau \left[a_i(\tau_i)\, a_k^\dagger(\tau_k) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j)\, a_l^\dagger(\tau_l) \right] \right\rangle_0 \\ = & -\left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_k^\dagger(\tau_k)\, a_j(\tau_j) \right\rangle_0 - \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l) \right\rangle_0 \end{aligned} \tag{33.39, 33.40}$$

with the minus sign in the first term because we had to exchange the order in one of the time-ordered products.

General proof: For the general proof, we follow Fetter and Walecka [73]. As in Eq.(33.28) above, it suffices to prove the theorem for a given time order. And as in Eq.(33.18), it suffices to go to the diagonal basis. In the diagonal basis then, we need to evaluate

$$\mathrm{Tr}\left[\rho_G A_\alpha A_\beta A_\gamma \cdots A_\nu \right] \tag{33.41}$$

where $\rho_G = e^{-\beta H_0}/Z$ is the density matrix and where, for now, A_α can be either creation or annihilation operators. The proof for fermions is easily generalized to bosons. Anticommuting the first operator all the way to the right-hand sied, you find

$$\begin{aligned} \mathrm{Tr}\left[\rho_G A_\alpha A_\beta A_\gamma \cdots A_\nu \right] = & \mathrm{Tr}\left[\rho_G \{A_\alpha, A_\beta\} A_\gamma \cdots A_\nu \right] - \mathrm{Tr}\left[\rho_G A_\beta \{A_\alpha, A_\gamma\} \cdots A_\nu \right] \\ & + \cdots + \mathrm{Tr}\left[\rho_G A_\beta A_\gamma \cdots \{A_\alpha, A_\nu\} \right] - \mathrm{Tr}\left[\rho_G A_\beta A_\gamma \cdots A_\nu A_\alpha \right] \end{aligned} \tag{33.42}$$

The sign in the last two terms follows from the fact that the number of A operators has to be even, otherwise the expectation value vanishes. Following the steps in Eq.(29.59) we have that

$$e^{\beta H_0} A_\alpha e^{-\beta H_0} = A_\alpha e^{\lambda_\alpha \zeta_\alpha} \tag{33.43}$$

where $\lambda_\alpha = -1$ if A_α is a destruction operator, and $\lambda_\alpha = +1$ if it is a creation operator. The above equation is then equivalent to

$$A_\alpha \rho_G = \rho_G A_\alpha e^{\lambda_\alpha \beta \zeta_\alpha} . \tag{33.44}$$

Using the cyclic property of the trace,

$$\begin{aligned} \mathrm{Tr}\left[\rho_G A_\beta A_\gamma \cdots A_\nu A_\alpha \right] = & \mathrm{Tr}\left[A_\alpha \rho_G A_\beta A_\gamma \cdots A_\nu \right] \\ = & e^{\lambda_\alpha \beta \zeta_\alpha} \mathrm{Tr}\left[\rho_G A_\alpha A_\beta A_\gamma \cdots A_\nu \right] \end{aligned} \tag{33.45}$$

so that the last trace on the right-hand side of Eq.(33.42) can be combined with the left-hand side to yield

$$\begin{aligned} \mathrm{Tr}\left[\rho_G A_\alpha A_\beta A_\gamma \cdots A_\nu \right] = & \frac{\{A_\alpha, A_\beta\}}{1 + e^{\lambda_\alpha \beta \zeta_\alpha}} \mathrm{Tr}\left[\rho_G A_\gamma \cdots A_\nu \right] - \frac{\{A_\alpha, A_\gamma\}}{1 + e^{\lambda_\alpha \beta \zeta_\alpha}} \mathrm{Tr}\left[\rho_G A_\beta \cdots A_\nu \right] \\ & + \cdots + \frac{\{A_\alpha, A_\nu\}}{1 + e^{\lambda_\alpha \beta \zeta_\alpha}} \mathrm{Tr}\left[\rho_G A_\beta A_\gamma \cdots \right] . \end{aligned} \tag{33.46}$$

Then it becomes convenient to define a contraction by

$$A_{\alpha}^{\cdot}A_{\beta}^{\cdot} = \frac{\{A_\alpha, A_\beta\}}{1+e^{\lambda_\alpha \beta \zeta_\alpha}}. \tag{33.47}$$

The only non-vanishing contributions are of the form

$$a_{\alpha}^{\dagger\cdot}a_{\alpha}^{\cdot} = \frac{\left\{a_\alpha^\dagger, a_\alpha\right\}}{1+e^{\beta\zeta_\alpha}} = \frac{1}{e^{\beta\zeta_\alpha}+1} = \left\langle a_\alpha^\dagger a_\alpha \right\rangle \tag{33.48}$$

$$a_{\alpha}^{\cdot}a_{\alpha}^{\dagger\cdot} = \frac{\left\{a_\alpha, a_\alpha^\dagger,\right\}}{1+e^{-\beta\zeta_\alpha}} = \left(1-\frac{1}{e^{\beta\zeta_\alpha}+1}\right) = \left\langle a_\alpha a_\alpha^\dagger \right\rangle \tag{33.49}$$

so that quite generally

$$A_{\alpha}^{\cdot}A_{\beta}^{\cdot} = \langle A_\alpha A_\beta \rangle \tag{33.50}$$

and

$$\begin{aligned}\mathrm{Tr}\left[\rho_G A_\alpha A_\beta A_\gamma \cdots A_\nu\right] &= \langle A_\alpha A_\beta\rangle \,\mathrm{Tr}\left[\rho_G A_\gamma \cdots A_\nu\right] - \langle A_\alpha A_\gamma\rangle \,\mathrm{Tr}\left[\rho_G A_\beta \cdots A_\nu\right] \\ &\quad + \cdots + \langle A_\alpha A_\nu\rangle \,\mathrm{Tr}\left[\rho_G A_\beta A_\gamma \cdots\right].\end{aligned} \tag{33.51}$$

Continuing this process, the expectation value is equal to the set of all complete contractions of operators with signs determined from the signature of the permutations. For a time ordered product, as in Eq.(33.28), it suffices to include the time-ordering operator on the left-hand side and in everyone of the contractions. The overall number of plus and minus signs will be the same on the left and on the right of the equation. The return to the original basis is easily performed as in Eqs.(33.18) and (33.26).

Recalling the definition of the Green function and of the determinant, Wick's theorem can also be written in the following form

$$\begin{aligned}&\left\langle T_\tau \psi\left(\tau_1\right)\psi\left(\tau_2\right)\cdots\psi\left(\tau_n\right)\psi^\dagger\left(\tau_n'\right)\cdots\psi^\dagger\left(\tau_2'\right)\psi^\dagger\left(\tau_1'\right)\right\rangle \\ &= (-1)^n \det\begin{bmatrix} \mathcal{G}\left(\tau_1,\tau_1'\right) & \mathcal{G}\left(\tau_1,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_1,\tau_n'\right) \\ \mathcal{G}\left(\tau_2,\tau_1'\right) & \mathcal{G}\left(\tau_2,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_2,\tau_n'\right) \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{G}\left(\tau_n,\tau_1'\right) & \mathcal{G}\left(\tau_n,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_n,\tau_n'\right) \end{bmatrix}.\end{aligned} \tag{33.52}$$

Spatial indices and spin labels can easily be added. The antisymmetry of the time-ordered product under interchange of creation operators translates into the antisymmetry of the determinant under the interchange of columns. And similarly, the antisymmetry under interchange of destruction operators translates into antisymmetry under interchange of lines.

Remark 240 *Wick's theorem can also be proven [132] using the functional methods that we develop in the next part of these notes.*

33.2 Linked cluster theorems

Suppose we want to evaluate the Green's function by expanding the time-ordered product in the evolution operator Eq.(33.3). The expansion has to be done both in the numerator and in the denominator of the general expression for the average Eq.(33.1). This is a very general problem that forces us to introduce the notion

of connected graphs. A generalization of this problem also occurs if we want to compute the free-energy from

$$\ln Z = \ln\left(\mathrm{Tr}\left[e^{-\beta H_0} U_I(\beta,0)\right]\right) = \ln\left(Z_0 \left\langle U_I(\beta,0)\right\rangle_0\right) \tag{33.53}$$

$$= \ln\left(\left\langle T_\tau\left[\exp\left(-\int_0^\beta d\tau_1 V_I(\tau_1)\right)\right]\right\rangle_0\right) + \ln Z_0 \tag{33.54}$$

In probability theory this is like computing the cumulant expansion of the characteristic function. Welcome to linked cluster theorems.

These problems are special cases of much more general problems in the theory of random variables which do not even refer to specific Feynman diagrams or to quantum mechanics. The theorems, and their corollary that we prove below, are amongst the most important theorems used in many-body Physics or Statistical Mechanics in general. Linked cluster theorems lead to observables that are expressed in terms of connected diagrams.

Remark 241 *The value of connected diagrams scales like the volume of the system. If observables were to contain contributions from disconnected diagrams, we would obtain non-extensive quantities, that is results that scale like higher powers of the volume, which clearly does not make sense.*

33.2.1 Linked cluster theorem for normalized averages

Consider the calculation of

$$\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} \tag{33.55}$$

where the expectation $\langle\rangle$ is computed over a multivariate probability distribution function for the variables collectively represented by $\mathbf{x}$. The function $f(\mathbf{x})$ is arbitrary, as is the function $A(\mathbf{x})$. Expanding the exponential, we may write

$$\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} = \frac{\sum_{n=0}^\infty \frac{1}{n!}\left\langle (-f(\mathbf{x}))^n A(\mathbf{x})\right\rangle}{\sum_{n=0}^\infty \frac{1}{n!}\left\langle (-f(\mathbf{x}))^n\right\rangle} \tag{33.56}$$

When computing a term of a given order n, such as $\frac{1}{n!}\left\langle (-f(\mathbf{x}))^n A(\mathbf{x})\right\rangle$, we may always write

$$\frac{1}{n!}\left\langle (-f(\mathbf{x}))^n A(\mathbf{x})\right\rangle = \sum_{\ell=0}^\infty \sum_{m=0}^\infty \delta_{n,m+\ell} \frac{1}{n!}\frac{n!}{\ell! m!}\left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x})\right\rangle_c \left\langle (-f(\mathbf{x}))^m\right\rangle \tag{33.57}$$

where the subscript c on the average means that none of the terms in $\left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x})\right\rangle_c$ can be factored into lower order correlation functions, such as for example $\left\langle (-f(\mathbf{x}))^\ell\right\rangle \langle A(\mathbf{x})\rangle$ or $\left\langle (-f(\mathbf{x}))^{\ell-1}\right\rangle \langle (-f(\mathbf{x}))\, A(\mathbf{x})\rangle$ etc... The combinatorial factor corresponds to the number of ways the $(-f(\mathbf{x}))^n$ can be grouped into a group of ℓ terms and a group of $n-\ell$ terms, the $\delta_{n,m+\ell}$ Kronecker delta function ensuring that indeed $m = n - \ell$. Using the last equation in the previous one, the sum over n is now trivially performed with the help of $\delta_{n,m+\ell}$ and one is left with

$$\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} = \frac{\sum_{\ell=0}^\infty \sum_{m=0}^\infty \frac{1}{m!\ell!}\left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x})\right\rangle_c \left\langle (-f(\mathbf{x}))^m\right\rangle}{\sum_{n=0}^\infty \frac{1}{n!}\left\langle (-f(\mathbf{x}))^n\right\rangle} \tag{33.58}$$

The numerator can now be factored so as to cancel the denominator which proves the theorem

Theorem 25 *Linked cluster theorem for normalized averages:*

$$\boxed{\frac{\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle}=\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}A\left(\mathbf{x}\right)\right\rangle_{c}=\left\langle e^{-f(\mathbf{x})}A\left(\mathbf{x}\right)\right\rangle_{c}} \tag{33.59}$$

This result can be applied to our calculation of the Green's function since within the time-ordered product, the exponential may be expanded just as an ordinary exponential, and the quantity which plays the role of $(-f(\mathbf{x}))$, namely $\left(-\int_0^\beta d\tau V_I(\tau)\right)$ can be moved within the T_τ product without costing any additional minus sign.

33.2.2 Linked cluster theorem for characteristic functions or free energy

We now wish to show the following general theorem for a multivariate probability distribution.

Theorem 26 *Linked cluster theorem (cumulant expansion).*

$$\boxed{\ln\left\langle e^{-f(\mathbf{x})}\right\rangle=\sum_{n=1}^{\infty}\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}\right\rangle_{c}=\left\langle e^{-f(\mathbf{x})}\right\rangle_{c}-1} \tag{33.60}$$

The proof is inspired by Enz[11]. When $f(\mathbf{x})=i\mathbf{k}\cdot\mathbf{x}$, the quantity $\left\langle e^{-i\mathbf{k}\cdot\mathbf{x}}\right\rangle$ is called the characteristic function of the probability distribution. It is the generating function for the moments. The quantities on the right-hand side, which as above are connected averages, are usually called *cumulants* in ordinary probability theory and $\ln\left\langle e^{-i\mathbf{k}\cdot\mathbf{x}}\right\rangle$ is the generating function for the cumulant averages.

Proof: To prove the theorem, we introduce first an auxiliary variable λ

$$\frac{\partial}{\partial\lambda}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle=\left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle \tag{33.61}$$

We can apply to the right-hand side the theorem we just proved

$$\left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle=\left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle_{c}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle \tag{33.62}$$

so that

$$\frac{1}{\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle}\frac{\partial}{\partial\lambda}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle=\left\langle\frac{\partial}{\partial\lambda}e^{-\lambda f(\mathbf{x})}\right\rangle_{c}. \tag{33.63}$$

Integrating both sides from 0 to 1, we obtain

$$\ln\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle|_{0}^{1}=\left\langle e^{-f(\mathbf{x})}\right\rangle_{c}-1 \tag{33.64}$$

QED

Remark 242 *The above results tell us that derivatives of the logarithm of the partition function will in general yield cumulants. This is indeed what we found from* $\delta^2\ln Z\left[\phi\right]/\left(\delta\phi\left(2,1\right)\delta\phi\left(4,3\right)\right)=-\delta G\left(1,2\right)/\delta\phi\left(4,3\right)$ *since it corresponds to the average of a four-point function with the disconnected piece (product of Green functions) subtracted out.*

Example 27 *It is instructive to check the meaning of the above result explicitly to second order*

$$\ln\left\langle e^{-\lambda f(x)}\right\rangle \approx \ln\left\langle 1-\lambda f\left(x\right)+\frac{1}{2}\left(\lambda f\left(x\right)\right)^{2}\right\rangle \approx\left(-\left\langle \lambda f\left(x\right)\right\rangle +\frac{1}{2}\left\langle \left(\lambda f\left(x\right)\right)^{2}\right\rangle \right)-\frac{1}{2}\left\langle \lambda f\left(x\right)\right\rangle ^{2} \tag{33.65}$$

$$\left\langle e^{-\lambda f(x)}\right\rangle _{c}-1\approx-\left\langle \lambda f\left(x\right)\right\rangle _{c}+\frac{1}{2}\left\langle \left(\lambda f\left(x\right)\right)^{2}\right\rangle _{c} \tag{33.66}$$

so that equating powers of λ*, we find as expected,*

$$\left\langle \left(f\left(\mathbf{x}\right)\right)^{2}\right\rangle _{c}=\left\langle \left(f\left(\mathbf{x}\right)\right)^{2}\right\rangle -\left\langle f\left(\mathbf{x}\right)\right\rangle ^{2}. \tag{33.67}$$

The above results will help us in the calculation of the free energy since we find, as in the first equations of the section on linked cluster theorems,

$$F=-T\ln\left[Z_{0}\left\langle T_{\tau}\left[e^{-\int_{0}^{\beta}d\tau V_{I}(\tau)}\right]\right\rangle _{0}\right]=-T\sum_{n=1}^{\infty}\frac{1}{n!}\left\langle T_{\tau}\left[-\int_{0}^{\beta}d\tau V_{I}\left(\tau\right)\right]^{n}\right\rangle _{0c}-T\ln Z_{0} \tag{33.68}$$

$$\boxed{F=-T\ln Z=-T\left[\left\langle T_{\tau}\left[e^{-\int_{0}^{\beta}d\tau V_{I}(\tau)}\right]\right\rangle _{0c}-1\right]-T\ln Z_{0}.} \tag{33.69}$$

the subscript 0 stands for averages with the non-interacting density matrix. The above proof applies to our case because the time-ordered product of an exponential behaves exactly like an ordinary exponential when differentiated, as we know from the differential equation that leads to its definition.

33.3 Variational principle and application to Hartree-Fock theory

It is legitimate to ask if there is a one-body Hamiltonian, in other words an effective Hamiltonian with a time-independent potential, whose solution is as close as possible to the true solution. To address this question, we also need to define what we mean by "as close as possible". The answer to both of these queries is provided by the variational principle for thermodynamic systems. We discuss below how Hartree-Fock theory comes out naturally from the variational principle. Also, it is an unavoidable starting point when there is a broken symmetry, as we will discuss more fully in a later chapter.

33.3.1 Thermodynamic variational principle

A proof of the variational principle for both classical and quantum systems can be obtained by starting from the following inequality for the entropy[16]

$$\boxed{S=-\mathrm{Tr}\left[\varrho\ln\varrho\right]\leq-\mathrm{Tr}\left[\varrho\ln\varrho'\right].} \tag{33.70}$$

Proof Let $|m\rangle$ and $|m'\rangle$ be the basis that diagonalize respectively ϱ and ϱ'. Then by inserting the closure relation, and defining $p_m = \langle m|\,\varrho\,|m\rangle$ with the analogous definition for p'_m, we find

$$\begin{aligned}\mathrm{Tr}\left[-\varrho\ln\varrho+\varrho\ln\varrho'\right] &= -\sum_m p_m\ln p_m+\sum_{m,m'}p_m\langle m\,|m'\rangle\ln p'_{m'}\,\langle m'\,|m\rangle \\ &= \sum_{m,m'}\langle m\,|m'\rangle\,\langle m'\,|m\rangle\,p_m\ln\frac{p'_{m'}}{p_m}. \end{aligned} \tag{33.71}$$

In this sum, $\langle m\,|m'\rangle\,\langle m'\,|m\rangle\,p_m$ is positive or zero. We can now use $\ln y \leq y-1$. (This inequality follows from the fact that the first derivative of $\ln y - y$ vanishes at $y=1$ and that the second derivative, $-1/y^2$ is negative everywhere. Hence, $\ln y - y$ has a maximum at $y=1$ and the value there is -1.) Using this inequality above, we find

$$\mathrm{Tr}\left[-\varrho\ln\varrho+\varrho\ln\varrho'\right]\leq\sum_{m,m'}\langle m\,|m'\rangle\,\langle m'\,|m\rangle\,(p'_m-p_m)=\mathrm{Tr}\left[\varrho'\right]-\mathrm{Tr}\left[\varrho\right]=0. \tag{33.72}$$

The last equality follows from the fact that the trace of a density matrix is unity. The equality occurs only if $\langle m\,|m'\rangle = 0$ or if $p'_{m'}/p_m = 1$ for all possible choices of $|m\rangle$ and $|m'\rangle$.

To prove Feynman's variational principle Eq.(33.73) it suffices to take $\varrho' = e^{-\beta(H-\mu N)}/Z$ and $\varrho = \varrho_0$, a trial density matrix. Then, the inequality for the entropy, Eq.(33.70) becomes

$$\boxed{-T\ln Z\leq\mathrm{Tr}\left[\varrho_0\left(H-\mu N\right)\right]+T\mathrm{Tr}\left[\varrho_0\ln\varrho_0\right]} \tag{33.73}$$

which looks as if we had the function $(E-\mu N)-TS$ to minimize, quite a satisfactory state of affairs.

Another useful form is obtained by replacing ϱ_0 by $\varrho_0 = e^{-\beta\left(\widetilde{H}_0-\mu N\right)}/Z_0$ with $\widetilde{H}_0$ the trial Hamiltonian. Then the above equation reduces to

$$\boxed{-T\ln Z\leq -T\ln Z_{\widetilde{0}}+\left\langle H-\widetilde{H}_0\right\rangle_{\widetilde{0}}} \tag{33.74}$$

where $\langle O\rangle_{\widetilde{0}}$ refers to an average of the operator O with the density matrix $\varrho_0 = e^{-\beta\left(\widetilde{H}_0-\mu N\right)}/Z_{0.}$.

33.3.2 Thermodynamic variational principle for classical systems based on the linked-cluster theorem

One can base the thermodynamic variational principle for classical systems on the inequality

$$\boxed{e^x\geq 1+x} \tag{33.75}$$

which is valid for all x, whether $x>0$, or $x<0$. This inequality is a convexity inequality which appears obvious when the two functions are plotted. We give two proofs.

Proof 1: e^x is a convex function, *i.e.* $d^2e^x/d^2x \geq 0$ for all values of x. At $x=0$ the functions e^x and $1+x$ as well as their first derivatives are equal. Since a straight line tangent to a convex curve at a point cannot intersect it anywhere else, the theorem is proven. *QED*

Algebraically, the proof goes as follows.

Proof 2: The function $e^x - 1 - x$ has an absolute minimum at $e^x = 1$ since its first derivative vanishes there while its second derivative is everywhere positive. At its minimum $e^x - 1 - x = 0$. This proves the inequality. *QED*

Moving back to our initial purpose, let $\widetilde{H}_0$ be a trial Hamiltonian. Then take $e^{-\beta\left(\widetilde{H}_0 - \mu N\right)}/Z_0$ as the trial density matrix corresponding to averages $\langle\rangle_{\widetilde{0}}$. We will use the above inequality Eq.(33.75) to prove the variational principle Eq.(33.74)

$$\boxed{-T \ln Z \leq -T \ln Z_{\widetilde{0}} + \left\langle H - \widetilde{H}_0 \right\rangle_{\widetilde{0}}}. \tag{33.76}$$

This inequality is a variational principle because $\widetilde{H}_0$ is arbitrary, meaning that we are free to parametrize it and then to minimize with respect to the set of all parameters to find the best one-particle Hamiltonian in our Physically chosen space of Hamiltonians.

Proof Our general result for the free energy in terms of connected terms, Eq.(33.69), is obviously applicable to classical systems. The simplification that occurs there is that since all operators commute, we do not need to worry about the time-ordered product, thus with

$$\widetilde{V} = H - \widetilde{H}_0 \tag{33.77}$$

we have

$$F = -T \ln Z = -T \left[\left\langle e^{-\beta \widetilde{V}} \right\rangle_{\widetilde{0},c} - 1 \right] - T \ln Z_{\widetilde{0}}. \tag{33.78}$$

Using our basic inequality Eq.(33.75) for $e^{-\beta \widetilde{V}}$ we immediately obtain the desired result

$$F \leq -T \left\langle -\beta \widetilde{V} \right\rangle_{\widetilde{0},c} + F_{\widetilde{0}} \tag{33.79}$$

which is just another way of rewriting Eq.(33.74).

It is useful to note that in the language of density matrices, $\varrho_0 = e^{-\beta\left(\widetilde{H}_0 - \mu N\right)}/Z_0$ the variational principle Eq.(33.74) reads,

$$\boxed{-T \ln Z \leq \mathrm{Tr}\left[\varrho_0 \left(H - \mu N\right)\right] + T \mathrm{Tr}\left[\varrho_0 \ln \varrho_0\right]} \tag{33.80}$$

which looks as if we had the function $(E - \mu N) - TS$ to minimize, quite a satisfactory state of affairs.

33.3.3 Application of the variational principle to Hartree-Fock theory

Writing down the most general one-body Hamiltonian with *orthonormal* eigenfunctions left as variational parameters, the above variational principle leads to the usual Hartree-Fock eigenvalue equation. Such a general one-body Hamiltonian would look like

$$\widetilde{H}_0 = \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}^{*}\left(\mathbf{x}\right) \left(-\frac{\nabla^2}{2m} \right) \phi_{\alpha}\left(\mathbf{x}\right) c_{\alpha}^{+} c_{\alpha} \tag{33.81}$$

with $\phi_\alpha(\mathbf{x})$ as variational wave-functions. In the minimization problem, one must add Lagrange multipliers to enforce the constraint that the wave-functions are not only orthogonal but also normalized.

In a translationally invariant system, the one-body wave functions will be plane waves usually, so only the eigenenergies need to be found. This will be done in the following chapter.

It does happen however that symmetry is spontaneously broken. For example, in an anti-ferromagnet the periodicity is halved so that the Hartree-Fock equations will correspond to solving a 2×2 matrix, even when Fourier transforms are used. The matrix becomes larger and larger as we allow more and more general non-translationally invariant states. In the extreme case, the wave functions are different on every site! This is certainly the case in ordinary Chemistry with small molecules or atoms!

34. EXERCICES FOR PART IV

34.0.4 Bosonic Matsubara frequencies.

The Green's function for bosons is defined with a commutator instead of an anti-commutator. Correspondingly, there is no sign change associated with the time-ordering operator. This is like for the susceptibilities we defined in part II. Show that for bosons, the Green's function is periodic instead of antiperiodic. Consequently we have $q_n = 2n\pi T = \frac{2n\pi}{\beta}$ in that case.

34.0.5 First quantization from the second

The results are identical whether we assume that field operators obey bosonic or fermionic statistics. We will suppose that they obey bosonic statistics.

a) Using

$$\left[\psi(\mathbf{r},t), \psi^{\dagger}(\mathbf{r},t)\right] = \delta(\mathbf{r}-\mathbf{r}')$$

show that

$$\left[\int d^3\mathbf{r}'\ \psi^{\dagger}(\mathbf{r}',t)\ \psi(\mathbf{r}',t), \psi^{\dagger}(\mathbf{r},t)\right] = \psi^{\dagger}(\mathbf{r},t) \tag{34.1}$$

$$\left[\int d^3\mathbf{r}'\ \psi^{\dagger}(\mathbf{r}',t)\ \psi(\mathbf{r}',t), \psi(\mathbf{r},t)\right] = -\psi(\mathbf{r},t) \tag{34.2}$$

b) then defining the position operator X and its conjugate momentum P_x by

$$\int d^3\mathbf{r}\ \psi^*(\mathbf{r},t)\ \mathbf{r}_x\ \psi(\mathbf{r},t) = X(t) \tag{34.3}$$

$$\int d^3\mathbf{r}\ \psi^*(\mathbf{r},t)\ \frac{\hbar}{i}\nabla_x\ \psi(\mathbf{r},t) = P_x(t) \tag{34.4}$$

show that

$$[X(t), P_x(t)] = i\hbar \int d^3\mathbf{r}\ \psi^{\dagger}(\mathbf{r},t)\ \psi(\mathbf{r},t). \tag{34.5}$$

c) How can the theorem on commutators of ladder operators be used to show that $\int d^3\mathbf{r}\ \psi^{\dagger}(\mathbf{r},t)\ \psi(\mathbf{r},t)$ can take only integers as eigenvalues?

d) How does this recover first quantization?

34.0.6 Retrouver la première quantification à partir de la seconde

Le résultat est identique, peu importe qu'on suppose que les opérateurs de champ obéissent à des statistiques bosoniques ou des fermioniques. Nous allons supposer que les opérateurs de seconde quantification sont bosoniques.

a) Utilisant

$$\left[\psi\left(\mathbf{r},t\right),\psi^{\dagger}\left(\mathbf{r},t\right)\right]=\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

montrez que

$$\left[\int d^{3}\mathbf{r}'\ \psi^{\dagger}\left(\mathbf{r}',t\right)\ \psi\left(\mathbf{r}',t\right),\psi^{\dagger}\left(\mathbf{r},t\right)\right] = \psi^{\dagger}\left(\mathbf{r},t\right) \tag{34.6}$$

$$\left[\int d^{3}\mathbf{r}'\ \psi^{\dagger}\left(\mathbf{r}',t\right)\ \psi\left(\mathbf{r}',t\right),\psi\left(\mathbf{r},t\right)\right] = -\psi\left(\mathbf{r},t\right) \tag{34.7}$$

b) puis définissant l'opérateur position X et son moment conjugué P_x par

$$\int d^{3}\mathbf{r}\ \psi^{*}\left(\mathbf{r},t\right)\ \mathbf{r}_{x}\ \psi\left(\mathbf{r},t\right) = X\left(t\right) \tag{34.8}$$

$$\int d^{3}\mathbf{r}\ \psi^{*}\left(\mathbf{r},t\right)\ \frac{\hbar}{i}\nabla_{x}\ \psi\left(\mathbf{r},t\right) = P_{x}\left(t\right) \tag{34.9}$$

montrez qu'on retrouve le résultat suivant.

$$\left[X\left(t\right),P_{x}\left(t\right)\right]=i\hbar\int d^{3}\mathbf{r}\ \psi^{\dagger}\left(\mathbf{r},t\right)\ \psi\left(\mathbf{r},t\right). \tag{34.10}$$

b) Comment le théorème sur les commutateurs d'opérateurs d'échelle peut-il être utilisé pour arguer que $\int d^{3}\mathbf{r}\ \psi^{\dagger}\left(\mathbf{r},t\right)\ \psi\left(\mathbf{r},t\right)$ ne peut prendre que des valeurs entières comme valeur propre.
c) Comment ce qui précède permet-il de retrouver le résultat de la première quantification.

34.0.7 Non interacting Green's function from the spectral weight and analytical continuation

Find $\mathcal{G}_{0}\left(\mathbf{k};ik_{n}\right)$ starting from the spectral weight for non-interacting particles and analytical continuation.

34.0.8 Sum over bosonic Matsubara frequencies

Derive the analog of the above results for the bosonic case.

34.0.9 Représentation de Lehman et prolongement analytique

Soit la définition habituelle à l'aide d'un commutateur pour la susceptibilité de charge retardée

$$\chi_{\rho\rho}^{R}\left(\mathbf{q};t-t'\right)=i\theta\left(t-t'\right)\left\langle\left[\rho\left(\mathbf{q},t\right),\rho\left(-\mathbf{q},t'\right)\right]\right\rangle \tag{34.11}$$

Soit aussi la susceptibilité de charge correspondante de Matsubara

$$\chi_{\rho\rho}\left(\mathbf{q};\tau-\tau'\right) = \left\langle T_{\tau}\rho\left(\mathbf{q},\tau\right)\rho\left(-\mathbf{q},0\right)\right\rangle \tag{34.12}$$

$$= \theta\left(\tau\right)\left\langle\rho\left(\mathbf{q},\tau\right)\rho\left(-\mathbf{q},0\right)\right\rangle+\theta\left(-\tau\right)\left\langle\rho\left(-\mathbf{q},0\right)\rho\left(\mathbf{q},\tau\right)\right\rangle \tag{34.13}$$

Les moyennes sont prises dans l'ensemble grand-canonique.

a) Trouvez les conditions de périodicité en temps imaginaire pour la fonction de Matsubara et déduisez-en un développement en fréquences discrètes.

b) Trouvez la représentation de Lehman pour chacune de ces deux fonctions de réponse et déduisez-en la règle permettant de faire le prolongement analytique d'une fonction à l'autre.

c) Vérifiez à partir de la représentation de Lehman que le poids spectral satisfait à la condition $\omega\chi''_{\rho\rho}(\mathbf{q},\omega) > 0$.

d) Pourquoi n'a-t-on pas besoin d'un facteur de convergence pour calculer $\sum_{n=-\infty}^{\infty} \chi_{\rho\rho}(\mathbf{q};iq_n)$.

34.0.10 Représentation de Lehman et prolongement analytique pour les fermions

Obtenez la représentation de Lehman pour la fonction de Green de Matsubara $\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)$ puis celle pour la fonction de Green retardée $G^R(\mathbf{r},\mathbf{r}';\omega)$ et utilisez ces résultats pour montrer que $G^R(\mathbf{r},\mathbf{r}';\omega)$ s'obtient de $\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)$ simplement en remplaçant ik_n par $\omega + i\eta$ dans la fonction de Green de Matsubara.

34.0.11 Fonction de Green pour les phonons

Soient $a_{\lambda k}$ et $a^+_{\lambda k}$ les opérateurs de destruction et de création pour des phonons (statistiques de Bose) de polarisation λ et de nombre d'onde k. L'amplitude quantifiée correspondante est

$$Q_{\lambda,k} = \frac{1}{\sqrt{2\omega_{\lambda k}}}\left(a_{\lambda,k} + a^+_{\lambda,-k}\right)$$

($\hbar = 1$). Definissons le propagateur de phonon de Matsubara par:

$$D_{\lambda\lambda'}(k,k';\tau-\tau') = -2\sqrt{\omega_{\lambda k}\omega_{\lambda' k'}} < T_\tau\left[Q_{\lambda,k}(\tau)\, Q_{\lambda',-k'}(\tau')\right] > .$$

Notez que pour les quantités bosoniques il n'y a pas de changement de signe lorsqu'on réordonne les opérateurs avec le produit chronologique.

a)

-Prouvez que $D_{\lambda\lambda'}(k,k';\tau-\tau')$ ne dépend que de $\tau-\tau'$.

- Dérivez la condition de périodicité en temps imaginaire.

- Donnez le développement de $D_{\lambda\lambda'}(k,k';\tau-\tau')$ en fréquences discrètes.

b) Soit

$$H = \sum_{k,\lambda} \omega_{\lambda k}[a^+_{\lambda,k}a_{\lambda,k} + \frac{1}{2}]$$

- Calculez le $D_\lambda(k,iq_n) \equiv D_{\lambda\lambda}(k,k;iq_n)$ correspondant.

- Trouvez le poids spectral.

- Montrez que le poids spectral s'annule à fréquence nulle. (Ceci est le cas général pour les bosons. Ceci permet de faire le prolongement analytique de la représentation spectrale sans rencontrer de problèmes avec la fréquence de Matsubara nulle.)

- Faites le prolongement analytique pour obtenir la fonction de Green retardée correspondante.

- Utilisez un contour dans le plan complexe et la formule de Cauchy pour évaluer

$$T\sum_{n=-\infty}^{\infty} D_{\lambda\lambda}\left(k,k;iq_n\right)e^{-iq_n0^{\pm}} \tag{34.14}$$

Pourquoi le résultat ne dépend-t-il pas du facteur de convergence choisi, $e^{iq_n0^+}$ ou $e^{iq_n0^-}$?

34.0.12 Oscillateur harmonique en contact avec un réservoir

Un oscillateur harmonique de fréquence Ω interagissant avec un réservoir d'oscillateurs de fréquences ω_i est décrit par l'hamiltonien

$$H=\Omega a^+a+\sum_i \omega_i b_i^+b_i+\sum_i g_i\left(a^+b_i+ab_i^+\right)$$

Définissons les propagateurs de Matsubara suivants:

$$D\left(\tau\right)=-<T_\tau[a\left(\tau\right)a^+(0)]>$$

$$F_i\left(\tau\right)=-<T_\tau[b_i\left(\tau\right)a^+(0)]>$$

a) Ecrivez les equations du mouvement pour ces propagateurs.

b) Prenez la transformée de Fourier pour obtenir les équations du mouvement pour $D\left(iq_n\right)$ et $F_i\left(iq_n\right)$ et résolvez ces équations.

c) Faites le prolongement analytique pour obtenir les propagateurs retardés.

d) Décrivez la structure analytique de $D^R\left(\omega\right)$ dans le plan complexe, en montrant où sont les pôles et autres singularités. Vous pouvez aussi supposer que i peut prendre les valeurs de 1 à N et montrer que $D^R\left(\omega\right)$ s'écrit comme le rapport de deux polynômes, un de degré N au numérateur et un de degré $N+1$ au dénominateur.

e) Tracez un shéma permettant d'obtenir graphiquement la position des nouveaux pôles de $D^R\left(\omega\right)$ en présence du réservoir (concentrez-vous sur le dénominateur de $D^R\left(\omega\right)$). Pour simplifier la discussion, supposez qu'il n'y a que deux oscillateurs dans le réservoir et trouvez ce qui arrive si Ω est plus petit, plus grand, ou entre les deux fréquences des oscillateurs du réservoir.

34.0.13 Limite du continuum pour le réservoir, et irréversibilité

Continuons le problème précédent. Supposons que le nombre d'oscillateurs du réservoir augmente sans limite de telle sorte que la fonction

$$\Gamma\left(\omega\right)\equiv\sum_i g_i^2\delta\left(\omega-\omega_i\right)$$

devienne continue

a) Montrez que si Γ et ses dérivées sont petites, la partie imaginaire du pôle de $D^R\left(\omega\right)$ est à $-i\pi\Gamma\left(\Omega\right)$. Donnez une expression intégrale pour le déplacement de la fréquence (encore une fois à l'ordre dominant en Γ).

b) Montrez que $D^R(t)$ décroît exponentiellement dans le temps. La fréquence d'oscillation est-elle déplacée? Dans cette limite nous avons un oscillateur quantique amorti! Pourquoi ce résultat est-il si différent de celui du problème précédent? Que se passe-t-il si le nombre d'oscillateurs est grand mais pas infini? Discutez la façon dont l'irréversibilité est apparue dans le problème, en particulier notez que la limite du volume infini (nombre d'oscillateurs infini) est prise avant $\eta \to 0$.

c) Si $\Gamma(\omega)$ est donné par

$$\Gamma(\omega) = \frac{\epsilon}{1 + \omega^2 \tau^2}$$

trouvez, à l'ordre dominant en ϵ, la fréquence renormalisée et l'amortissement.

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Part V

The Coulomb gas

The electron gas with long-range forces and a neutralizing background, also known as the jellium model, is probably the first challenge that was met by quantum many-body theory in the context of Solid State physics. It is extremely important conceptually since it is crucial to understand how, in a solid, the long-range Coulomb force becomes effectively short-range, or screened, at low energy. Other models, such as the Hubbard model that we will discussed later on, have their foundation rooted in the physics of screening. In fact, one of the most useful methods in modern electronic structure calculations uses perturbation theory to compute single-particle excitations, and the method they rely on, called the GW approach, is just an adaptation of what was developed for the Coulomb gas.

In this part, we assume that the uniform neutralizing background has infinite inertia. In a subsequent part of this book we will allow it to move, in other words to support sound waves, or phonons. We will consider electron-phonon interactions and see how these eventually lead to superconductivity.

The main physical phenomena to account for here in the immobile background, are screening and plasma oscillations, at least as far as collective modes are concerned. The surprises come in when one tries to understand single-particle properties. Hartree-Fock theory is a disaster since it predicts that the effective mass of the electron at the Fermi level vanishes. The way out of this paradox will indicate to us how important it is to take screening into account.

We will start by describing the source formalism due to the Schwinger-Martin school[1, 2] and then start to do calculations. The advantage of this approach is that it allows more easily to devise non-perturbative approximations and to derive general theorems. It gives a systematic algebraic way to formulate perturbation theory when necessary, without explicit use of Wick's theorem. With this formalism, so-called conserving approximations can also be formulated naturally. The source, or functional derivative formalism, is however less appealing than Feynman rules for the Feynmann diagram approach to perturbation theory. When these two competing approaches were invented, it was forbidden to the practitioners of the source approach to draw Feynamnn diagrams, but nothing really forbids it. The students, anyway, drew the forbidden pictures hiding in the basement. The two formalisms are strictly equivalent.

After we introduce the formalism, we discuss first the density oscillations, where we will encounter screening and plasma oscillations. This will allow us to discuss the famous Random Phase Approximation (RPA). Then we move on to single particle properties and end with a general discussion of what would be needed to go beyond RPA. The electron gas is discussed in detail in a very large number of textbooks. The discussion here is brief and incomplete, its main purpose being to illustrate the physics involved.

35. THE FUNCTIONAL DERIVATIVE APPROACH

We basically want to compute correlation functions. In the first section below, we show, in the very simple context of classical statistical mechanics, how introducing artificial external fields (source fields) allows one to compute correlation functions of arbitrary order for the problem without external fields. This is one more example where enlarging the space of parameters of interest actually simplifies matters in the end. In the other section, we show how to obtain Green's functions with source fields and then give an impressionist's view of how we plan to use this idea for our problem.

35.1 External fields to compute correlation functions

In elementary statistical mechanics, we can obtain the magnetization by differentiating the free energy with respect to the magnetic field. To be more specific, let

$$Z_h = \mathrm{Tr}\left[e^{-\beta(K-hM)}\right] \tag{35.1}$$

then

$$\frac{\partial \ln Z_h}{\beta \partial h} = \frac{1}{Z_h}\mathrm{Tr}\left[e^{-\beta(K-hM)}M\right] = \langle M\rangle_h . \tag{35.2}$$

The indice h on $\langle M\rangle_h$ and Z_h reminds us that the magnetic field is non zero. We can obtain correlation fucntions of higher order by continuing the process

$$\begin{aligned}\frac{\partial^2 \ln Z_h}{\beta^2 \partial h^2} &= \langle MM\rangle_h - \mathrm{Tr}\left[e^{-\beta(K-hM)}M\right]\frac{1}{Z_h^2}\frac{\partial \mathrm{Tr}\left[e^{-\beta(K-hM)}\right]}{\beta\partial h} &(35.3)\\ &= \langle MM\rangle_h - \langle M\rangle_h \langle M\rangle_h . &(35.4)\end{aligned}$$

The second term clearly comes from the fact that Z_h in the denominator of the equation for $\langle M\rangle_h$ depends on h. One can clearly continue this process to find higher and higher order correlation functions. At the end, we can set $h = 0$. Clearly then, if one can compute $\langle M\rangle_h$ or Z_h, one can obtain higher order correlation functions just by differentiating.

Suppose now that we want for example $\langle M(\mathbf{x}_1) M(\mathbf{x}_2)\rangle - \langle M(\mathbf{x}_1)\rangle \langle M(\mathbf{x}_2)\rangle$ .That can still be achieved if we impose a position dependent-external field:

$$Z[h] = \mathrm{Tr}\left[e^{-\beta\left(K-\int d^3\mathbf{x} h(\mathbf{x})M(\mathbf{x})\right)}\right]. \tag{35.5}$$

It is as if at each position $\mathbf{x}$, there were an independent variable $h(\mathbf{x})$. The position is now just a label. The notation $Z[h]$ means that Z is a functional of $h(\mathbf{x})$.

Definition 28 *A functional takes a function and maps it into a scalar.*

To obtain the magnetization at a single point, we introduce the notion of functional derivative, which is just a simple generalization to the continuum of the idea of partial derivative. To be more specific,

$$\frac{\delta}{\delta h\left(\mathbf{x}_1\right)}\int d^3\mathbf{x}h\left(\mathbf{x}\right)M\left(\mathbf{x}\right) = \int d^3\mathbf{x}\frac{\delta h\left(\mathbf{x}\right)}{\delta h\left(\mathbf{x}_1\right)}M\left(\mathbf{x}\right) \tag{35.6}$$

$$= \int d^3\mathbf{x}\delta\left(\mathbf{x}_1-\mathbf{x}\right)M\left(\mathbf{x}\right)=M\left(\mathbf{x}_1\right). \tag{35.7}$$

In other words, the partial derivative for two independent variables y_1 and y_2

$$\frac{\partial y_1}{\partial y_2}=\delta_{1,2} \tag{35.8}$$

where $\delta_{1,2}$ is the Kroenecker delta, is replaced by

$$\frac{\delta h\left(\mathbf{x}\right)}{\delta h\left(\mathbf{x}_1\right)}=\delta\left(\mathbf{x}_1-\mathbf{x}\right). \tag{35.9}$$

Very simple.

Armed with this notion of functional derivative, one finds that

$$\frac{\delta \ln Z\left[h\right]}{\beta\delta h\left(\mathbf{x}_1\right)}=\left\langle M\left(\mathbf{x}_1\right)\right\rangle_h \tag{35.10}$$

and the quantity we want is obtained from one more functional derivative

$$\frac{\delta^2 \ln Z\left[h\right]}{\beta^2\delta h\left(\mathbf{x}_1\right)\delta h\left(\mathbf{x}_2\right)}=\left\langle M\left(\mathbf{x}_1\right)M\left(\mathbf{x}_2\right)\right\rangle_h-\left\langle M\left(\mathbf{x}_1\right)\right\rangle_h\left\langle M\left(\mathbf{x}_2\right)\right\rangle_h. \tag{35.11}$$

The $[h]$ near Z reminds us that Z is a functional of the function $h\left(\mathbf{x}\right)$, i.e. it maps this function to a scalar, namely Z.

Definition 29 *Connected response functions: Correlation functions such as the one above are called connected. This means that the "trivial" part, which would be the result if there were no correlations, is subtracted. In probability theory, these are cumulants.*

Remark 243 *The approach outlined above is in a sense an application of the fluctuation-dissipation theorem since the fluctuations are obtained from the response to a source field, here h.*

35.2 Green's functions and higher order correlations from functional derivatives

In our case, we are interested in correlation functions that depend not only on space but also on real or imaginary time. In addition, we know that time-ordered products are relevant. Hence, you will not be surprized to learn that we use as our partition function with source fields $\phi\left(1,2\right)$:

$$Z\left[\phi\right]=\mathrm{Tr}\left[e^{-\beta K}T_\tau\exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\right] \tag{35.12}$$

where we used the short-hand

$$(1) = (\mathbf{x}_1, \tau_1; \sigma_1) \tag{35.13}$$

with the overbar indicating integrals over space-time coordinates and spin sums. More specifically,

$$\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right) =$$

$$\sum_{\sigma_1,\sigma_2}\int d^3\mathbf{x}_1\int_0^\beta d\tau_1\int d^3\mathbf{x}_2\int_0^\beta d\tau_2\psi^\dagger_{\sigma_1}\left(\mathbf{x}_1,\tau_1\right)\phi_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1,\mathbf{x}_2,\tau_2\right)\psi_{\sigma_2}\left(\mathbf{x}_2,\tau_2\right).$$

We can think of $\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)$ as vector-matrix-vector multiplication. Some of the matrix or vector indices are continuous, but that should not confuse you I think. All the operators above evolve in imaginary time with the same $\hat{K} = \hat{H} - \mu\hat{N}$ that enters the Boltzmann weight $e^{-\beta\hat{K}}$.

With the definition,

$$\mathcal{S}\left[\phi\right] = \exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right) \tag{35.14}$$

we can write the Matsubara Green's function as a functional derivative of the generating function $\ln Z\left[\phi\right]$,

$$\begin{aligned} -\frac{\delta \ln Z\left[\phi\right]}{\delta\phi\left(2,1\right)} &= -\frac{\left\langle T_\tau \mathcal{S}\left[\phi\right]\psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle}{\left\langle T_\tau \mathcal{S}\left[\phi\right]\right\rangle} \\ &\equiv -\left\langle T_\tau \psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle_\phi = \mathcal{G}\left(1,2\right)_\phi . \end{aligned} \tag{35.15}$$

To obtain this result, we used the fact that the functional derivative with respect to ϕ does not influence at all the time order, so one can differentiate the exponential inside the time-ordered product. (See Sec. 29.2) The thermal average on the first line is with respect to $e^{-\beta\hat{K}}$. In the average with a subscript, $\left\langle T_\tau \psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle_\phi$, one does not write $\mathcal{S}\left[\phi\right]$ explicitly. Note the reversal in the order of indices in $\mathcal{G}$ and in ϕ. We have also used the fact that in a time ordered product we can displace operators as we wish, as long as we keep track of fermionic minus signs. Finally, the functional derivative with respect to ϕ is defined by

$$\frac{\delta\phi\left(\overline{1},\overline{2}\right)}{\delta\phi\left(1,2\right)} = \delta\left(\overline{1}-1\right)\delta\left(\overline{2}-2\right) \tag{35.16}$$

where the delta function is a mixture of Dirac and Kronecker delta functions

$$\delta\left(\overline{1}-1\right) = \delta^3\left(\mathbf{x}_{\overline{1}}-\mathbf{x}_1\right)\delta\left(\tau_{\overline{1}}-\tau_1\right)\delta_{\sigma_{\overline{1}},\sigma_1}. \tag{35.17}$$

Remark 244 *You should keep your mathematician friend as far as possible from you when looking at this notation, because in this notation, the equality* $1 = 2$ *is allowed. What it means is that two different sets of coordinates are equal, so that it is rather innocuous. It is nevertheless a bit disturbing if you are not aware of the context.*

Higher order correlation functions can be obtained by taking further functional

derivatives

$$\begin{aligned}
\frac{\delta \mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= -\frac{\delta}{\delta\phi(3,4)}\frac{\left\langle T_\tau \mathcal{S}[\phi]\,\psi(1)\,\psi^\dagger(2)\right\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle} \\
&= \frac{\left\langle T_\tau \mathcal{S}[\phi]\,\psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle} \\
&\quad -\frac{\left\langle T_\tau \mathcal{S}[\phi]\,\psi(1)\,\psi^\dagger(2)\right\rangle\left\langle T_\tau \mathcal{S}[\phi]\,\psi^\dagger(3)\,\psi(4)\right\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle^2} \qquad (35.18) \\
&= \left\langle T_\tau \psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi\,. \qquad (35.19)
\end{aligned}$$

The first term is called a four-point correlation function. The last term comes from differentiating $\langle T_\tau \mathcal{S}[\phi]\rangle$ in the denominator. To figure out the minus signs in that last term note that there is one from $-1/Z^2$, one from the derivative of the argument of the exponential and one from ordering the field operators in the order corresponding to the definition of $\mathcal{G}_\sigma$. The latter is absorbed in the definition of $\mathcal{G}_\sigma$.

Remark 245 *The results of this section are independent of the explicit form of* $\hat{K} = \hat{H} - \mu\hat{N}$.

Remark 246 *Translational invariance: It is very important to understand that even when the system is translationally invariant, you should not assume that it is when using this formalism in the presence of the source term* $\phi(1,2)$*. This is because* $\phi(1,2)$ *has to break translational invariance to generate the correlation functions that are needed. Translational invariance is recovered at the end, when you have all the equations that you need. Only then can you set* $\phi = 0$ *and recover all the symmetries of the Hamiltonian.*

35.3 Source fields for Green's functions, an impressionist view

Before we enter into even more indices and lenghty expressions, it is useful to have an impressionist view, a sort of road map that we will follow. We will need to put all indices back for this to make any sense, but anyway, I hope you stick with me for a while.

We are addressing here the question of how can that formalism possibly be helpful. It is helpful because the self-energy will be expressed in terms of a four point correlation function which in turn can be found from a functional derivative of $\mathcal{G}_\sigma(,)_\phi$. It will be possible to find this functional derivative if we know $\mathcal{G}_\sigma(,)_\phi$. We do have an expression for that quantity so that, in a sense, it closes the loop. We will see things are not so simple in practice, but at least that is a start.

How do we find $\mathcal{G}_\sigma(,)_\phi$? It suffices to write the equations of motion. This is the first time in this Chapter that the explicit form of the Hamiltonian comes in. What is different from the non-interacting case is the presence of ϕ and of interactions. When we compute $\frac{\partial\psi(1)}{\partial\tau_1} = [K, \psi(1)]$, there will be a term coming from the commutator of the interaction term with $\psi(1)$. That will be a term proportional to $V\psi^\dagger\psi\psi$ with V the potential energy. Using this result in the

definition of $\mathcal{G}$, which has an extra $\psi^\dagger$ tagged on the right, the equation of motion for $\mathcal{G}$ will read something like

$$\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 - V\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger \right\rangle. \tag{35.20}$$

Using our notion of irreducible self-energy, we define

$$\begin{aligned} \Sigma\mathcal{G} &= -V\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger \right\rangle \\ \Sigma &= -V\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger \right\rangle \mathcal{G}^{-1}. \end{aligned} \tag{35.21}$$

so that when you use this definition and put everything on the left-hand side, except for unity, you recognize

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma. \tag{35.22}$$

which is equivalent to Dyson's equation

$$\mathcal{G} = \mathcal{G}_{0\phi} + \mathcal{G}_{0\phi}\Sigma\mathcal{G} \tag{35.23}$$

with $\mathcal{G}_{0\phi} = \left(\mathcal{G}_0^{-1} - \phi\right)^{-1}$. The four-point correlation function entering the definition of Σ is then obtained from a functional derivative of $\mathcal{G}$ since

$$\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger \right\rangle = \frac{\delta\mathcal{G}}{\delta\phi} - \mathcal{G}\mathcal{G} \tag{35.24}$$

as we saw in the previous section.

To find that functional derivative we start from the equation of motion Eq.(35.20) which gave us Dyson's equation Eq.(35.22) which is easy to differentiate with respect to ϕ. Then, we can take advantage of this and $\mathcal{G}^{-1}\mathcal{G} = 1$ to find the functional derivative of $\mathcal{G}$. Indeed,

$$\frac{\delta\left(\mathcal{G}^{-1}\mathcal{G}\right)}{\delta\phi} = \frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} + \mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\phi} = 0 \tag{35.25}$$

or, left multiplying by $\mathcal{G}$

$$\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} \tag{35.26}$$

which can be evaluated with the help of Dyson's equation Eq.(35.22)

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}. \tag{35.27}$$

Remark 247 $\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}$ *is a useful way to differentiate matrices. Note that in the special case* $\mathcal{G} = (ik_n - \zeta_{\mathbf{k}})^{-1}$, *the previous formula gives the expected result when we use* $\frac{\partial\mathcal{G}}{\partial\zeta_{\mathbf{k}}} = -\mathcal{G}\frac{\partial\mathcal{G}^{-1}}{\partial\zeta_{\mathbf{k}}}\mathcal{G}$.

The last equation suggests that the functional dependence of Σ on ϕ comes only from the dependence of $\mathcal{G}$ on ϕ. The self-energy has no explicit dependence on ϕ. Hence, using the chain rule

$$\frac{\delta\Sigma}{\delta\phi} = \frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi} \tag{35.28}$$

we have an integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$

$$\boxed{\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G}.} \tag{35.29}$$

If we can solve this, we can find $\mathcal{G}$ Eq.(35.20)

$$\boxed{\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 + \Sigma\mathcal{G}} \tag{35.30}$$

with the self-energy Eq.(35.21) written in terms of the four-point function Eq.(35.24)

$$\boxed{\Sigma = -V\left(\frac{\delta\mathcal{G}}{\delta\phi} - \mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1}.} \tag{35.31}$$

Since the integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$ requires that we know both $\mathcal{G}$ and $\frac{\delta\Sigma}{\delta\mathcal{G}}$ there will be some iteration process involved. The last three equations can be solved for $\phi = 0$, since ϕ has played its role and is no longer necessary at that point.

One physical point that will become clearer when I put all indices back, is that the self-energy contains information about the fact that the medium is polarizable, i.e. it depends on the four-point correlation function $\frac{\delta\mathcal{G}}{\delta\phi}$ and hence on the density-density correlation function, or equivalently the longitudinal dielectric constant, as we shall verify.

I can also write an equation that looks as a closed functional equation for Σ by using the expression Eq.(35.27) relating $\frac{\delta\mathcal{G}}{\delta\phi}$ and $\frac{\delta\Sigma}{\delta\phi}$:

$$\begin{aligned}\Sigma &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G} - \mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1}. \\ &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi} - \mathcal{G}\right)\end{aligned} \tag{35.32}$$

An alternate useful form that uses the fact that all the functional dependence of Σ on ϕ is implicit through its dependence on $\mathcal{G}$ is

$$\boxed{\Sigma = -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi} - \mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)} \tag{35.33}$$

Since Σ is already linear in V, it is tempting to use $\Sigma = -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi} - \mathcal{G}\right)$ as a first approximation. This is the Hartree-Fock approximation.

Remark 248 *$\frac{\delta\Sigma}{\delta\mathcal{G}}$ in the equation for the functional derivative Eq.(35.29) is called the irreducible vertex in the particle-hole channel. The reason for this will become clear later. The term that contains this irreducible vertex is called a vertex correction.*

Remark 249 *Note that $\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\right)\mathcal{G}$ plays the role of a self-energy for the four-point function $\frac{\delta\mathcal{G}}{\delta\phi}$. For the same reason that it was profitable to resum infinite series for $\mathcal{G}$ by using the concept of a self-energy, it will be preferable to do the same here and use $\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\right)\mathcal{G}$ as a self-energy instead of iterating the equation for $\frac{\delta\mathcal{G}}{\delta\phi}$ at some finite order.*

Remark 250 *If I had written an equation of motion for the four-point function, we would have seen that it depends on a six point function, and so on, so that is not the way to go. This would have been the analog of the so-called BBGKY hierarchy [115] in classical transport theory. In the quantum context, it is called the Martin-Schwinger hierarchy [132].*

36. EQUATIONS OF MOTION TO FIND $\mathcal{G}$ IN THE PRESENCE OF SOURCE FIELDS

Here we try to do everything more rigorously with all the bells and whistles. It is clear that the first step is to derive the equations of motion for the Green's function in the jellium model. That was one of the ways to find the Green's function in the non-interacting case, without source fields. That begins with the Hamiltonian and equations for motion for $\psi_\sigma(1)$ which will enter the equation of motion for $\mathcal{G}$.

36.1 Hamiltonian and equations of motion for $\psi(1)$

The Hamiltonian we consider contains the kinetic energy and the electron-electron interaction. Note that we now introduce spin indices denoted by Greek indices:

$$\hat{K} = \hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{V} + \hat{V}_n - \mu\hat{N} \tag{36.1}$$

$$\hat{H}_0 = \frac{-1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\boldsymbol{\nabla}^2\psi_{\sigma_1}(\mathbf{x}_1) \tag{36.2}$$

$$\hat{V} = \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1)$$

$$\hat{V}_n = -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n \tag{36.3}$$

The last piece, V_n represents the interaction between a "neutralizing background" of the same uniform density n as the electrons. The potential is the Coulomb potential

$$v(\mathbf{x}_1-\mathbf{x}_2) = \frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|} \tag{36.4}$$

To derive the equations of motion for the Green's function, we first need those for the field operators.

$$\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} = \left[\hat{K},\psi_\sigma(\mathbf{x},\tau)\right] \tag{36.5}$$

Using $[AB,C] = A\{B,C\} - B\{A,C\}$ and Eq.(36.1) for $\hat{K}$ we have

$$\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} = \frac{\nabla^2}{2m}\psi_\sigma(\mathbf{x},\tau) + \mu\psi_\sigma(\mathbf{x},\tau) - \sum_{\sigma_2}\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\psi^\dagger_{\sigma_2}(\mathbf{x}_2,\tau)\psi_{\sigma_2}(\mathbf{x}_2,\tau)\psi_\sigma(\mathbf{x},\tau) \tag{36.6}$$

The last term does not have the 1/2 factor that appeared in the Hamiltonian

because

$$\begin{aligned}\left[\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\,\psi^{\dagger}_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1),\psi_{\sigma}(\mathbf{x})\right] &= \left[\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\,\psi^{\dagger}_{\sigma_2}(\mathbf{x}_2),\psi_{\sigma}(\mathbf{x})\right]\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1)\\ &= -\delta_{\sigma_1,\sigma}\delta(\mathbf{x}-\mathbf{x}_1)\,\psi^{\dagger}_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1)\\ &\quad +\delta_{\sigma_2,\sigma}\delta(\mathbf{x}-\mathbf{x}_2)\,\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1).\end{aligned}$$

Anticommuting the destruction operators in the last term, substituting and changing dummy indices, the two contributions are identical.

The equation of motion can be rewritten in the more matrix-like form

$$\boxed{\frac{\partial\psi(1)}{\partial\tau_1}=\frac{\nabla_1^2}{2m}\psi(1)+\mu\psi(1)-\psi^{\dagger}\left(\overline{2}\right)\psi\left(\overline{2}\right)V\left(\overline{2}-1\right)\psi(1)} \tag{36.7}$$

if we define a time- and spin-dependent potential

$$\boxed{V(1,2)=V_{\sigma_1,\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2)\equiv\frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|}\delta(\tau_1-\tau_2).} \tag{36.8}$$

In reality the potential is independent of spin and is instantaneous but introducing these dependencies simplifies the notation.

Remark 251 *We assume that the potential has no $q=0$ component because of the compensating effect of the positive background. The argument for the neutralizing background is as follows. If we had kept it, the above equation would have had an extra term*

$$+n\left[\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\right]\psi_{\sigma}(\mathbf{x},\tau). \tag{36.9}$$

We will see that there is a contribution to the self-energy, the Hartree contribution that cancels this term. To an excellent degree of approximation we may say that the only effect of the neutralizing background is to remove the $q=0$ component of the Coulomb potential. The result that we are about to derive would be different in other models, such as the Hubbard model, where the $q=0$ component of the interaction potential is far from negligible.

36.2 Equations of motion for $\mathcal{G}_{\phi}$ and definition of $\sum_{\phi}$

We expect that the equation for motion for $\mathcal{G}(1,2)_{\phi}$

$$\mathcal{G}(1,2)_{\phi}=-\frac{\left\langle T_{\tau}\mathcal{S}[\phi]\,\psi(1)\,\psi^{\dagger}(2)\right\rangle}{\langle T_{\tau}\mathcal{S}[\phi]\rangle}$$

will have the following structure $\mathcal{G}^{-1}(1,2)_{\phi}=\mathcal{G}_0^{-1}(1,2)-\phi(1,2)-\Sigma(1,2)_{\phi}$. In detail, it is obtained by taking an imaginary-time derivative. There will be three contributions. One from $\frac{\partial\psi(1)}{\partial\tau_1}$, that we found above, one from the time derivative of the two Heaviside functions $\theta(\tau_1-\tau_2)$ and $\theta(\tau_2-\tau_1)$ entering the definition of the time-ordered product (that gives the usual delta function), and one from the fact that terms in $\mathcal{S}[\phi]$ have to be ordered with respect to τ_1. The only unfamiliar contribution is the latter one. To understand how to compute it,

we write explicitely the time integral associated with the creation operator in the exponential and order it properly:

$$\left\langle T_\tau \mathcal{S}\left[\phi\right]\psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle = \left\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\overline{2}\right)\psi\left(\overline{2}\right)\right)\right.$$
$$\left.\psi\left(1\right)\exp\left(-\int_{0}^{\tau_1} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\overline{2}\right)\psi\left(\overline{2}\right)\right)\psi^\dagger\left(2\right)\right\rangle$$

Since we moved an even number of fermion operators, we do not need to worry about sign. We do not need to worry about the destruction operator in the exponential either since it anticommutes with $\psi\left(1\right)$: The time-ordered product will eventually take care of the proper order (see also the first remark below). We thus have a contribution to the time derivative with respect to τ_1 that comes from acting on the exponentials and reads

$$\begin{aligned}
&\left\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\overline{2}\right)\psi\left(\overline{2}\right)\right)\right.\\
&\int d^3\mathbf{x}_{1'}\left[\psi^\dagger\left(\mathbf{x}_{1'},\tau_1\right)\phi\left(\mathbf{x}_{1'},\tau_1,\overline{2}\right)\psi\left(\overline{2}\right),\psi\left(\mathbf{x}_1,\tau_1\right)\right]\\
&\left.\exp\left(-\int_{0}^{\tau_1} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\overline{2}\right)\psi\left(\overline{2}\right)\right)\psi^\dagger\left(2\right)\right\rangle\\
= \;& -\phi\left(1,\overline{2}\right)\left\langle T_\tau \mathcal{S}\left[\phi\right]\psi\left(\overline{2}\right)\psi^\dagger\left(2\right)\right\rangle.
\end{aligned}$$

We had to take the derivative of the arguments of the exponentials and to be careful about order of operators at equal time. Collecting all the contributions, we can write

$$\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\mathcal{G}\left(1,2\right)_\phi = -\delta\left(1-2\right)+\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)V\left(1-\overline{2}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle_\phi$$
$$-\phi\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},2\right)_\phi. \tag{36.10}$$

Note that we had to specify $\psi^\dagger\left(\overline{2^+}\right)$ in the term with the potential energy. The superscript $+$ specifies that the time in that field operator is later than the time in $\psi\left(\overline{2}\right)$. In other words

$$2^+ \equiv \left(\mathbf{x}_2,\tau_2+0^+;\sigma_2\right)$$

Equal time does not mean anything in a time ordered product, we have to specify the order. The choice to take $\psi^\dagger\left(\overline{2^+}\right)$ keeps the field in the order it was in to begin with.

The equations of motion can be written in a compact form if we define

$$\boxed{\mathcal{G}_0^{-1}\left(1,\overline{2}\right)\equiv-\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\delta\left(1-\overline{2}\right).} \tag{36.11}$$

With this definition, the equation of motion Eq.(36.10) takes the form

$$\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right)-\phi\left(1,\overline{2}\right)\right)\mathcal{G}\left(\overline{2},2\right)_\phi=\delta\left(1-2\right)-V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle_\phi \tag{36.12}$$

Comparing with Dyson's equation, we have an explicit form for the self-energy,

$$\boxed{\Sigma\left(1,\overline{2}\right)_\phi\mathcal{G}\left(\overline{2},2\right)_\phi=-V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle_\phi.} \tag{36.13}$$

The equation of motion can then also be written as

$$\boxed{\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right)-\phi\left(1,\overline{2}\right)-\Sigma\left(1,\overline{2}\right)_\phi\right)\mathcal{G}\left(\overline{2},2\right)_\phi=\delta\left(1-2\right)}$$

which also reads

$$\boxed{\mathcal{G}^{-1}\left(1,2\right)_\phi=\mathcal{G}_0^{-1}\left(1,2\right)-\phi\left(1,2\right)-\Sigma\left(1,2\right)_\phi.} \tag{36.14}$$

Remark 252 *$T_\tau\left[e^{A+B}\right]=T_\tau\left[e^Ae^B\right]$ even when A and B are operators that do not commute, as long as A and B have bosonic commutation relations: Let us consider the first few terms of the power series:*

$$\begin{aligned} T_\tau\left[e^Ae^B\right] &= T_\tau\left[\left(1+A+\frac{1}{2}A^2+\ldots\right)\left(1+B+\frac{1}{2}B^2+\ldots\right)\right] &(36.15)\\ &= T_\tau\left[\left(1+(A+B)+\frac{1}{2}A^2+AB+\frac{1}{2}B^2\ldots\right)\right] &(36.16)\end{aligned}$$

while

$$\begin{aligned} T_\tau\left[e^{A+B}\right] &= T_\tau\left[1+(A+B)+\frac{1}{2}(A+B)^2+\ldots\right] &(36.17)\\ &= T_\tau\left[1+(A+B)+\frac{1}{2}(A^2+AB+BA+B^2)+\ldots\right]. &(36.18)\end{aligned}$$

Now, let the time order operator do his job. If A is at a later time than B, then $AB+BA$ in the last equation will become $2AB$ and we recover the result also obtained from $T_\tau\left[e^Ae^B\right]$. You can convince yourself that equality will also follow if B is at a time later than A.

Remark 253 *The self-energy is related to a four-point function and we note in passing that the trace of the defining equation (36.13) is related to the potential energy. That can be seen as follows. In the limit $2\rightarrow 1^+$ the right-hand side becomes*

$$\left\langle T_\tau\left[\psi^\dagger\left(1^+\right)\psi^\dagger\left(\overline{1'^+}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(1\right)\right]\right\rangle.$$

Recalling the definition of the average potential energy

$$2\left\langle V\right\rangle=\sum_{\sigma_1}\int d^3\mathbf{x}_1\left\langle T_\tau\left[\psi^\dagger\left(1^+\right)\psi^\dagger\left(\overline{1'^+}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(1\right)\right]\right\rangle \tag{36.19}$$

this special case of our general formula gives

$$\sum_{\sigma_1}\int d^3\mathbf{x}_1\int_{1'}\Sigma\left(1,1'\right)\mathcal{G}\left(1',1^+\right)=2\left\langle V\right\rangle. \tag{36.20}$$

We have the freedom to drop the time-ordered product when we recall that the operators are all at the same time and in the indicated order. Using time-translational invariance the last result may also be written

$$\boxed{\Sigma\left(\overline{1},\overline{1'}\right)\mathcal{G}\left(\overline{1'},\overline{1^+}\right)=2\left\langle V\right\rangle\beta=\left\langle T_\tau\left[\psi^\dagger\left(\overline{1^+}\right)\psi^\dagger\left(\overline{1'^+}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(\overline{1}\right)\right]\right\rangle} \tag{36.21}$$

Remark 254 *The 1^+ on the left-hand side is absolutely necessary for this expression to make sense. Indeed, taken from the point of view of Matsubara frequencies, one knows that the self-energy goes to a constant at infinite frequency while the Green's function does not decay fast enough to converge without ambiguity. On the right-hand side of the above equation, all operators are at the same time, in the order explicitly given.*

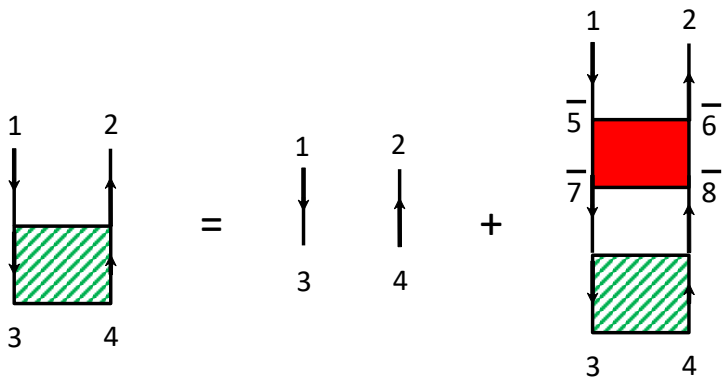


Figure 36-1 Diagrammatic representation of the integral equation for the four point function represented on the left of the equation. The two lines on the right of the equal sign and on top of the last block are Green's function. The filled box is the functional derivative of the self-energy. It is called the particle-hole irreducible vertex. It plays, for the four-point function the role of the self-energy for the Green's function.

36.3 Four-point function from functional derivatives

Since we need a four-point function to compute the self-energy and we know $\mathcal{G}_\phi$ if we know the self-energy, let us find an equation for the four-point function in terms of functional derivatives as we saw at length in Eq.(35.19)

$$\boxed{\frac{\delta \mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \left\langle T_\tau \psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi.} \tag{36.22}$$

The equation for the functional derivative is then easy to find using $\mathcal{G}\mathcal{G}^{-1}=1$ and our matrix notation,

$$\frac{\delta\left(\mathcal{G}\mathcal{G}^{-1}\right)}{\delta\phi} = 0 \tag{36.23}$$

$$\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1} + \mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi} = 0 \tag{36.24}$$

$$\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}. \tag{36.25}$$

With Dyson's equation Eq. (36.14) for $\mathcal{G}^{-1}$ we find the right-hand side of that equation

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}. \tag{36.26}$$

Just to make sure what we mean, let us restore indices. This then takes the form

$$\begin{aligned}\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= \mathcal{G}\left(1,\overline{1}\right)_\phi \frac{\delta\phi\left(\overline{1},\overline{2}\right)}{\delta\phi(3,4)}\mathcal{G}\left(\overline{2},2\right)_\phi + \mathcal{G}\left(1,\overline{5}\right)_\phi \frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_\phi}{\delta\phi(3,4)}\mathcal{G}\left(\overline{6},2\right)_\phi \\ &= \mathcal{G}(1,3)_\phi\,\mathcal{G}(4,2)_\phi + \mathcal{G}\left(1,\overline{5}\right)_\phi \frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_\phi}{\delta\phi(3,4)}\mathcal{G}\left(\overline{6},2\right)_\phi .\end{aligned} \tag{36.27}$$

If you take the convention that $\mathcal{G}(1,2)$ is represented by an arrow going from 1 to 2 from left to right, then we can represent $\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)}$ as $\mathcal{G}(1,2)$ being pinched by $\phi(3,4)$, i.e. having an arrow starting at 1 and ending at 2 with $3,4$ at the bottom.

This last equation shows that Σ has no explicit dependence on ϕ. It depends on ϕ only through its dependence on $\mathcal{G}$. We will see this is a self-consistent assumption. Taking that into account, and using the chain rule, this last equation can also be written in the form

$$\begin{aligned}\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi} \\ &+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_{\phi}. \end{aligned} \tag{36.28}$$

This general equation can also be written in short-hand notation

$$\frac{\delta\mathcal{G}}{\delta\phi}=\mathcal{G}\hat{\cdot}\mathcal{G}+\ \mathcal{G}\ \begin{matrix}\frac{\delta\Sigma}{\delta\mathcal{G}}\\ \frac{\delta\mathcal{G}}{\delta\phi}\end{matrix}\ \mathcal{G}\ , \tag{36.29}$$

where the caret $\hat{\cdot}$ reminds us that the indices adjacent to it are the same as those of ϕ and where the two terms on top of one another are matrix multiplied top down as well. In the top down multiplication, it is pairs of indices of $\mathcal{G}$ that are considered as a single matrix index. Fig. 36-1 illustrates the equation with the indices. The diagrams go from top to bottom to remind ourselves of where the indices are in the algebraic equation, but we may rotate the diagrams in any direction we want.

Definition 30 *In the jargon, $\frac{\delta\Sigma}{\delta\mathcal{G}}$ is the vertex function which is irreducible in a particle-hole channel. (There are two particle-hole channels). This means that if we iterate the equation for $\frac{\delta\mathcal{G}}{\delta\phi}$, we generate all the diagrams that have Green's function lines going in opposite direction. Those diagrams for $\frac{\delta\mathcal{G}}{\delta\phi}$ can thus be cut in two by cutting these two lines. They are reducible. $\frac{\delta\Sigma}{\delta\mathcal{G}}$ contains the diagrams that cannot be cut in two in this way. It sort of plays the role of a self-energy for response functions.*

Remark 255 *Connection between labels (that we also call indices) in the Green's function and the direction of the arrow in the diagram: We take the convention that for $\mathcal{G}\left(1,2\right)_{\phi}$ the arrow begins at the annihilation operator 1 and ends at the creation operator 2. It might have been natural to begin at the creation operator instead. In fact it does not matter, as long as one is consistent. Both conventions can be found in the literature.*

Remark 256 $\frac{\delta\mathcal{G}\left(1,1^{+}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)}$ *in Eq. (36.22) is related to minus the density-density correlation function:*

$$-\left[\left\langle\psi^{\dagger}\left(1^{+}\right)\psi\left(1\right)\psi^{\dagger}\left(2^{+}\right)\psi\left(2\right)\right\rangle_{\phi}-\left\langle\psi^{\dagger}\left(1^{+}\right)\psi\left(1\right)\right\rangle_{\phi}\left\langle\psi^{\dagger}\left(2^{+}\right)\psi\left(2\right)\right\rangle_{\phi}\right]. \tag{36.30}$$

Using the exact result for this quantity, namely Eq. (36.28), we see that even when there are no interactions, this quantity is $\mathcal{G}\left(1,2\right)_{\phi}\mathcal{G}\left(2,1\right)_{\phi}$. We thus see the necessity to know Green's functions to compute observables, even in the non-interacting case. Physically, this term is a so-called exchange term. It makes sure that two electrons with the same spin are not on top of exach other. This comes from the Pauli exclusion principle.

36.4 Self-energy from functional derivatives

To compute the self-energy, according to Eq.(36.13), what we need is

$$\boxed{\Sigma\left(1,3\right)_{\phi}=-V\left(1-\overline{2}\right)\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{2^{+}}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^{\dagger}\left(\overline{4}\right)\right]\right\rangle_{\phi}\mathcal{G}_{\phi}^{-1}\left(\overline{4},3\right).} \tag{36.31}$$

We write the four-point function with the help of the functional derivative Eq.(36.22) by replacing in the latter equation $3\rightarrow\overline{2^{+}}$, $4\rightarrow\overline{2}$, $1\rightarrow1$, $2\rightarrow\overline{4}$ so that

$$\Sigma\left(1,3\right)_{\phi}=-V\left(1-\overline{2}\right)\left[\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(1,\overline{4}\right)_{\phi}\right]\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi} \tag{36.32}$$

Remark 257 *Mnemotechnic: The first label of the $V\left(1-\overline{2}\right)$ is the same as the first label of $\mathcal{G}\left(1,\overline{4}\right)_{\phi}$ on the numerator and the same as the first label on the left-hand side of the equation. The second label is summed over and is the same as the label on the denominator of $\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}$. The two Green's function in $\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(1,\overline{4}\right)_{\phi}$ can be arranged on top of one another so that this rule is preserved.*

The final expression is easy to obtain if we change the labels of the exact four-point function Eq.(36.28) so that they correspond to those above. Namely, we write

$$\begin{aligned}\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)} &= \mathcal{G}\left(1,\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(\overline{2},\overline{4}\right)_{\phi}\\ &\quad+\mathcal{G}\left(1,\overline{7}\right)_{\phi}\left(\frac{\delta\Sigma\left(\overline{7},\overline{8}\right)_{\phi}}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}\right)\mathcal{G}\left(\overline{8},\overline{4}\right)_{\phi}.\end{aligned} \tag{36.33}$$

Substituting in the expression for the self-energy Eq.(36.32) using $\mathcal{G}\left(1,\overline{4}\right)_{\phi}\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi}=\delta\left(1-3\right)$ (and changing the dummy label $\overline{7}\rightarrow\overline{4}$) this yields,

$$\begin{aligned}\Sigma\left(1,3\right)_{\phi} &= -V\left(1-3\right)\mathcal{G}\left(1,3^{+}\right)_{\phi}-V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}\\ &\quad+V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right).\end{aligned} \tag{36.34}$$

The second term is the only one that will give a frequency dependence, and hence an imaginary part, to the self-energy. The other two terms in the above equation are the Hartree-Fock contribution that we will discuss at length later on. Note that $V\left(1-\overline{2}\right)$ is instantaneous, i.e. there is a delta function $\delta\left(\tau_{1}-\tau_{\overline{2}}\right)$, and whether we have $V\left(1-3\right)$ or $V\left(1-3^{+}\right)$ is irrelevant. In the Green's functions however, it is important to keep track of the $+$. Indeed, that reflects the fact that in the Hamiltonian, the creation operators are always to the left of the annihilation operators. That is the way to preserve that property in a time-ordered product.

The equation for the self-energy is represented schematically in Fig. 36-2. Note that the diagrams are one-particle irreducible, i.e. they cannot be cut in two seperate pieces by cutting a single propagator.

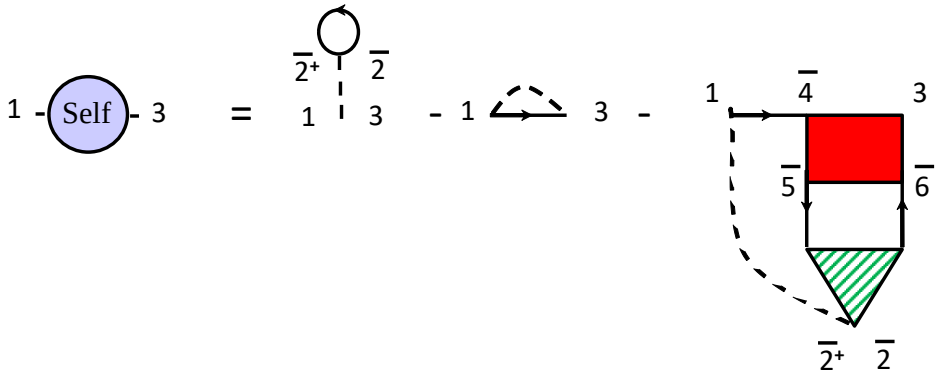


Figure 36-2 Diagrams for the self-energy. The dashed line represent the interaction. The first two terms are, respectively, the Hatree and the Fock contributions. The textured square appearing in the previous figure for the four-point function has been squeezed to a triangle to illustrate the fact that two of the indices (coordinates) are identical.

Remark 258 *Historically, the expressions "self-energy" is inspired by the fact that it is the electromagnetic field of the electron itself that leads to modifications of the properties of the electron even when it is moving in a vacuum. In the latter case, the electromagnetic field of the electron contains virtual photons that can in turn create virtual electron-positron pairs, the analog of electron-hole excitations.*

36.5 The self-energy, one-particle irreducibility and Green's function

It is clear from the diagrammatic illustration of the self-energy in Fig. 36-2 that all internal indices are integrated over, as the Feynman rules would specify. In addition, the diagrams are connected and none of them can be cut into two distinct pieces by cutting one Green's function line. We say that the self-energy contains all the diagrams that are one-particle irreducible. The Feynman rules tell us that the self-energy contains all the topologically distinct connected diagrams that end and begin with an interaction and a Green's function at the same point. There are rules for their sign as well: One minus sign for each order in perturbation theory and one minus sign for every closed loop. The Feynman rules are generally formulated in terms of bare Green's functions. Here, the dressed Green's functions appear but, as you will check in an exercise, it is also possible to recover the perturbation theory in terms of bare Green's functions.

Finally notice that if we iterate the Dyson equation,

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G} \tag{36.35}$$

$$= \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0+\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \dots \tag{36.36}$$

it becomes clear that the Green's function is given by the sum of all diagrams that end at the destruction operator and begin at the annihilation operator and contains all possible topologically distinct diagrams. The Green's function diagrams are, however, one-particle reducible.

37. FIRST STEPS WITH FUNCTIONAL DERIVATIVES: HARTREE-FOCK AND RPA

These are the two most famous approximations: Hartree-Fock for the self-energy and RPA for the density-density correlation function. We will see later on why these come out naturally from simple considerations, including the variational principle.

37.1 Functional derivatives can be used to generate perturbation theory

The Schwinger formalism generates very naturally an expansion in powers of the dressed Green's function. The diagrams that are found for the self-energy then do not include self-energy insertions. This is called the skeleton expansion. This is formally very nice and this expansion can be used to derive a number of exact results, such as the Luttinger theorem Sec. (74.2). However, it has some drawbacks that will be discussed for example in the section on the Luttinger theorem and in section (75) on the limitations of conserving approximations . The expansion in terms of the bare Green's function is often much better behaved, but it is a bit more ackward to generate with the Schwinger formalism. This is discussed in the following two subsections.

37.1.1 Skeleton expansion

The general equations (36.34) for the self-energy and (36.33) for the susceptibility can be used iteratively to generate perturbation theory for the self-energy in powers of the external potential. Since the leading term in Σ is already linear in external potential, the last term the general expression for the self-energy Eq.(36.34) is of second order at least since it have a product of V and Σ. To leading order then,

$$\Sigma\left(1,3\right)_{\phi}=V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)-V\left(1-3\right)\mathcal{G}\left(1,3^{+}\right)_{\phi}. \tag{37.1}$$

This is the Hartree-Fock approximation, on which I will comment much more later on.

To obtain the second order, it suffices to compute $\delta\Sigma\left(\overline{4},3\right)_{\phi}/\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}$ to first order, i.e. using the above equation and $\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}/\delta\phi\left(\overline{2^{+}},\overline{2}\right)$ to zero'th order in

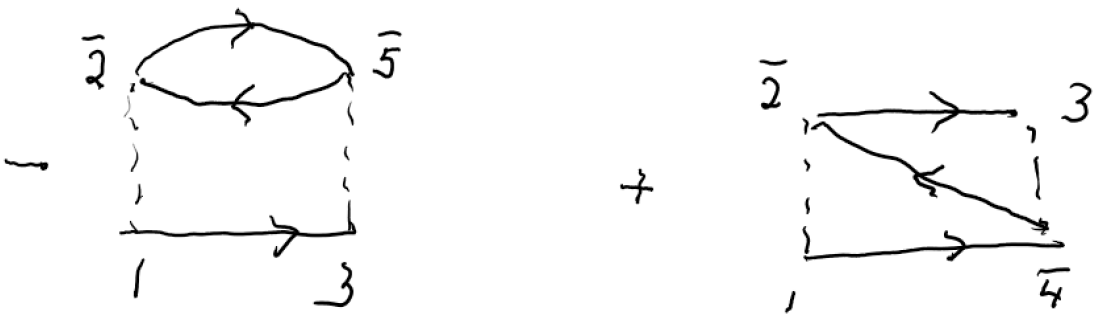


Figure 37-1 Second-order skeleton self-energy diagrams.

V. This means that we substitute on the right-hand side of Eq. (36.34)

$$\begin{aligned}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}} &= \frac{\delta}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}\left[V\left(\overline{4}-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(\overline{4}-3\right)-V\left(\overline{4}-3\right)\mathcal{G}\left(\overline{4},3^{+}\right)_{\phi}\right] \quad (37.2)\\ &= V\left(\overline{4}-\overline{2}\right)\delta\left(\overline{5}-\overline{2}\right)\delta\left(\overline{6}-\overline{2^{+}}\right)\delta\left(\overline{4}-3\right)-V\left(\overline{4}-3\right)\delta\left(\overline{5}-\overline{4}\right)\delta\left(\overline{6}-3^{+}\right)\end{aligned}$$

while

$$\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}=\mathcal{G}\left(\overline{5},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(\overline{2},\overline{6}\right)_{\phi}. \quad (37.3)$$

The second order contribution to the self-energy thus becomes

$$-V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)} \quad (37.4)$$

$$= -V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}V\left(\overline{4}-\overline{5}\right)\mathcal{G}\left(\overline{5},\overline{2^{+}}\right)\mathcal{G}\left(\overline{2},\overline{5}\right)_{\phi}\delta\left(\overline{4}-3\right) \quad (37.5)$$

$$+V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}V\left(\overline{4}-3\right)\mathcal{G}\left(\overline{4},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(\overline{2},3^{+}\right)_{\phi} \quad (37.6)$$

The second order diagrams thus looks as illustrated on Fig. (37-1).

The iterative process becomes more and more complicated as the order of perturbation increases, but it is clear that it can be done.

Remark 259 *With this approach, the algebraic expression is obtained directly. The sign of the diagram appears explicitly. With the Feynman rules, that can be found in Chapter (38), the sign is given by a rule: There is a minus sign for each order in perturbation theory, and a minus sign for each closed fermion loop. This corresponds to the sign of the diagrams in Fig. (37-1).*

Remark 260 *The perturbation theory that we have just found is in powers of the interaction with dressed propagators. This is the so-called skeleton expansion where self-energies never appear on a Green's function. The jargon is that there are non self-energy insertions. For example, a term such as the one illustrated in Fig. (37-2) does not appear. The following section shows that such diagrams appear when we expand in powers of the bare Green's function.*

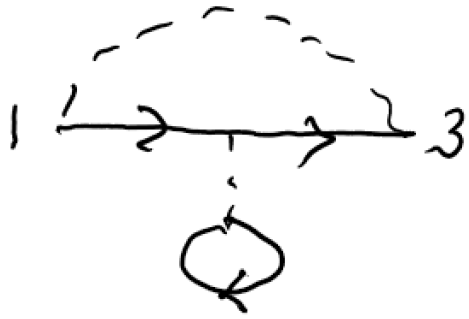


Figure 37-2 Example of a self-energy diagram that is not a skeleton self-energy diagram. One of the Green's functions is dressed with a self-energy.

37.1.2 Expansion in terms of the bare Green's function

The Feynman rules in Chapter (38) give a way to generate all self-energy diagrams, but it is easy to miss some terms. With the Schwinger formalism, one way is to start from the skeleton expansion, that can be found analytically, as I have show above.

The first-order diagrams for the self-energy in powers of the potential using $\mathcal{G}_0$ is obtained simply by replacing $\mathcal{G}$ by $\mathcal{G}_0$ in the skeleton expansion.

For the second-order diagram, we again replace $\mathcal{G}$ by $\mathcal{G}_0$ in the second-order skeleton expansion. But there are other diagrams that are obtained by replacing successively one of the $\mathcal{G}$ by $\mathcal{G}_0$ and the other $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ that was obtained previously to first order in V using $\mathcal{G}_0$.

Say we want the third order diagrams for the self-energy. The idea is to keep using the skeleton expansion and then recursively use Dyson's equation (35.23)

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G} \tag{37.7}$$

that can be iterated to give

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \cdots . \tag{37.8}$$

Assume that, as above, we have found the self-energy expansion to second order in the external potential with $\mathcal{G}_0$ propagators. To third order, we must *add all the contributions below:*

- Replace all $\mathcal{G}$ by $\mathcal{G}_0$ in the third order skeleton diagram.
- In the second-order skeleton diagram, replace in turn successively all but one of the $\mathcal{G}$ by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to first order with $\mathcal{G}_0$ propagators.
- In the first-order skeleton diagram,
    1. replace successively all $\mathcal{G}$ except one by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to second order in the external potential with $\mathcal{G}_0$ propagators.
    2. replace successively all $\mathcal{G}$ except one by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to first order in the external potential with $\mathcal{G}_0$ propagators.

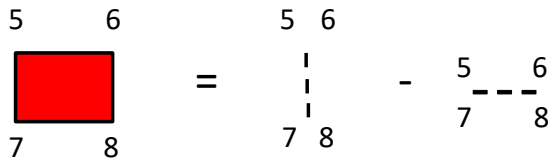


Figure 37-3 Expression for the irreducible vertex in the Hartree-Fock approximation. The labels on either side of the bare interaction represented by a dashed line are at the same point, in other words there is a delta function.

3. replace simultaneously the two $\mathcal{G}$ of the first-order skeleton expansion by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ to first order in the external potential with $\mathcal{G}_0$ propagators.

The procedure is clear but tedious. It suffices to keep track of perturbation order recursively, going back in the order of the skeleton expansion and using Dyson's equation to replace $\mathcal{G}$.

37.2 Hartree-fock and RPA in space-time

The expression for the self-energy and an iterative procedure can be used to compute $\frac{\delta\Sigma}{\delta\mathcal{G}}$ that appears both in the exact expression for the self-energy Eq.(36.34) and in the exact expression for the four-point function Eq.(36.28), four-point function that also appears in the self-energy. A look at the last two figures that we drew is helpful.

Refering to the exact expression for the four-point function Eq.(36.28), what we need to obtain the so-called Random Phase Approximation (RPA) is $\frac{\delta\Sigma(5,6)_\phi}{\delta\mathcal{G}(7,8)_\phi}$ evaluated from the the Hartree-Fock approximation Eq.(37.1), namely the first two terms in Fig. (36-2).

$$\begin{aligned}\frac{\delta\Sigma(5,6)_\phi}{\delta\mathcal{G}(7,8)_\phi} &= V(5-\overline{9})\,\delta(\overline{9}-7)\,\delta(\overline{9}-8)\,\delta(5-6) - V(5-6)\,\delta(7-5)\,\delta(8-6)\\ &= V(5-7)\,\delta(7-8)\,\delta(5-6) - V(5-6)\,\delta(7-5)\,\delta(8-6)\,.\end{aligned}$$

It is easier to imagine the result by looking back at the illustration of the Hartree-Fock term in Fig. 36-1. The result of the functional derivative is illustrated in Fig. 37-3. When two coordinates are written on one end of the interaction line, it is because there is a delta function. For example, there is a $\delta(5-6)$ for the vertical line.

Substituting back in the equation for the exact found-point function $\frac{\delta\mathcal{G}}{\delta\phi}$ Eq.(36.28), we find

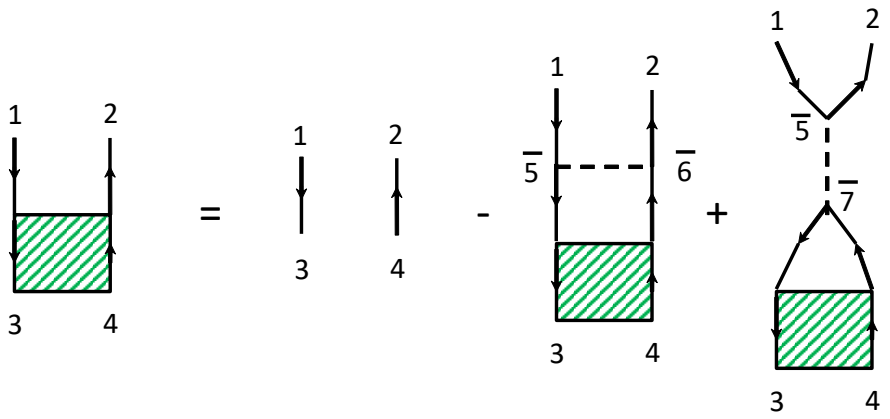


Figure 37-4 Integral equation for $\delta\mathcal{G}/\delta\phi$ in the Hartree-Fock approximation.

$$\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} = \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi}$$

$$+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta\mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{5},2\right)_{\phi} \tag{37.9}$$

$$-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_{\phi}. \tag{37.10}$$

This expression is easy to deduce from the general diagrammatic representation of the general integral equation Fig. 36-1 by replacing the irreducible vertex by that in Fig. 37-3 that follows from the Hartree-Fock approximation. This is illustrated in Fig. 37-4.

To compute a better approximation for the self-energy we will need $\delta\phi\left(2^{+},2\right)$ instead of $\delta\phi\left(3,4\right)$, as can be seen from our exact result Eq.(36.34). Although one might guess it from symmetry, we will also see that all that we will need is, $\delta\mathcal{G}\left(1,1^{+}\right)$, although it is not obvious at this point. It is quite natural however that the density-density correlation function plays an important role since it is related to the dielectric constant (Sec.13). From the previous equation, that special case can be written

$$\frac{\delta\mathcal{G}\left(1,1^{+}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)} = \mathcal{G}\left(1,2\right)_{\phi}\mathcal{G}\left(2,1\right)_{\phi} \tag{37.11}$$

$$+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta\mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{5},1\right)_{\phi} \tag{37.12}$$

$$-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{6},1\right)_{\phi}. \tag{37.13}$$

This equation is refered to as the generalized RPA. When the last term is neglected, this is the RPA. We will discuss this in more details later.

Remark 261 *Clearly, external points, such as* $1,2,3,4$ *are fixed, but the coordinates that appear inside diagrams must be integrated over. This is a simple rule for interpreting diagrams. There are analogous rules in momentum-Matsubara space when there is translational invariance, as we proceed to show.*

37.3 Hartree-Fock and RPA in Matsubara and momentum space with $\phi = 0$

We are ready to set $\phi = 0$. As we have discussed, it is important not to do that too soon. Once this is done, we can use translational invariance so that $\Sigma(1,2) = \Sigma(1-2)$ and $\mathcal{G}(1,2) = \mathcal{G}(1-2)$. In addition, spin rotational invariance implies that these objects are diagonal in spin space. We then Fourier transform to take advantage of the translational invariance. In that case, restoring spin indices we can define

$$\mathcal{G}_\sigma(k) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2)\, e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{ik_n(\tau_1-\tau_2)} \mathcal{G}_\sigma(1-2) \quad (37.14)$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. For clarity then, we have explicitly written a single spin label. We thus make the following rule:

- When in position space there is an arrow representing $\mathcal{G}(1-2)$ in the translationally invariant case, in momentum space, you can think of this arrow as carrying a momentum $\mathbf{k}$.

For the potential we define

$$V_{\sigma,\sigma'}(q) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2)\, e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(1-2) \quad (37.15)$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_n = 2n\pi T \quad (37.16)$$

with n an integer. Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}(1-2)$ is independent of spin.

- An interaction in a diagram is represented by a dotted line. Note that because $V(1-2) = V(2-1)$, in momentum space we are free to choose the direction of $\mathbf{q}$ on the dotted line at will. Once a convention is chosen, we stick with it.

Remark 262 *General spin-dependent interaction: In more general theories, there are four spin labels attached to interaction vertices. These labels correspond to those of the four fermion fields. Here the situation is simpler because the interaction not only conserves spin at each vertex but is also spin independent.*

Whether we compute $\mathcal{G}(1-2)$ or a susceptibility $\chi(1-2)$, when we go to momentum space, it is as if we were injecting a momentum (frequency) in the diagram. It is convenient to work completely in momentum space by starting from the above position space expressions, and their diagrammatic equivalent, and now write every $\mathcal{G}(1-2)$ and $V(1-2)$ entering the internal lines of a diagram also in terms of their Fourier-Matsubara transforms, namely

$$\mathcal{G}_\sigma(1-2) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-ik_n(\tau_1-\tau_2)} \mathcal{G}_\sigma(k) \quad (37.17)$$

$$V_{\sigma,\sigma'}(1-2) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(q) \quad (37.18)$$

or in the discrete version of momentum

$$\mathcal{G}_\sigma(1-2) = \frac{1}{V}\sum_{\mathbf{k}} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-ik_n(\tau_1-\tau_2)} \mathcal{G}_\sigma(k) \tag{37.19}$$

$$V_{\sigma,\sigma'}(1-2) = \frac{1}{V}\sum_{\mathbf{q}} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(q) \tag{37.20}$$

I hope the change of notation does not confuse you. I have taken out the spin index explicitly, so that now, $1 = (\mathbf{x}_1, \tau_1)$.

Then, consider an internal vertex, as illustrated in Fig.(37-5), where one has

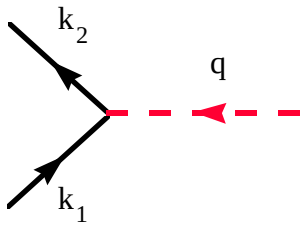


Figure 37-5 A typical interaction vertex and momentum conservation at the vertex.

to do the integral over the space-time position of the vertex, say 2 (in addition to the spin sum). Leaving aside the spin coordinates, that behave just as in position space, the integral to perform is

$$\int d\mathbf{x}_2 \int_0^\beta d\tau_2 e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_2} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_2} \tag{37.21}$$

$$= (2\pi)^3 \delta(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q}) \beta\delta_{(k_{2,n}-k_{1,n}),q_n} \tag{37.22}$$

$$= V\delta_{\mathbf{k}_1-\mathbf{k}_2,\mathbf{q}}\beta\delta_{(k_{2,n}-k_{1,n}),q_n} \tag{37.23}$$

$\delta_{\mathbf{k}_1-\mathbf{k}_2,\mathbf{q}}\delta_{(k_{2,n}-k_{1,n}),q_n}$ are Kronecker delta functions. The last line is for the discrete version of momentum. Note that the sum of two fermionic Matsubara frequencies is a bosonic Matsubara frequency since the sum of two odd numbers is necessarily even. This means that the integral over τ_1' is equal to β if $k_{1,n} - k_{2,n} + q_n = 0$ while it is equal to zero otherwise because $\exp(i(k_{1,n} - k_{2,n} + q_n)\tau_1')$is periodic in the interval 0 to β. The conclusion of this is that momentum and Matsubara frequencies are conserved at each interaction vertex. In other words, we obtain the following rule:

- *The sum of all wave vectors entering an interaction vertex vanishes. And similarly for Matsubara frequencies.*

This means that a lot of the momentum integrals and Matsubara frequency sums that occur in the replacements Eqs.(38.31) and (38.32) can be done by simply using conservation of momentum and of Matsubara frequencies at each vertex. We are left with the following rules:

- *One must integrate over the momenta and sum over Matsubara frequencies that are not determined by momentum conservation.* In general, there are as many integrals to perform as there are closed loops in a diagram.
- *We must also sum over spins that appear in internal indices, conserving spin at each interaction vertex when the interaction has this property.* The propagator $\mathcal{G}_\sigma$will then be diagonal in spin index.

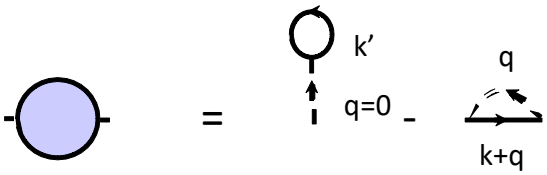


Figure 37-6 Diagram for the self-energy in momentum space in the Hartree-Fock approximation. There is an integral over all momenta and spins not determined by spin and momentum conservation.

Suppose we have $\mathcal{G}_\sigma(1-2)$ in terms of products of various $\mathcal{G}_\sigma$ and interactions. We want to write the corresponding expression in momentum space. This means that we take the Fourier-Matsubara transform of $\mathcal{G}_\sigma(1-2)$ to obtain $\mathcal{G}_\sigma(k)$. As mentioned above, a momentum k must flow in and out.

Example 31 *Writing*

$$k = (\mathbf{k}, ik_n), \tag{37.24}$$

the Hartree-Fock approximation for the self-energy Eq.(37.1) is

$$\Sigma(k) = -\frac{1}{\mathrm{V}}\sum_{\mathbf{q}} T\sum_{n=-\infty}^{\infty} V(q)\,\mathcal{G}(k+q)\,e^{-ik_n 0^-} + V(q=0)\,\frac{1}{\mathrm{V}}\sum_{\mathbf{k}} T\sum_{n=-\infty}^{\infty} e^{-ik_n 0^-}\mathcal{G}(k). \tag{37.25}$$

The sign of the wave vector q, or direction of the arrow in the diagram, must be decided once for each diagram but this choice is arbitrary since the potential is invariant under the interchange of coordinates, as mentioned above. This is illustrated in Fig. 37-6Note that here the $q=0$ contribution in the Hartree (so-called tadpole diagram) is cancelled by the positive ion background since $\mathcal{G}\left(\overline{2}, \overline{2^+}\right)$ is just the electron density, which is the same as the ion density. You can convince yourself that $\mathcal{G}\left(\overline{2}, \overline{2^+}\right) = \frac{1}{\mathrm{V}}\sum_{\mathbf{k}} T\sum_{n=-\infty}^{\infty} e^{ik_n 0^+}\mathcal{G}(k)$.

Example 32 *For the four-point function, there are four outside coordinates so we would need three independent outside momenta. However, all that we will need, as we shall see, are the density-density fluctuations. In other words, as we can see from the general expression for the self-energy in Fig. 36-2, we can identify two of the space-time points at the bottom of the graph. We have already written the expression in coordinates in Eq.(37.11). Writing the diagrams for that expression and using our rules for momentum conservation with a four-momentum q flowing top down, the four-point function in Fig. 37-4 becomes as illustrated in Fig. 37-7. You can skip the next chapter if you are satisfied with the functional derivative (source, or Schwinger) approach.*

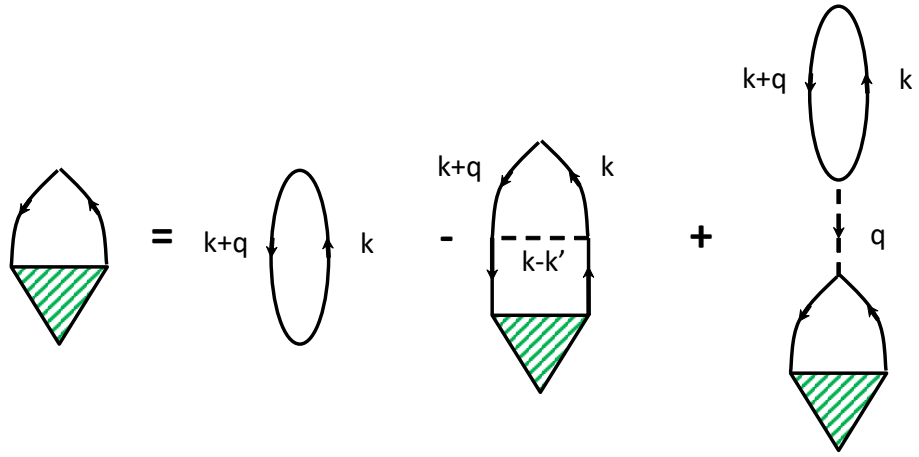


Figure 37-7 Diagrams for $\delta\mathcal{G}/\delta\phi$, which is minus the density-density correlation function. We imagine a momentum q flowing from the top of the diagram and conserve momentum at every vertex.

38. *FEYNMAN RULES FOR TWO-BODY INTERACTIONS

We have already encountered Feynman diagrams in the discussion of the impurity problem in the one-particle context. As we will see, perturbation theory is obtained simply by using Wick's theorem. This generates an infinite set of terms. Diagrams are a simple way to represent and remember the various terms that are generated. Furthermore, associating specific algebraic quantities and integration rules with the various pieces of the diagrams, allows one to write the explicit expression for a given term without returning to Wick's theorem. In case of doubt though, Wick's theorem is what should be used. The specific rules will depend on the type of interaction considered. This is described in a number of books [141],[73].

38.1 Hamiltonian and notation

The Hamiltonian we consider is the following. Note that we now introduce spin indices denoted by Greek indices:

$$\begin{aligned} K &= H-\mu N=H_0+V+V_n-\mu N \\ H_0 &= \frac{1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \boldsymbol{\nabla}\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\cdot\boldsymbol{\nabla}\psi_{\sigma_1}(\mathbf{x}_1) \qquad (38.1) \\ V &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\psi^{\dagger}_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1) \\ V_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^{\dagger}_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n \qquad (38.2) \end{aligned}$$

The last piece, V_n represents the interaction between a "neutralizing background" of the same uniform density n as the electrons. The potential is the Coulomb potential

$$v(\mathbf{x}_1-\mathbf{x}_2)=\frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|}. \qquad (38.3)$$

Let us say we want to compute the one-body Green's function in the interaction representation

$$\begin{aligned} \mathcal{G}_{\sigma_1\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) &= -\frac{Tr\left[e^{-\beta K_0}T_\tau\left(U_I(\beta,\tau_1)\psi_{I\sigma_1}(\mathbf{x}_1,\tau_1)U_I(\tau_1,\tau_2)\psi^{\dagger}_{I\sigma_2}(\mathbf{x}_2,\tau_2)U_I(\tau_2,0)\right)\right]}{Tr\left[e^{-\beta K_0}U_I(\beta,0)\right]} \\ &= -\frac{Tr\left[e^{-\beta K_0}T_\tau\left(U_I(\beta,0)\psi_{I\sigma_1}(\mathbf{x}_1,\tau_1)\psi^{\dagger}_{I\sigma_2}(\mathbf{x}_2,\tau_2)\right)\right]}{Tr\left[e^{-\beta K_0}U_I(\beta,0)\right]} \qquad (38.4) \end{aligned}$$

We do not write explicitly the interaction with the neutralizing background since it will be obvious later when it comes in. Then, the evolution operator is

$$U_I(\beta,0)=T_\tau\left[\exp\left(-\int_0^\beta d\tau_1 V_I(\tau_1)\right)\right]$$

Note that by definition of the interaction representation,

$$V_I(\tau_1) = e^{K_0\tau_1}\left[\frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\,\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1)\right]e^{-K_0\tau_1} \tag{38.5}$$

Inserting everywhere the identity operator $e^{-K_0\tau_1}e^{K_0\tau_1}$ this can be made to have a more symmetrical form

$$\begin{aligned} U_I(\beta,0) &= T_\tau\left[\exp\left(-\frac{1}{2}\sum_{\sigma_1,\sigma_2}\int_0^\beta d\tau_1\int d\mathbf{x}_1\int d\mathbf{x}_2 \quad\times\right.\right. \\ &\left.\left. v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^\dagger_{I\sigma_1}(\mathbf{x}_1,\tau_1)\,\psi^\dagger_{I\sigma_2}(\mathbf{x}_2,\tau_1)\,\psi_{I\sigma_2}(\mathbf{x}_2,\tau_1)\,\psi_{I\sigma_1}(\mathbf{x}_1,\tau_1)\right)\right] \end{aligned} \tag{38.6}$$

This can be made even more symmetrical by defining the potential,

$$\boxed{V_{\sigma_1,\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \tfrac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\delta(\tau_1-\tau_2)} \tag{38.7}$$

The right-hand side is independent of spin. In addition to being more symmetrical, this definition has the advantage that we can introduce the short-hand notation

$$V(1,2) \tag{38.8}$$

where

$$(1) = (\mathbf{x}_1,\tau_1;\sigma_1) \tag{38.9}$$

The evolution operator now systematically involves integrals over time space and a sum over spin indices, so it is possible to further simplify the notation by introducing

$$\int_1 = \int_0^\beta d\tau_1\int d\mathbf{x}_1\sum_{\sigma_1=\pm1} \tag{38.10}$$

and

$$\psi(1) = \psi_{I\sigma_1}(\mathbf{x}_1,\tau_1) \tag{38.11}$$

Note that we have taken this opportunity to remove subscript I on field operators. It should be clear that we are talking about the interaction representation all the time when we derive Feynman's rules.

With all these simplifications in notation, the above expressions for the Green's function Eq.(38.4) and the time evolution operator Eq.(38.6) take the simpler looking form

$$\boxed{\mathcal{G}(1,2) = -\frac{Tr\left[e^{-\beta K_0}T_\tau\left(U(\beta,0)\psi(1)\psi^\dagger(2)\right)\right]}{Tr\left[e^{-\beta K_0}U(\beta,0)\right]}} \tag{38.12}$$

$$\boxed{U(\beta,0) = T_\tau\left[\exp\left(-\tfrac{1}{2}\textstyle\int_1\int_2 V(1,2)\,\psi^\dagger(1)\,\psi^\dagger(2)\,\psi(2)\,\psi(1)\right)\right]} \tag{38.13}$$

38.2 *In position space

We now proceed to derive Feynman's rules in position space. Multiplying numerator and denominator of the starting expression for the Green's function by $1/Tr\left[e^{-\beta K_0}\right]$ we can use the linked cluster theorem in Subsection (33.2.1) to argue that we can forget about the power series expansion of the evolution operator in

the denominator, as long as in the numerator of the starting expression Eq.(38.12) only connected terms are kept. The perturbation expansion for the Green's function thus takes the form

$$\mathcal{G}(1,2) = -\left\langle T_\tau \left(U(\beta,0)\,\psi(1)\,\psi^\dagger(2) \right) \right\rangle_{0,c} \tag{38.14}$$

The average is over the unperturbed density matrix and only connected terms are kept. A typical term of the power series expansion thus has the form

$$-\frac{1}{n!}\left\langle T_\tau \left[\left(-\frac{1}{2}\int_{1'}\int_{2'} V(1',2')\,\psi^\dagger(1')\,\psi^\dagger(2')\,\psi(2')\,\psi(1') \right)^n \psi(1)\,\psi^\dagger(2) \right] \right\rangle_{0,c} \tag{38.15}$$

To evaluate averages of this sort, it suffices to apply Wick's theorem. Since this process becomes tedious and repetitive, it is advisable to do it once in such a way that simple systematic rules can be extracted that will allow us to write from the outset the simplest expression for a term of any given order. The trick is to write down diagrams and rules both to build them and to associate with them algebraic expressions. These are the Feynman rules.

Wick's theorem tells us that a typical average such as Eq.(38.15) is decomposed into a sum of products of single particle Green's function. Let us represent a Green's function by a straight line, as in Fig.(38-1). Following the convention of Ref. [6] the arrow goes from the left most to the right most label of the corresponding Green's function. Going from the creation to the annihilation operator might have been more natural and would have lead us to the opposite direction of the arrow, as for example in Ref. [7]. Nevertheless it is clear that it suffices to stick to one convention. In any case, contrary to older diagrammatic perturbation techniques, with Feynman diagrams the arrow represents the propagation of either and electron or a hole and the direction is irrelevant. The other building block for diagrams is the interaction potential which is represented by a dotted line. To either end of the dotted line, we have a Green's function that leaves and one that comes in, corresponding to the fact that there is one ψ and one $\psi^\dagger$ attached to any given end of a dotted line. The arrow heads in Fig.(38-1) just reminds us of this. They are not really part of the dotted line. Also, it does not matter whether the arrows come in from the top or from the bottom, or from left or right. It is only important that each end of the dotted line is attached to one incoming and one outgoing line.

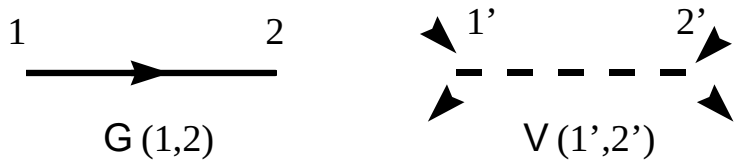


Figure 38-1 Basic building blocks of Feynman diagrams for the electron gas.

Let us give an example of how we can associate contractions and diagrams. For a term with $n = 1$, a typical term would be

$$-\left\langle T_\tau \left[-\frac{1}{2}\int_{1'}\int_{2'} V(1',2')\,\underset{1}{\psi^\dagger}(1')\,\underset{2}{\psi^\dagger}(2')\,\underset{3}{\psi}(2')\,\underset{2}{\psi}(1')\,\underset{1}{\psi}(1)\,\underset{3}{\psi^\dagger}(2) \right] \right\rangle_{0,c} \tag{38.16}$$

We have marked by a the same number every operator that belongs to the same contraction. The corresponding algebraic expression is

$$-\frac{1}{2}\int_{1'}\int_{2'} V(1',2')\,\mathcal{G}(1,1')\,\mathcal{G}(1',2')\,\mathcal{G}(2',2) \tag{38.17}$$

and we can represent it by a diagram, as in Fig.(38-2) Clearly, exactly the same

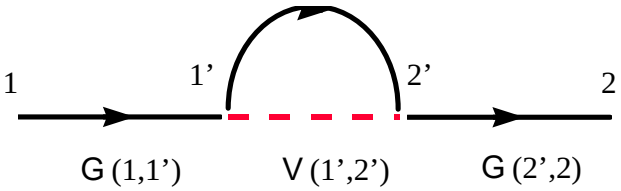


Figure 38-2 A typical contraction for the first-order expansion of the Green's function. THe Fock term.

contribution is obtained if the roles of the fields at the points $1'$ and $2'$ above are interchanged. More specifically, the set of contractions

$$-\left\langle T_\tau\left[-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\underset{2}{\psi^\dagger}\left(1'\right)\underset{1}{\psi^\dagger}\left(2'\right)\underset{2}{\psi}\left(2'\right)\underset{3}{\psi}\left(1'\right)\underset{1}{\psi}\left(1\right)\underset{3}{\psi^\dagger}\left(2\right)\right]\right\rangle_{0,c} \tag{38.18}$$

gives the algebraic expression

$$-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\mathcal{G}\left(2',1'\right)\mathcal{G}\left(1,2'\right)\mathcal{G}\left(1',2\right) \tag{38.19}$$

which, by a change of dummy integration variable, $1' \leftrightarrow 2'$ gives precisely the same contribution as the previous term.

We need to start to be more systematic and do some serious bookkeeping. Let us draw a diagram for each and every one of the possible contractions of this first order term. This is illustrated in Fig.(38-3). A creation operator is attached to point 2 while a destruction operator is attached to point 1. At either end of the interaction line, say at point $1'$, is attached one creation and one annihilation operators. We must link every destruction operator with a creation operator in all possible ways, as illustrated in the figure. The diagrams marked A and B are disconnected diagrams, so they do not contribute. On the other hand, by changing dummy integration variables, it is clear that diagrams C and D are equal to each other, as diagrams E and F are. The algebraic expressions for diagrams E and F are those given above, in Eqs.(38.17)(38.19). In other words, if we had given the rule that only connected and topologically distinct diagrams contribute and that there is no factor of $1/2$, we would have written down only diagram C and diagram E and obtained correctly all the first order contributions. Two diagrams are topologically distinct if they cannot be transformed one into the other by "elastic" changes that do not cut Green's functions lines.

For a general diagram of order n in the interaction, there are n interaction lines and $2n+1$ Green's functions. To prove the last statement, it suffices to notice that the four fermion fields attached to each interaction line correspond to four "half lines" and that the creation and annihilation operators corresponding to the "external" points 1 and 2 that are not integrated over yield one additional line. Consider two connected diagram of order three say, as in Fig.(38-4). The two diagrams there are clearly topologically equivalent, and they also correspond precisely to the same algebraic expression as we can see by doing the change of dummy integration variables $3' \leftrightarrow 5'$ and $4' \leftrightarrow 6'$. In fact, for any given topology, we can find $3! \times 2^3$ contractions that lead to diagrams with the same topology. The 3! corresponds to the number of ways of choosing the interaction lines to which four fermion lines attach, and the 2^3 corresponds to the fact that for every line there are two ends that one can interchange. For a diagram of order n, there are thus $2^n n!$ contractions that all have the same topology and that cancel the

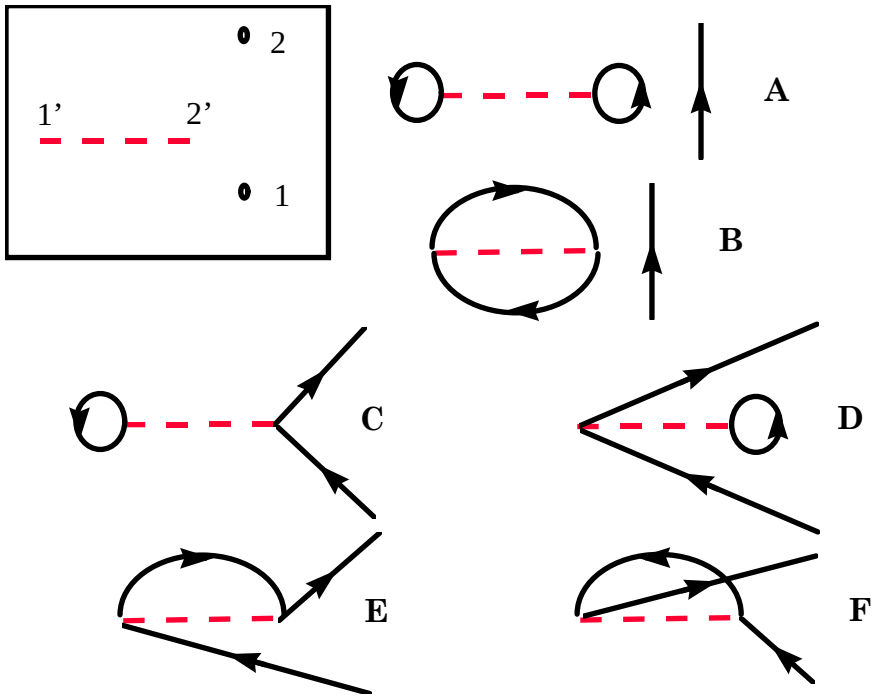


Figure 38-3 All possible contractions for the first-order contribution to the Green's function. A line must start at point 1 illustrated in the box on the left, and one line must end at 2. Lines must also come in and go out on either side of the dotted line.

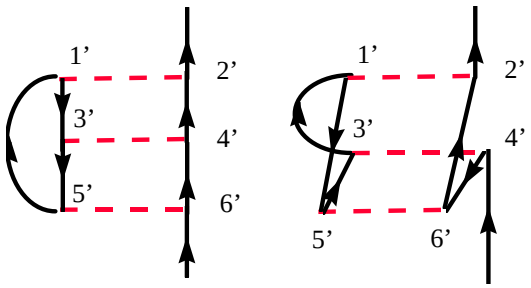


Figure 38-4 Two topologically equaivalent diagrams of order 3.

$1/\left(2^n n!\right)$ coming from the expansion of the exponential and the $1/2$ in front of each interaction $V\left(1',2'\right)$.

From what precedes then, it is clear that we can find all contributions for $\mathcal{G}\left(1,2\right)$ to order n by the following procedure that gives rules for drawing diagrams and for associating an algebraic expression to them.

1. Draw two "external" points, labeled 1 and 2 and n dotted lines with two ends (vertices). Join all external points and vertices with lines, so that each internal vertex has a line that comes in and a line that comes out while one line comes in external point 2 and one line comes out of point 1. The resulting diagrams must be *i)* Connected, *ii)* Topologically distinct (cannot be deformed one into the other).

2. Label all the vertices of interaction lines with dummy variables representing space, imaginary time and spin.

3. Associate a factor $\mathcal{G}\left(1,2\right)$ to every line going from a vertex or external point labeled 1 to a vertex or external point labeled 2.

4. Associate a factor $V\left(1',2'\right)$ to every dotted line between a vertex labeled $1'$ and a vertex labeled $2'$.

5. Integrate on all internal space, imaginary time and spin indices associated with interaction vertices. Notice that spin is conserved at each interaction vertex, as we can explicitly see from the original form of the interaction potential appearing in, say, Eq.(38.6). (And now the last two rules that we have not proven yet)

6. Associate a factor $\left(-1\right)^n\left(-1\right)^F$ to every diagram. The parameter n is the order of the diagram while F is the number of closed fermion loops.

7. Associate to every fermion line joining two of the vertices of the *same* interaction line (Fig.(38-5)) the factor

$$\mathcal{G}\left(1,2^+\right)\equiv\lim_{\eta\to 0}\mathcal{G}_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_1+\eta\right) \tag{38.20}$$

This last rule must be added because otherwise the rules given before are ambiguous since the Coulomb potential is instantaneous (at equal time) and Green's functions have two possible values at equal time. So it is necessary to specify which of these values it takes. The chosen order is discussed further in the following subsection.

Figure 38-5 Pieces of diagrams for which lead to equal-time Green's functions and for which it is necessary to specify how the $\tau\to 0$ limit is taken.

38.2.1 *Proof of the overall sign of a Feynman diagram

To prove the rule concerning the overall sign of a Feynman diagram, consider the expression for a $n'th$ order contribution before the contractions. We leave out the

factors of V and other factors to concentrate on field operators, their permutations and the overall sign.

$$-(-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \ldots \int_{2n-1} \int_{2n} \psi^\dagger(1') \psi^\dagger(2') \psi(2') \psi(1') \ldots \right. \right. \quad (38.21)$$

$$\left. \left. \ldots \psi^\dagger(2n-1) \psi^\dagger(2n) \psi(2n) \psi(2n-1) \psi(1) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (38.22)$$

This expression can be rearranged as follows without change of sign by permuting one destruction operator across two fermions in each group of four fermion fields appearing in interactions

$$-(-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \ldots \int_{2n-1} \int_{2n} \left(\psi^\dagger\left(1'^+\right) \psi(1') \right) \left(\psi^\dagger\left(2'^+\right) \psi(2') \right) \ldots \right. \right.$$

$$\left. \left. \ldots \left(\psi^\dagger\left((2n-1)^+\right) \psi(2n-1) \right) \left(\psi^\dagger\left((2n)^+\right) \psi(2n) \right) \psi(1) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (38.23)$$

We have grouped operators with parenthesis to illustrate the appearance of density operators, and we have added plus signs as superscripts to remind ourselves of the original order when we have two fields at equal time. By the way, this already justifies the equal-time rule Eq.(38.20) mentioned above. To clear up the sign question, let us now do contractions, that we will identify as usual by numbers under each creation-annihilation operator pair. We just make contractions in series so that there is a continuous fermion line running from point 1 to point 2 without fermion loops. More specifically, consider the following contractions

$$-(-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \ldots \int_{2n-1} \int_{2n} \underset{2n}{\psi^\dagger}\left(1'^+\right) \underset{1}{\psi}(1') \underset{1}{\psi^\dagger}\left(2'^+\right) \underset{2}{\psi}(2') \ldots_{\dot{2}} . \right. \right. \quad (38.24)$$

$$\left. \left. \underset{2n-2}{\ldots} \underset{2n-2}{\psi}^\dagger \left((2n-1)^+\right) \underset{2n-1}{\psi}(2n-1) \underset{2n-1}{\psi}^\dagger \left((2n)^+\right) \underset{2n+1}{\psi}(2n) \underset{2n}{\psi}(1) \underset{2n+1}{\psi}^\dagger(2) \right] \right\rangle_{0,c}$$

Not taking into account the $-(-1)^n$ already in front of the average, the contractions labeled 1 to $2n-1$ give a contribution

$$(-1)^{2n-1} \mathcal{G}(1',2') \mathcal{G}(2'3') \ldots \mathcal{G}(2n-1,2n) \quad (38.25)$$

where the overall sign comes from the fact that the definition of $\mathcal{G}$ has the creation and annihilation operators in the same order as they appear in the above contractions, but an overall minus sign in the definition. For the contraction labeled $2n$ one must do an even number of permutations to bring the operators in the order $\psi(1)\psi^\dagger(1'^+)$ so one obtains a factor $-\mathcal{G}(1,1'^+)$. Similarly, accounting for the new position of $\psi^\dagger(1'^+)$, an even number of permutations is necessary to bring to operators in the order $\psi(2n)\psi^\dagger(2)$ so that an overall factor $-\mathcal{G}(2n,2)$ is generated. The overall sign is thus

$$-(-1)^n (-1)^{2n-1} (-1)^2 = (-1)^n \quad (38.26)$$

In the contractions we have just done there is no closed fermion loop, as illustrated in Fig.(38-6) for the special case where $2n=4$.

Now all we need to show is that whenever we interchange two fermion operators we both introduce a minus sign and either form or destroy a closed fermion loop. The first part of the statement is easy to see. Consider,

$$\left\langle T_\tau \left[\psi^\dagger(1') \left(\psi^\dagger \psi \psi \ldots \psi \right) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (38.27)$$

Suppose we want to compare two sets of contractions that differ only by the fact that two creation operators (or two annihilation operators) interchange their respective role. In the time-ordered product above, bringing $\psi^\dagger(1')$ to the left of

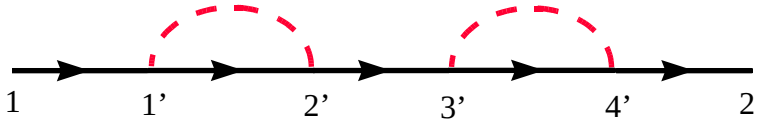


Figure 38-6 Example of a contraction without closed fermion loop.

$\psi^\dagger(2)$ produces a sign $(-1)^p$ where p is the number of necessary permutations. Then, when we take $\psi^\dagger(2)$ where $\psi^\dagger(1')$ was, we create an additional factor of $(-1)^{p+1}$ because $\psi^\dagger(2)$ has to be permuted not only with the operators that were originally there but also with $\psi^\dagger(1')$ that has been brought to its left. The overall sign is thus $(-1)^{2p+1} = -1$, which is independent of the number of operators originally separating the fields. That result was clear from the beginning given that what determines the sign of a permuation is the parity of the number of transpositions (interchange of two objects) necessary to obtain the given permutation. Hence, interchanging *any* pair of fermions gives an extra minus sign. Clearly there would have been something wrong with the formalism if we had not obtained this result.

Diagrammatically, if we start from the situation in Fig.(38-6) and interchange the role of two creation operators, as in Fig.(38-7), then we go from a situation with no fermion loops to one with one fermion loop. Fig.(38-8) illustrates the case where we interchange another pair of creation operators and clearly there also a fermion loop is introduced. In other words, by interchanging two creation operators (or two annihilation operators) we break the single fermion line, and the only way to do this is by creating a loop since internal lines cannot end at an interaction vertex. This completes the proof concerning the overall sign of a diagram.

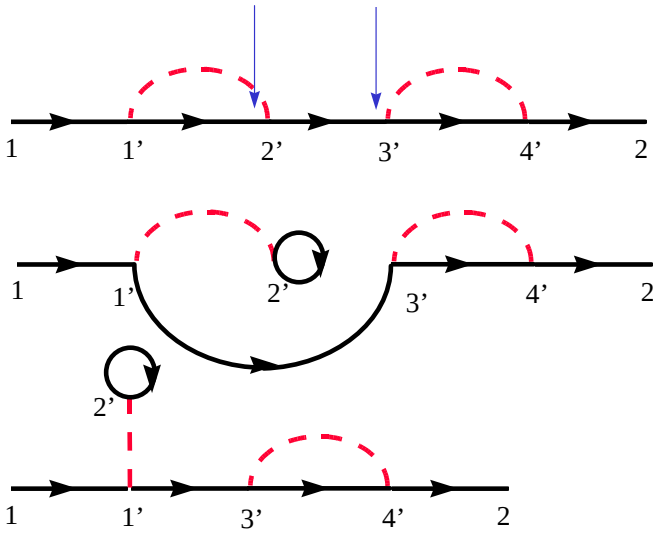


Figure 38-7 Creation of loops in diagrams by interchange of operators: The role of the two creation operators indicated by ligth arrows is interchanged, leading from a diagram with no loop, as on top, to a diagram with one loop. The diagram on the bottom is the same as the one in the middle. It is simply redrawn for clarity.

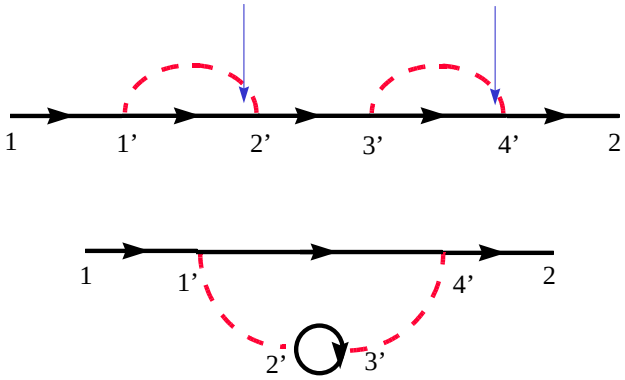


Figure 38-8 Interchange of two fermion operators creating a fermion loop.

Spin sums

A remark is in order concerning spin. In a diagram without loops, as in Fig.(38-6), there is a single spin label running from one end of the diagram to the other. Every time we introduce a loop, there is now a sum over the spin of the fermion in the loop. In the special case where $V(1,2)$ is independent of the spins at the vertices 1 and 2, as is the case for Coulomb interactions, then it is possible to simply disregard spin and add the rule that there is a factor of 2 associated with every fermion loop.

38.3 In momentum space

Starting from our results for Feynman's rule in position space, we can derive the rules in momentum space.[10] First introduce, for a translationally and spin rotationally invariant system, the definition

$$\mathcal{G}_\sigma(k) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2)\, e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{ik_n(\tau_1-\tau_2)} \mathcal{G}_\sigma(1-2) \quad (38.28)$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. For clarity then, we have explicitly written a single spin label. For the potential we define

$$V_{\sigma,\sigma'}(q) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2)\, e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(1-2) \quad (38.29)$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_n = 2n\pi T \quad (38.30)$$

with n and integer. Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}(1-2)$ is independent of spin. The spin σ is the same as the spin of the two propagators attaching to the vertex 1 while σ' is the same as the spin of the two propagators attaching to the vertex 2.

Remark 263 *General spin-dependent interaction: In more general theories, there are four spin labels attached to interaction vertices. These labels correspond to*

those of the four fermion fields. Here the situation is simpler because the interaction not only conserves spin at each vertex but is also spin independent.

To find the Feynman rules in momentum space, we start from the above position space diagrams and we now write $\mathcal{G}(1-2)$ and $V(1-2)$ in terms of their Fourier-Matsubara transforms, namely

$$\mathcal{G}_\sigma(1-2) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-ik_n(\tau_1-\tau_2)} \mathcal{G}_\sigma(k) \tag{38.31}$$

$$V_{\sigma,\sigma'}(1-2) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(q) \tag{38.32}$$

Then we consider an internal vertex, as illustrated in Fig.(38-9), where one has to

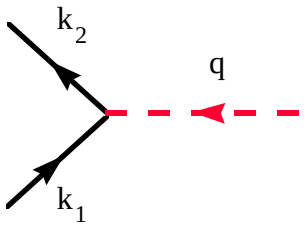


Figure 38-9 A typical interaction vertex and momentum conservation at the vertex.

do the integral over the space-time position of the vertex, $1'$. Note that because $V(1-2) = V(2-1)$, we are free to choose the direction of $\mathbf{q}$ on the dotted line at will. Leaving aside the spin coordinates, that behave just as in position space, the integral to perform is

$$\int d\mathbf{x}_1' \int_0^\beta d\tau_1' e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_1'} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_1'} \tag{38.33}$$

$$= (2\pi)^3 \delta(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q}) \beta \delta_{(k_{1,n}-k_{2,n}),q_n} \tag{38.34}$$

The last delta is a Kronecker delta. Indeed, the sum of two fermionic Matsubara frequencies is a bosonic Matsubara frequency since the sum of two odd numbers is necessarily even. This means that the integral over τ_1' is equal to β if $k_{1,n}-k_{2,n}+q_n = 0$ while it is equal to zero otherwise because $\exp(i(k_{1,n}-k_{2,n}+q_n)\tau_1')$is periodic in the interval 0 to β. The conclusion of this is that momentum and Matsubara frequencies are conserved at each interaction vertex. In other words, the sum of all wave vectors entering an interaction vertex vanishes. And similarly for Matsubara frequencies. This means that a lot of the momentum integrals and Matsubara frequency sums that occur in the replacements Eqs.(38.31) and (38.32) can be done by simply using conservation of momentum and of Matsubara frequencies at each vertex.

The Feynman rules for the perturbation expansion of the Green's function in momentum space thus read as follows.

1. For a term of order n, draw all connected, topologically distinct diagrams with n interaction lines and $2n+1$ oriented propagator lines, taking into account that at every interaction vertex one line comes in and one line comes out.

2. Assign a direction to the interaction lines. Assign also a wave number and a discrete frequency to each propagator and interaction line, conserving momentum and Matsubara frequency at each vertex.

3. To each propagator line, assign

$$\boxed{\mathcal{G}_\sigma^0(k) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)}} \tag{38.35}$$

(We have to remember that the propagator is independent of spin but still carries a spin label that is summed over.)

4. To each interaction line, associate a factor $V_{\sigma,\sigma'}(q)$, with iq_n a bosonic Matsubara frequency. Note that each of the spin labels is associated with one of the vertices and that it is the same as the spin of the fermion lines attached to it.

5. Perform an integral over wave vector and a sum over Matsubara frequency, namely $\int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty}$ for each momentum and frequency that is not fixed by conservation at the vertex.

6. Sum over all spin indices that are not fixed by conservation of spin.

7. Associate a factor $(-1)^n (-1)^F$ where F is the number of closed Fermion loops to every diagram of order n.

8. For Green's functions whose two ends are on the same interaction line, as in Fig.(38-5), associate a convergence factor $e^{ik_n\eta}$ before doing the sum over Matsubara frequency k_n. (This corresponds to the choice $\mathcal{G}(1, 2^+)$ in the position-space rules above).

The remark done at the end of the previous section concerning spin sums also applies here.

38.4 *Feynman rules for the irreducible self-energy

As in the one-body case that we studied in a preceding chapter, straight perturbation theory for the Green's function is meaningless because

- It involves powers of $\mathcal{G}_\sigma^0(k)$ and hence the analytically continued function has high order poles at the same location as the unperturbed system whereas the Lehmann representation tells us that the interacting Green's function has simple poles.
- High order poles can lead to negative spectral weight.[9] For example, the first order contribution to the spectral weight $A(k) = -2\,\mathrm{Im}\,G^R$ would be given by a term proportional to

$$\begin{aligned} -2\,\mathrm{Im}\left(\frac{1}{(\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu))^2}\right) &= 2\,\mathrm{Im}\,\frac{\partial}{\partial\omega}\left(\frac{1}{\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu)}\right) \\ &= -2\pi\frac{\partial}{\partial\omega}\delta(\omega - (\varepsilon_{\mathbf{k}} - \mu)) \end{aligned} \tag{38.36}$$

The derivative of the delta function can be infinitely positive or negative.

As before, the way out of this difficulty is to resum infinite subsets of diagrams and to rewrite the power series as

$$\boxed{\mathcal{G}_\sigma(k) = \mathcal{G}_\sigma^0(k) + \mathcal{G}_\sigma^0(k)\,\Sigma_\sigma(k)\,\mathcal{G}_\sigma(k)} \tag{38.37}$$

or

$$\mathcal{G}_\sigma(k) = \frac{1}{\left(\mathcal{G}^0_\sigma(k)\right)^{-1} - \Sigma_\sigma(k)} \tag{38.38}$$

This is the so-called Dyson equation. The iterative solution of this equation

$$\mathcal{G}_\sigma(k) = \mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\,\Sigma_\sigma(k)\,\mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\,\Sigma_\sigma(k)\,\mathcal{G}^0_\sigma(k)\,\Sigma_\sigma(k)\,\mathcal{G}^0_\sigma(k) + \ldots$$

clearly shows that all diagrams that can be cut in two pieces by cutting one fermion line $\mathcal{G}^0_\sigma(k)$ will automatically be generated by Dyson's equation. In other words, we define the *one-particle irreducible self-energy* by the set of diagrams that are generated by Feynman's rules for the propagator but that, after truncating the two external fermion lines, cannot be cut in two disjoint pieces by cutting a $\mathcal{G}^0_\sigma(k)$ line. As an example, the diagram on the left of Fig.(38-10) is one-particle reducible and hence does not belong to the one-particle irreducible self-energy, but the two diagrams on the right of this figure do.

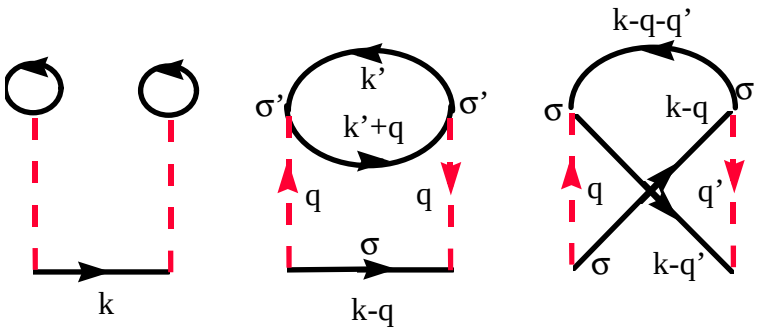


Figure 38-10 Diagram on the left is one-particle reducible, and hence is not an acceptable contribution to the self-energy. The two diagrams on the right however are acceptable contributions to the one-particle irreducible self-energy. In these diagrams, k is the external momentum and Matsubara frequency label while σ is the external spin label. There is a sum over the variables k', q and q' and over the spin σ'.

Remark 264 *Terminology: To be shorter, one sometimes refers to the one-particle irreducible self-energy using the term "proper self-energy". In almost everything that follows, we will be even more concise and refer simply to the self-energy. We will mean one-particle irreducible self-energy. The other definitions that one can give for the self-energy do not have much interest in practice.*

38.5 *Feynman diagrams and the Pauli exclusion principle

Since operators can be anticommuted at will in a time-ordered product at the price of a simple sign change, it is clear that whenever there are two destruction operators or two creation operators for the same state, the contraction should vanish. This is just the Pauli exclusion principle. On the other hand, if we look at a self-energy diagram like the middle one in Fig.(38-10) there are contributions that violate the Pauli exclusion principle. Indeed, suppose we return to imaginary

time but stay in momentum space. When we perform the sum over wave vectors and over spins in the closed loop, the right-going line with label $\mathbf{k}' + \mathbf{q}$ in the loop will eventually have a value of $\mathbf{k}'$ and of spin such that it represents the same state as the bottom fermion line. Indeed, when $\mathbf{k}' + \mathbf{q} = \mathbf{k} - \mathbf{q}$ and spins are also identical, we have two fermion lines in the same state attached to the same interaction line (and hence hitting it at the same time) with two identical creation operators. Similarly we have two identical destruction operators at the same time attached to the other interaction line. This means that this contribution should be absent if the Pauli exclusion principle is satisfied. What happens in diagrams is that this contribution is exactly canceled by the diagram where we have exchanged the two right-going lines, in other words the last diagram on this figure. Indeed, this diagram has opposite sign, since it has one less fermion loop, and the special case $\mathbf{q} = \mathbf{q}'$ precisely cancels the unwanted contribution from the middle graph in Fig.(38-10). That this should happen like this is no surprise if we return to our derivation of Wick's theorem. We considered separately the case where two fermions were in the same state and we noticed that if we applied Wick's theorem blindly, the Pauli violating terms would indeed add up to zero when we add up all terms.

The important lesson of this is that unless we include all the exchange graphs, there is no guarantee in diagrammatic techniques that the Pauli exclusion principle will be satisfied. We are tempted to say that this does not matter so much because it is a set of measure zero but in fact we will see practical cases in short-range models where certain approximate methods do unacceptable harm to the Pauli exclusion principle.

39. PARTICLE-HOLE EXCITATIONS IN THE NON-INTERACTING LIMIT AND THE LINDHARD FUNCTION

We will come back later to the calculation of the self-energy for the electron gas. It is preferable to look first at collective modes. Since single-particle excitations scatter off these collective modes, it is important to know those first. It is true that collective modes are also influenced by the actual properties of single-particles, but conservation laws, long-range forces and/or the presence of broken symmetries strongly influence the behavior of collective modes, while the details of single-particle excitations that lead to them are less relevant.

The main physical quantity we want to compute and understand for collective modes of the electron gas is the longitudinal dielectric constant. Indeed, we have seen in the chapter on correlation functions that inelastic electron scattering Eq.(13.16) measures

$$S_{\rho\rho}(\mathbf{q},\omega) = \frac{2}{1-e^{-\beta\omega}} \operatorname{Im}\left[\chi^R_{\rho\rho}(\mathbf{q},\omega)\right] = -\frac{2}{1-e^{-\beta\omega}} \frac{q^2}{4\pi} \operatorname{Im}\left[\frac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)}\right]. \quad (39.1)$$

The longitudinal dielectric constant itself obtained in Sec.(13.2) is

$$\boxed{\frac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)} = 1 - \frac{1}{\varepsilon_0 q^2}\chi^R_{\rho\rho}(\mathbf{q},\omega)}. \quad (39.2)$$

The physical phenomenon of screening will manifest itself in the zero-frequency limit of the longitudinal dielectric constant, $\varepsilon^L(\mathbf{q},0)$. Interactions between electrons will be screened, hence it is important to know the dielectric constant. Plasma oscillations should come out from the finite frequency zeros of this same function $\varepsilon^L(\mathbf{q},\omega) = 0$, as we expect from our general discussion of collective modes.

We will start this section by a discussion of the Lindhard function, namely $\chi^R_{nn}(\mathbf{q},\omega) = \chi^R_{\rho\rho}(\mathbf{q},\omega)/e^2$ for the free electron gas. We will interpret the poles of this function. Then we introduce interactions with a simple physical discussion of screening and plasma oscillations. A diagrammatic calculation in the so-called Random phase approximation (RPA) will then allow us to recover in the appropriate limiting cases the phenomena of screening and of plasma oscillations.

It is noteworthy that even for the non-interacting electron gas, the density-density correlation function is not simply the product of two independent densities. Fundamentally, this is because even in the absence of interactions, the Pauli exclusion principle prohibits two electrons of being in the same state. That leads to correlations, whose origin is due to quantum statistics. This is illustrated by Fig.(39-1) that shows that density excitation corresponds to the excitation of a particle-hole pair that is created and then destroyed in the same measurement process.

Remark 265 *The result $\chi^R_{nn}(\mathbf{q},\omega) = \chi^R_{\rho\rho}(\mathbf{q},\omega)/e^2$ holds only when electrons are the sole degrees of freedom. For example, assume that neutrons are scattering from neutral atoms through the nuclear force. They will see phonons that can be neutral and contribute to $\chi^R_{nn}(\mathbf{q},\omega)$ but not to $\chi^R_{\rho\rho}(\mathbf{q},\omega)$.*

39.1 Definitions and analytic continuation

We want the Fourier transform of the density-density response function. First note that

$$n_{\mathbf{q}} \equiv \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} n(\mathbf{r}) = \sum_{\sigma=\pm 1} \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \psi^{\dagger}_{\sigma}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \tag{39.3}$$

$$= \frac{1}{\left(\sqrt{\mathcal{V}}\right)^2} \sum_{\sigma} \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \mathbf{e}^{i\mathbf{k}'\cdot\mathbf{r}} \mathbf{e}^{-i\mathbf{k}\cdot\mathbf{r}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} \tag{39.4}$$

$$= \sum_{\sigma} \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma}. \tag{39.5}$$

As before, $\mathcal{V}$ is the quantization volume of the system. We can obtain the retarded density-density response function from

$$\boxed{\chi^R_{nn}(\mathbf{q},\omega) = \lim_{iq_n \to \omega + i\eta} \chi_{nn}(\mathbf{q}, iq_n)} \tag{39.6}$$

with iq_n a bosonic Matsubara frequency, as required by the periodic boundary condition obeyed by the Matsubara density response in imaginary time. The above two functions are defined by

$$\chi_{nn}(\mathbf{q}, iq_n) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_0^{\beta} d\tau e^{iq_n\tau} \langle T_{\tau} [\delta n(\mathbf{r},\tau) \delta n(\mathbf{r}',0)] \rangle \tag{39.7}$$

$$= \frac{1}{\mathcal{V}} \int_0^{\beta} e^{iq_n\tau} \quad \langle T_{\tau} [\delta n_{\mathbf{q}}(\tau) \delta n_{-\mathbf{q}}(0)] \rangle \quad d\tau \tag{39.8}$$

$$\chi^R_{nn}(\mathbf{q},\omega) = \frac{1}{\mathcal{V}} \int_{-\infty}^{\infty} e^{i\omega t} \quad i \langle [\delta n_{\mathbf{q}}(t), \delta n_{-\mathbf{q}}(0)] \rangle \theta(t) \quad dt \tag{39.9}$$

Analytic continuation for density response If you did not read Sec.(30.1) that addresses this problem, consider the following. To prove the analytic continuation formula for the density response Eq.(39.6), one can simply use the Lehmann representation or deform the integration contour in the Matsubara representation, as we did for propagators in Sec.(26.4). (See Eqs.(29.33) and (29.29) in particular). The fact that we have bosonic Matsubara frequencies means that we will have a commutator in real frequency instead of an anticommutator because this time $e^{iq_n\beta} = 1$ instead of -1. Furthermore, notice that whether the retarded density response is defined with $n(\mathbf{q},t)$ or with

$$\delta n(\mathbf{q},t) = n(\mathbf{q},t) - \langle n(\mathbf{q},t) \rangle = n(\mathbf{q},t) - n (2\pi)^3 \delta(\mathbf{q})$$

is irrelevant since a constant commutes with any operator.

Remark 266 *The charge response function is also called charge susceptibility.*

39.2 Density response in the non-interacting limit in terms of $\mathcal{G}^0_{\sigma}$

The density response can be expressed in terms of Green's function starting either from the Feynman or from the functional derivative approach. In this section we

arrive at the same result both ways.

39.2.1 *The Feynman way

If you have followed the route of Fenynann, to do the calculation in the non-interacting case, it suffices to use Wick's theorem.

$$\chi^0_{nn}(\mathbf{q},iq_n) = \frac{1}{\mathcal{V}}\int_0^\beta d\tau e^{iq_n\tau}\sum_\sigma\sum_{\mathbf{k}}\sum_{\sigma'}\sum_{\mathbf{k}'} \left[\left\langle T_\tau\left[\underset{1}{c^\dagger_{\mathbf{k},\sigma}}(\tau)\underbrace{\underset{2}{c_{\mathbf{k}+\mathbf{q},\sigma}}(\tau)\underset{2}{c^\dagger_{\mathbf{k}',\sigma'}}}\underset{1}{c_{\mathbf{k}'-\mathbf{q},\sigma'}}\right]\right\rangle_0 - \left\langle c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0\left\langle c^\dagger_{\mathbf{k}',\sigma'}c_{\mathbf{k}',\sigma'}\right\rangle_0\delta_{\mathbf{q},0}\right] \tag{39.10}$$

Only the contractions indicated survive. The other possible set of contractions is canceled by the disconnected piece $\left\langle c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0\left\langle c^\dagger_{\mathbf{k}',\sigma'}c_{\mathbf{k}',\sigma'}\right\rangle_0$. Using momentum conservation, all that is left is

$$\chi^0_{nn}(\mathbf{q},iq_n) = -\frac{1}{\mathcal{V}}\int_0^\beta d\tau e^{iq_n\tau}\sum_\sigma\sum_{\mathbf{k}}\mathcal{G}^0_\sigma(\mathbf{k}+\mathbf{q},\tau)\,\mathcal{G}^0_\sigma(\mathbf{k},-\tau) \tag{39.11}$$

Going to the Matsubara frequency representation for the Green's functions, and using again the Kronecker delta that will arise from the τ integration, we are left with something that looks like what could be obtained from the theorem for Fourier transform of convolutions

$$\chi^0_{nn}(\mathbf{q},iq_n) = -\frac{1}{\mathcal{V}}\sum_\sigma\sum_{\mathbf{k}}T\sum_{ik_n}\mathcal{G}^0_\sigma(\mathbf{k}+\mathbf{q},ik_n+iq_n)\,\mathcal{G}^0_\sigma(\mathbf{k},ik_n) \tag{39.12}$$

where as usual we will do the replacement in the infinite volume limit

$$\frac{1}{\mathcal{V}}\sum_{\mathbf{k}} \to \int\frac{d^3\mathbf{k}}{(2\pi)^3} \tag{39.13}$$

Remark 267 *Although we have not derived Feynman rules for χ_{nn} it is clear that the last expression could have been written down directly from the diagram in Fig.(39-1) if we had followed trivial generalizations of our old rules. There is even an overall minus sign for the closed loop and a sum over wave vectors, Matsubara frequency and spin inside the loop since these are not determined by momentum conservation. However, we needed to perform the contractions explicitly to see this. In particular, it was impossible to guess the overall sign and numerical factors since Feynman's rules that we have developed were for the Green's function, not for the susceptibility. Now that we have obtained the zeroth order term it is clear how to apply Feynman rules for the terms of the perturbation series. But this is the subject of another subsection below.*

39.2.2 The Schwinger way (source fields)

Start from the expression for the four-point function Eq.(36.22) for $\phi = 0$ and point $2 = 1^+$ and $3 = 2^+$, and $4 = 2$. Then we find

$$\frac{\delta\mathcal{G}(1,1^+)}{\delta\phi(2^+,2)} = -\left\langle T_\tau\psi^\dagger(1^+)\,\psi(1)\,\psi^\dagger(2^+)\,\psi(2)\right\rangle + \mathcal{G}(1,1^+)\,\mathcal{G}(2,2^+). \tag{39.14}$$

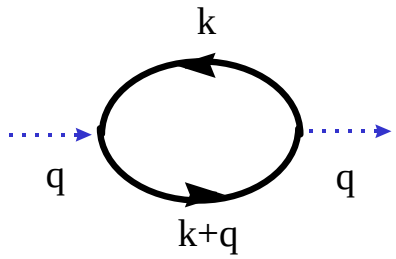


Figure 39-1 Diagram for non-interacting charge susceptibility. Note that the dotted lines just indicate the flow of momentum. No algebraic expression is associated with them.

If we sum over the spins associated with point 1 and the spins associated with point 2 and recall that once we sum over spins, we have $\mathcal{G}(1,1^+) = \mathcal{G}(2,2^+) = n$ where n is the average density, then

$$
\begin{aligned}
-\sum_{\sigma_1,\sigma_2} \frac{\delta \mathcal{G}(1,1^+)}{\delta\phi(2^+,2)} &= \sum_{\sigma_1,\sigma_2} \left\langle T_\tau \psi^\dagger(1^+)\psi(1)\psi^\dagger(2^+)\psi(2)\right\rangle - n^2 \quad (39.15)\\
&= \langle T_\tau n(1)\, n(2)\rangle - n^2 \quad (39.16)\\
&= \langle T_\tau (n(1)-n)(n(2)-n)\rangle \\
&= \chi_{nn}(1-2). \quad (39.17)
\end{aligned}
$$

The last expression is from the definition of the density-density correlation function in Eq.(39.7).

The non-interacting contribution is given by the first term in Fig. 37-7 (taking into account the minus sign above) or, if you want, from the first term in Eq.(37.11) for the functional derivative. It takes the form

$$
\chi_{nn}(1-2) = -\sum_\sigma \mathcal{G}^0_\sigma(1-2)\,\mathcal{G}^0_\sigma(2-1)\,. \quad (39.18)
$$

Only one spin sum is left because the spins corresponding the label 1 are identical in $\frac{\delta\mathcal{G}(1,1^+)}{\delta\phi(2^+,2)}$, as are the spin labels for label 2. Furthermore, spin is conserved, so the spin cannot flip in going from 1 to 2 in $\mathcal{G}^0_\sigma(1-2)$. Taking the Fourier transform and using the convolution theorem, one obtains,

$$
\chi^0_{nn}(\mathbf{q}, iq_n) = -\frac{1}{\mathcal{V}}\sum_\sigma \sum_{\mathbf{k}} T\sum_{ik_n} \mathcal{G}^0_\sigma(\mathbf{k}+\mathbf{q}, ik_n+iq_n)\,\mathcal{G}^0_\sigma(\mathbf{k}, ik_n)\,. \quad (39.19)
$$

One of the sums over spins has disappeared because we should think of $\mathcal{G}^0_\sigma$ as a matrix that is diagonal in spin indices. This is the so-called Lindhard function. It is also known as the bubble diagram .

Remark 268 *To obtain the above result from the first term in Fig. 37-7, note that it is as if we were injecting a momentum (Matsubara-frequency)* $\mathbf{q}$ *on one side of the diagram and using our rules for momentum conservation at each vertex.*

39.3 Density response in the non-interacting limit: Lindhard function

To compute

$$\chi^0_{nn}(\mathbf{q}, iq_n) = -\frac{1}{\mathcal{V}} \sum_\sigma \sum_{\mathbf{k}} T \sum_{ik_n} \mathcal{G}^0_\sigma (\mathbf{k}+\mathbf{q}, ik_n + iq_n)\, \mathcal{G}^0_\sigma (\mathbf{k}, ik_n) \tag{39.20}$$

the sums over Matsubara frequency should be performed first and they are easy to do. The technique is standard. First introduce the notation

$$\boxed{\zeta_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu} \tag{39.21}$$

and note that

$$T \sum_{ik_n} \mathcal{G}^0_\sigma (\mathbf{k}+\mathbf{q}, ik_n + iq_n)\, \mathcal{G}^0_\sigma (\mathbf{k}, ik_n) = T \sum_{ik_n} \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \frac{1}{ik_n - \zeta_{\mathbf{k}}}. \tag{39.22}$$

Substituting in the expression for the susceptibility and decomposing in partial fractions, we find.

$$\chi^0_{nn}(\mathbf{q}, iq_n) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \left[\frac{1}{ik_n - \zeta_{\mathbf{k}}} - \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \right] \frac{1}{iq_n - \zeta_{\mathbf{k}+\mathbf{q}} + \zeta_{\mathbf{k}}}. \tag{39.23}$$

The factor of two comes from the sum over spin σ. After the decomposition in partial fractions, it seems that now we need a convergence factor to do each sum individually. Using the general results of the preceding chapter for Matsubara sums, Eqs.(29.85) and (29.86), it is clear that as long as we take the same convergence factor for both terms, the result is

$$\chi^0_{nn}(\mathbf{q}, iq_n) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{iq_n + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \tag{39.24}$$

independently of the choice of convergence factor. Before the partial fractions, the terms in the ik_n series decreased like $(ik_n)^{-2}$ so, in fact, no convergence factor is needed.

The retarded function is easy to obtain by analytic continuation. It is the so-called Lindhard function

$$\boxed{\chi^{0R}_{nn}(\mathbf{q}, \omega) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}}} \tag{39.25}$$

This form is very close to the Lehmann representation for this response function. Clearly *at zero temperature* poles will be located at $\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}}$ as long as the states $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ are not on the same side of the Fermi surface. These poles are particle-hole excitations instead of single-particle excitations as in the case of the Green's function. The sign difference between $\zeta_{\mathbf{k}+\mathbf{q}}$ and $\zeta_{\mathbf{k}}$ comes from the fact that one of them plays the role of a particle while the other plays the role of a hole.

Remark 269 *Summing over ik_n first: Note that the iq_n in the denominator of $\frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}}$ did not influence the result for the sum over Matsubara frequencies ik_n because iq_n is bosonic, which means that $ik_n + iq_n$ is a fermionic frequency: an odd number plus an even number is an odd number and the sum is from minus to plus infinity. The sums over Matsubara freuencies must be performed first, before analytic continuation (unless the sums and integrals are uniformly convergent, and that is rare).*

Remark 270 *Diagrammatic form of particle-hole excitations: If we return to the diagram in Fig.(39-1), we should notice the following general feature. If we cut the diagram in two by a vertical line, we see that it is crossed by lines that go in opposite directions. Hence, we have a particle-hole excitation. In particle-particle or hole-hole excitations, the lines go in the same direction and the two single-particle energies* $\zeta_{\mathbf{k}+\mathbf{q}}$ *and* $\zeta_{\mathbf{k}}$ *add up instead of subtract.*

Remark 271 *Absorptive vs reactive part of the response, real vs virtual excitations: There is a contribution to the imaginary part, in other words absorption, if for a given* $\mathbf{k}$ *and* $\mathbf{q}$ *energy is conserved in the intermediate state, i.e. if the condition* $\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}}$ *is realized. If this condition is not realized, the corresponding contribution is reactive, not dissipative, and it goes to the real part of the response only. The intermediate state then is only virtual. To understand the type of excitations involved in the imaginary part, rewrite* $f(\zeta_{\mathbf{k}}) - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right) = \left(1 - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right) f(\zeta_{\mathbf{k}}) - (1 - f(\zeta_{\mathbf{k}})) f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)$. *We see that either* $\zeta_{\mathbf{k}}$ *can correspond to a hole and* $\zeta_{\mathbf{k}+\mathbf{q}}$ *to a particle or the other way around. In other words a single Green function line contains both the hole and the particle propagation, as we expect from its definition that allows either a creation operator or a destruction operator to act first.*

Remark 272 *When there are many Green's functions, partial fractions are always an option, but it can be much more efficient to use the Fermi function and contour integration as in Fig. (29-7) and to deform it around the poles using Cauchy's theorem.*

39.3.1 Zero-temperature value of the Lindhard function: the particle-hole continuum

To evaluate the integral appearing in the Lindhard function, which is what Lindhard did, it is easier to evaluate the imaginary part first and then to obtain the real part using Kramers-Kronig. Let us begin

$$\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) = 2\pi \int \frac{d^3\mathbf{k}}{(2\pi)^3}\left[f(\zeta_{\mathbf{k}}) - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\delta\left(\omega + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}\right) \tag{39.26}$$

With $\mathbf{k} \to \mathbf{k} - \mathbf{q}$ in the second term this becomes

$$\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) = 2\pi \int \frac{d^3\mathbf{k}}{(2\pi)^3} f(\zeta_{\mathbf{k}})\left[\delta\left(\omega + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}\right) - \delta\left(\omega + \zeta_{\mathbf{k}-\mathbf{q}} - \zeta_{\mathbf{k}}\right)\right].$$

Doing the replacement $f(\zeta_{\mathbf{k}}) = \theta(k_F - k)$, going to polar coordinates with $\mathbf{q}$ along the polar axis and doing the replacement $\varepsilon_{\mathbf{k}} = k^2/2m$, we have

$$\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) = \frac{1}{2\pi}\int_0^{k_F} k^2 dk \int_{-1}^{1} d(\cos\theta)\,\frac{m}{kq}\left[\delta\left(\frac{\omega - \varepsilon_{\mathbf{q}}}{kq/m} - \cos\theta\right) - \delta\left(\frac{\omega + \varepsilon_{\mathbf{q}}}{kq/m} - \cos\theta\right)\right]. \tag{39.27}$$

The angle θ is between $\mathbf{k}$ and $\mathbf{q}$. It is clear that this strategy in fact allows one to do the integrals in any spatial dimension. One finds, for an arbitrary ellipsoidal dispersion [13]

$$\varepsilon_{\mathbf{k}} = \sum_{i=1}^{d} \frac{k_i^2}{2m_i} \tag{39.28}$$

$$\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) = \frac{\prod_{i=1}^{d}\left(\sqrt{2m_i}\right)}{2^d \pi^{(d-1)/2}\Gamma\left(\frac{d+1}{2}\right)\sqrt{\varepsilon_{\mathbf{q}}}} \times \tag{39.29}$$

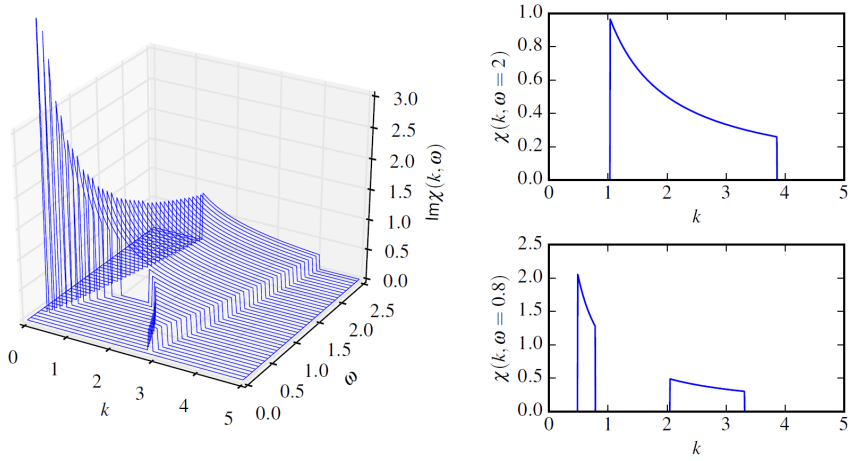


Figure 39-2 Imaginary part of the Lindhard function in $d = 1$ on the vertical axis. Frequency increases from left to right and wave vector from back to front.

$$\left\{\theta\left(\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}}-\theta\left(\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}}\right\}.$$

The real part is also calculable [13] but we do not quote it here.

The functional form of this function in low dimension is quite interesting. Figures (39-2)(39-3) and (39-4) show the imaginary part of the Lindhard function in, respectively, $d = 1, 2, 3$. The small plots on the right show a cut in wave vector at fixed frequency while the plots on the left show $\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$ on the vertical axis, frequency going from left to right and wave vector going from back to front. In all cases, at finite frequency it takes a finite wave vector $\mathbf{q}$ to have absorption. If the wave vector is too large however the delta function cannot be satisfied and there is no absorption either. The one-dimensional case is quite special since at low frequency there is absorption only in a narrow wave vector band. This has a profound influence on the interacting case since it will allow room for collective modes to propagate without absorption. In fact, in the interacting one-dimensional case the collective modes become eigenstates. This leads to the famous spin-charge separation [81]. In two dimensions, there is a peak at $q = 2k_F$ that becomes sharper and sharper as the frequency decreases as we can more clearly see from the small plot on the right.[13] By contrast, the three-dimensional function is smoother, despite a discontinuity in slope at $q = 2k_F$.

Definition 33 *The region in* $\mathbf{q}$ *and* ω *space where there is absorption is referred to as the particle-hole continuum.*

To understand the existence of the particle-hole continuum and its shape, it is preferable to return to the original expression Eq.(39.26). In Fig.(39-5) we draw the geometry for the *three-dimensional case*.[14] The two "spheres" represent the domain where each of the Fermi functions is non-vanishing. We have to integrate over the wave vector $\mathbf{k}$ while $\mathbf{q}$ is fixed. The energy conservation tells us that when $\zeta_{\mathbf{k}+\mathbf{q}} > 0$ and $\zeta_{\mathbf{k}} < 0$ then $\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}} > 0$ and all wave vectors $\mathbf{k}$ located in the plane

$$\omega - \frac{q^2}{2m} = \frac{kq}{m}\cos\theta \tag{39.30}$$

are allowed. This plane in $\mathbf{k}$ space with normal $\mathbf{q}$ must be inside the left-most sphere and outside the right-most one. It cannot however be inside both or outside

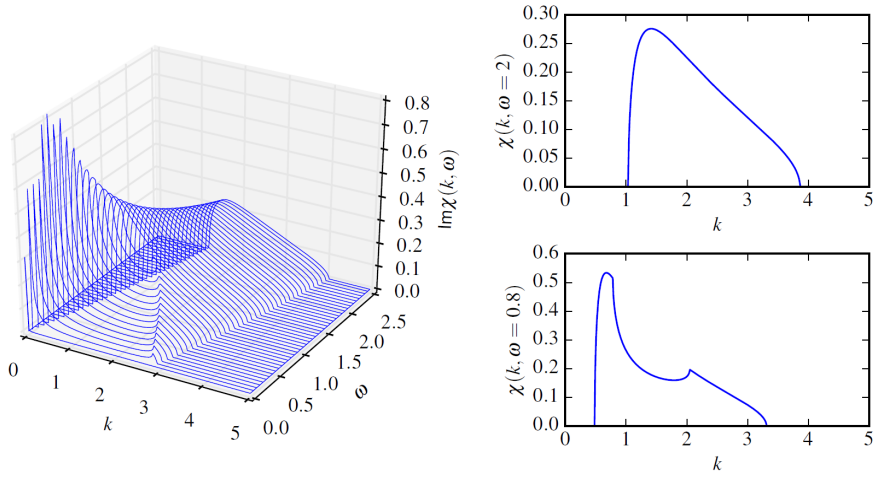


Figure 39-3 Imaginary part of the Lindhard function in $d = 2$. Axes like in the $d = 1$ case.

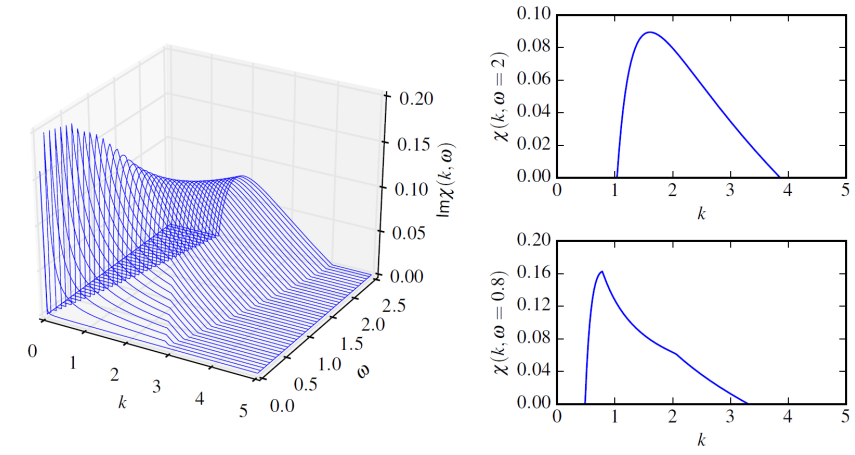


Figure 39-4 Imaginary part of the Lindhard function in $d = 3$. Axes like in the $d = 1$ case.

both. We study the case $\omega > 0$. The case $\omega < 0$ follows from the properties of the charge susceptibility under a change of sign of ω.

Consider first the case $q > 2k_F$. Take the two Fermi spheres, one where $\mathbf{k}$ on the left is occupied and $\mathbf{k}+\mathbf{q}$ on the right is not occupied. Since $q > 2k_F$, the two spheres do not overlap. Hence, there is a minimum value for ω, given by the case where $\mathbf{k}+\mathbf{q}$ and $\mathbf{k}$ are antiparallel and $\mathbf{k}$ is on the Fermi surface of the occupied Fermi sphere. We find then,

$$\omega_{\min} = \frac{(k_F - q)^2}{2m} - \frac{k_F^2}{2m} = \varepsilon_{\mathbf{q}} - v_F q; \quad q > 2k_F. \tag{39.31}$$

There is also a maximum value of ω, namely when $\mathbf{k}$ and $\mathbf{q}$ are parallel and $\mathbf{k}$ is on the Fermi surface of the occupied sphere. This gives,

$$\omega_{\max} = \frac{(k_F + q)^2}{2m} - \frac{k_F^2}{2m} \tag{39.32}$$

$$= \varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q > 2k_F. \tag{39.33}$$

When $q < 2k_F$, the two spheres overlap. There is still a maximum value, as illustrated in Fig. (39-5), given by the case where $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ are parallel:

$$\omega_{\max} = \frac{(k_F + q)^2}{2m} - \frac{k_F^2}{2m} \tag{39.34}$$

$$= \varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q < 2k_F. \tag{39.35}$$

This line continues without discontinuity the $\omega_{\max}$ line found above for $q > 2k_F$. When the plane of integration defined by Eq. (39.30) intersects the region where both spheres overlap, the domain of integration is an annulus instead of a filled circle. When this occurs, there is a discontinuous change in slope of $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$. This occurs when the vectors $\mathbf{k}+\mathbf{q}$ and $\mathbf{k}$ are antiparallel to each other and when $q = k_F - k$ while $k = k_F - q$ is inside the left Fermi surface. The corresponding energy is

$$\omega_{change} = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}} = \frac{k_F^2}{2m} - \frac{(k_F - q)^2}{2m} = v_F q - \varepsilon_{\mathbf{q}} \tag{39.36}$$

This line, $\omega_{change}(q)$, is shown in Fig.(39-6). The minimum allowed value of ω vanishes since both arrows can be right at the Fermi surface in the annulus region.

$$\omega_{\min} = 0 \quad ; \quad q < 2k_F \tag{39.37}$$

The region in ω and q space where $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is non-vanishing, the particle-hole continuum, is illustrated schematically in Fig.(39-6) for positive frequency. Since $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is odd in frequency, there is a symmetrical region at $\omega < 0$.

Remark 273 $2k_F$ *singularities: The sudden changes in the Lindhard functions at* $q = 2k_F$ *have numerous consequences on observable quantities. They lead to Kohn anomalies in the phonon spectrum and to Friedel oscillations, for example.*

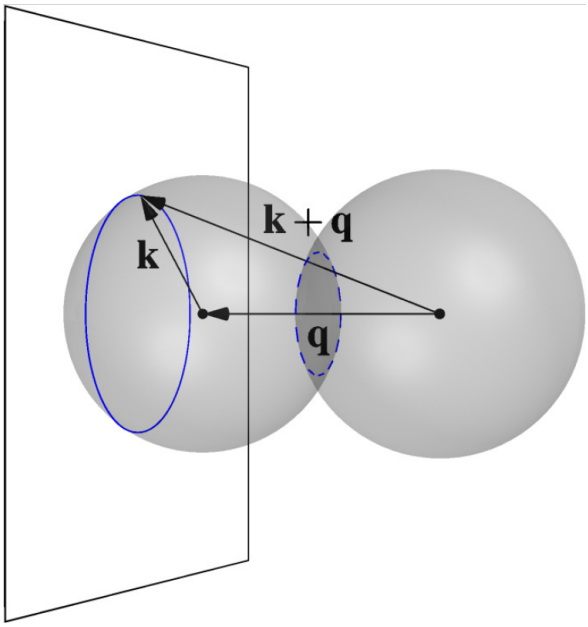


Figure 39-5 Geometry for the integral giving the imaginary part of the $d = 3$ Lindhard function. The wave vectors in the plane satisfy energy conservation as well as the restrictions imposed by the Pauli principle. The plane located symmetrically with respect to the miror plane of the spheres corresponds to energies of opposite sign.

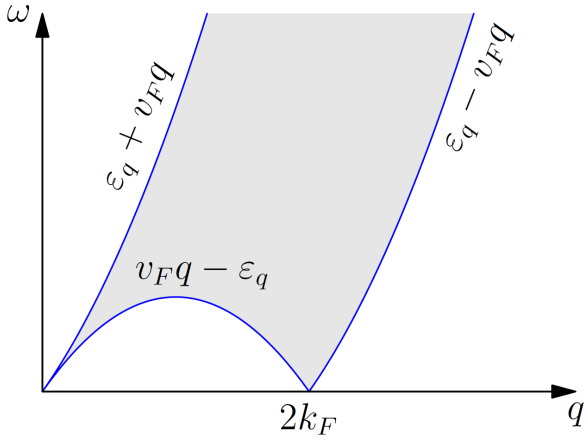


Figure 39-6 Schematic representation of the domain of frequency and wave vector where there is a particle-hole continuum.

40. INTERACTIONS AND COLLECTIVE MODES IN A SIMPLE WAY

Before I start the whole machinery to take into account interactions and perhaps make you lose track of the physics with too much formalism, it is helpful to recall some of the simple results that we should obtain. We begin by identifying the expansion parameter.

40.1 Expansion parameter in the presence of interactions: r_s

In the presence of interactions, it is convenient to define a dimensionless constant that measures the strength of interactions relative to the kinetic energy. If the kinetic energy is very large compared with the interaction strength, perturbative methods may have a chance. Let us begin by recalling some well known results. In the hydrogen atom, potential and kinetic energy are comparable. That defines a natural distance for interacting electrons, namely the Bohr radius. Let us remind ourselves of what this number is. Using the uncertainty principle, we have $\Delta k \sim a_0^{-1}$ so that the kinetic energy can be estimated as $1/\left(ma_o^2\right)$ and the value of a_0 itself is obtained by equating this to the potential energy

$$\frac{1}{ma_o^2} = \frac{e^2}{4\pi\varepsilon_0 a_0} \tag{40.1}$$

giving us for the Bohr radius, in standard units,

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10} m \sim 0.5\,\text{Å} \tag{40.2}$$

It is standard practice to define the dimensionless parameter r_s by setting the density of electrons n equal to 1/(volume of the sphere of radius $r_s a_0$ occupied by a single electron). In other words, we have

$$\boxed{n \equiv \frac{1}{\frac{4\pi}{3} r_s^3 a_0^3}} \tag{40.3}$$

where

$$n = \frac{k_F^3}{3\pi^2} \tag{40.4}$$

is the density of electrons. Another way to write r_s is then

$$\boxed{r_s \equiv \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{k_F a_0}} \tag{40.5}$$

In a way, r_s is the average distance between electrons measured in units of the Bohr radius. Large r_s means that the electrons are far apart, hence that the kinetic

energy is small. Using the same uncertainty relation as in the hydrogen atom, this means that interactions are more important than kinetic energy. Conversely, at small r_s kinetic energy is large compared with interactions and the interactions are much less important than the kinetic energy. It is natural then to expect that r_s is a measure of the relative strength of the interactions or, if you want, an expansion parameter. A way to confirm this role of r_s is to show that

$$\frac{Potential}{Kinetic} \sim \frac{\frac{e^2}{4\pi\varepsilon_0}k_F}{k_F^2/2m} \sim \frac{m\frac{e^2}{4\pi\varepsilon_0}}{k_F} \sim \frac{1}{k_F a_0} \sim \left(\frac{1}{na_0^3}\right)^{1/3} \sim r_s \tag{40.6}$$

These estimates are obtained as follows. The average momentum exchanged in interactions is of order k_F so that $\frac{e^2}{4\pi\varepsilon_0 r} \sim \frac{e^2}{4\pi\varepsilon_0}k_F$ should be a sensible value for the average potential energy while the kinetic energy as usual is estimated from E_F.

It may be counterintuitive at first to think that interactions are less important at large densities but that is a consequence of the uncertainty principle, not a concept of classical mechanics.

40.2 Thomas-Fermi screening

The elementary theory of screening is the Thomas-Fermi theory.[12] In this approach, Poisson's equation is solved simultaneously with the electrochemical equilibrium equation to obtain an expression for the potential. The screening will not occur over arbitrarily short distance because localizing the electron's wave functions costs kinetic energy. In fact, at very short distance the potential will be basically unscreened.

Consider Poisson's equation for our electron gas in the presence of an external charge ρ_e. You can think of this external charge as being for example an impurity positive charge added to the medium. In the Landau gauge, where $\nabla \cdot \mathbf{A} = \mathbf{0}$, the result is

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\left[\rho_e(\mathbf{r}) + \delta\rho(\mathbf{r})\right] \tag{40.7}$$

The quantity $\delta\rho(\mathbf{r})$ is the change in charge density of the background produced by the charged impurity

$$\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0 = -e\left[n(\mathbf{r}) - n\right] \tag{40.8}$$

We need to find $n(\mathbf{r}) - n$.

Original phenomenological derivation valid in the non-linear case: We will consider only the linearized case, so if you are in a hurry, you can skip the discussion in this paragraph which is more phenomenological but also more general.

Since density and Fermi wave vector are related, kinetic energy will come in. Assuming that the Fermi energy and the potential both vary slowly in space, the relation

$$\frac{n(\mathbf{r})}{n} = \frac{k_F^3(\mathbf{r})}{k_F^3} \tag{40.9}$$

and electrochemical equilibrium

$$\frac{k_F^2(\mathbf{r})}{2m} + (-e\phi(\mathbf{r})) = E_F = \frac{k_F^2}{2m} \tag{40.10}$$

where E_F is the value of the Fermi energy infinitely far from the impurity potential, lead immediately to the relation between density and electrostatic potential

$$\frac{n(\mathbf{r})}{n} = \frac{k_F^3(\mathbf{r})}{k_F^3} = \left[\frac{k_F^2(\mathbf{r})/2m}{k_F^2/2m}\right]^{3/2} = \left[1 - \frac{(-e\phi(\mathbf{r}))}{E_F}\right]^{3/2}. \tag{40.11}$$

Substituting this back into Poisson's equation, we have a closed equation for potential

$$\boxed{-\nabla^2\phi(\mathbf{r}) = \tfrac{1}{\varepsilon_0}\rho_e(\mathbf{r}) - \tfrac{1}{\varepsilon_0}ne\left[\left(1 - \tfrac{(-e\phi(\mathbf{r}))}{E_F}\right)^{3/2} - 1\right]}. \tag{40.12}$$

In general it is important to solve this full non-linear equation because otherwise at short distances the impurity potential is unscreened $\phi(\mathbf{r}) \sim 1/r$ which leads to unphysical negative values of the density in the linearized expression for the density,

$$\frac{n(\mathbf{r})}{n} \approx \left[1 - \frac{3}{2}\frac{(-e\phi(\mathbf{r}))}{E_F}\right] \tag{40.13}$$

Nevertheless, if we are interested only in long-distance properties, the linear approximation turns out to be excellent. In this approximation, Poisson's equation Eq.(40.12) becomes

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\rho_e(\mathbf{r}) + \frac{1}{\varepsilon_0}\frac{3}{2}\frac{ne}{E_F}(-e\phi(\mathbf{r})). \tag{40.14}$$

Since we will need only the linearized version, we can immediately obtain the final result from linear response in Poisson's equation Eq.(40.7). Fourier transforming, we find

$$q^2\phi(\mathbf{q},\omega) = \frac{1}{\varepsilon_0}\left[\rho_e(\mathbf{q},\omega) - \chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)\,\phi(\mathbf{q},\omega)\right]. \tag{40.15}$$

The susceptibility appears with a negative sign because the coupling to charge density to scalar potential is with a positive sign. Since it gives the density response to the self-consistent potential, it is called the irreducible susceptibility for reasons that will become clear in the next section. Since n scales as k_F^3 and E_F scales like k_F^2, it is easy to compute $\partial n/\partial\mu = \partial n/\partial E_F$. If we then define

$$\boxed{q_{TF}^2 = \tfrac{3}{2}\tfrac{ne^2}{\varepsilon_0 E_F} = \tfrac{e^2}{\varepsilon_0}\tfrac{\partial n}{\partial\mu}}, \tag{40.16}$$

both ways of doing the calculation lead to the same result

$$\boxed{\phi(\mathbf{q}) = \tfrac{1}{\varepsilon_0}\tfrac{\rho_e(\mathbf{q})}{q^2+q_{TF}^2}}. \tag{40.17}$$

if we use $\chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega) = e^2\chi_{nn}^{irr,R}(\mathbf{q},\omega)$ and the leading term of low-frequency, long-wavelength limit, namely $\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\chi_{nn}^{irr,R} = \frac{\partial n}{\partial\mu}$ that follows from a thermodynamic sum rule discussed in Sec.(10.10.1) when it is generalized to charged systems, a rather subtle point[1]. We can also define a Thomas-Fermi longitudinal dielectric constant by

$$\boxed{\varepsilon^L(\mathbf{q},0) = \varepsilon_0\tfrac{q^2+q_{TF}^2}{q^2} = \varepsilon_0\left(1 + \tfrac{q_{TF}^2}{q^2}\right)}. \tag{40.18}$$

[1] See the first remark below.

Let us pause to give a physical interpretation of this result. At small distances (large q) the charge is unscreened since $\varepsilon_L \to 1$. On the contrary, at large distance (small q) the sreening is very effective. In real space, one finds an exponential decrease of the potential over a length scale q_{TF}^{-1}, the Thomas-Fermi screening length. Let us write this length in terms of r_s using the definition Eq.(40.3) or (40.5) with $\hbar$ appearing explicitly now so that $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$

$$\lambda^2 \equiv q_{TF}^{-2} = \frac{2\varepsilon_0 E_F}{3ne^2} = \frac{2\varepsilon_0 k_F^2/2m}{3ne^2} = \frac{k_F^2 a_0}{12\pi n} \tag{40.19}$$

$$= \frac{k_F^2 a_0^4}{12\pi}\left(\frac{4\pi}{3}r_s^3\right) = a_0^2\left(\frac{1}{9}\left(\frac{9\pi}{4}\right)^{2/3}\right) r_s \tag{40.20}$$

Roughly speaking then, for $r_s \ll 1$ we have that the screening length

$$\boxed{\lambda \sim \left(a_0\sqrt{r_s} = \frac{a_0 r_s}{\sqrt{r_s}}\right)} \tag{40.21}$$

is larger than the interelectronic distance $a_0 r_s$. In this limit our long wavelength Thomas-Fermi reasoning makes sense. On the other hand, for $r_s \gg 1$ the screening length is much smaller than the interelectronic distance. This is counter intuitive: When the distance λ over which electrons see each other is short, λ small, the potential energy is larger than kinetic energy, i.e. $r_s \gg 1$. This is because kinetic energy decreases faster with separation between electrons $1/(r_s a_0)^2$ than potential energy $1/(r_s a_0)$. It makes less sense to think that the free electron Hamiltonian is a good perturbative starting point when $r_s \gg 1$. Electrons start to localize. Note however, that we mean by large r_s can be pretty large. For sodium, $r_s \sim 4$ while for aluminum, $r_s \sim 2$ but still, these are good metals.

Remark 274 *The thermodynamic sum-rule that I have proven in Section (10.10.1) is that* $\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\chi^R_{nn} = \frac{\partial n}{\partial \mu}$. *In the next section, in remark 276, I discuss under what assumptions the equalities* $\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\chi^R_{nn} = \lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\chi^{irr,R}_{nn} = \frac{\partial n}{\partial \mu}$ *are satisfied.*

Remark 275 *Two dimensional case: As an exercise, note that if the material is two dimensional, then the density is confined to a surface so that* $n \to n_s\delta(z)$ *and* $\rho \to \rho_s\delta(z)$ *where* n_s *and* ρ_s *are surface density and charge surface density. Then, Eq.(40.15) in Fourier space becomes*

$$\left(q_z^2 + q_{||}^2\right)\phi(\mathbf{q}) = \frac{1}{\varepsilon_0}\left[\rho_s(\mathbf{q}_{||}) - e\frac{\partial n_s}{\partial \mu}\left(+e\phi(\mathbf{q}_{||}, z=0)\right)\right] \tag{40.22}$$

Dividing by $q_z^2 + q_{||}^2$ *we obtain*

$$\int \phi(\mathbf{q})\frac{dq_z}{2\pi} = \phi(\mathbf{q}_{||}, z=0)$$

$$= \frac{1}{\varepsilon_0}\left[\rho_s(\mathbf{q}_{||}) - e\frac{\partial n_s}{\partial \mu}\left(e\phi(\mathbf{q}_{||}, z=0)\right)\right]\int \frac{1}{q_z^2 + q_{||}^2}\frac{dq_z}{2\pi} \tag{40.23}$$

The last integral is equal to $(2q_{||})^{-1}$ *so that*

$$\left[1 + \frac{e^2}{2\varepsilon_0 q_{||}}\frac{\partial n_s}{\partial \mu}\right]\phi(\mathbf{q}_{||}, z=0) = \frac{\rho_s(\mathbf{q}_{||})}{2\varepsilon_0 q_{||}} \tag{40.24}$$

and

$$\phi(\mathbf{q}_{||}, z=0) = \frac{\rho_s(\mathbf{q}_{||})}{2\varepsilon^L(\mathbf{q}_{||})q_{||}} = \frac{1}{2\varepsilon_0}\frac{\rho_s(\mathbf{q}_{||})}{q_{||} + \frac{e^2}{2\varepsilon_0}\frac{\partial n_s}{\partial \mu}} \tag{40.25}$$

$$\frac{\varepsilon^L(\mathbf{q}_{||})}{\varepsilon_0} = 1 + \frac{e^2}{2\varepsilon_0 q_{||}} \frac{\partial n_s}{\partial \mu}. \tag{40.26}$$

This result was obtained by Stern [226].

40.3 Reducible and irreducible susceptibilities: another look at the longitudinal dielectric constant

The calculation of the longitudinal dielectric constant for a homogeneous isotropic medium proceeds, in the Landau gauge $\nabla \cdot \mathbf{A} = \mathbf{0}$, from the following equalities

$$q^2 \phi(\mathbf{q},\omega) = \frac{1}{\varepsilon_0}\left(\rho_e(\mathbf{q},\omega) + \delta\rho(\mathbf{q},\omega)\right) \equiv \frac{1}{\varepsilon^L(\mathbf{q},\omega)} \rho_e(\mathbf{q},\omega). \tag{40.27}$$

In the linear approximation we obtained $\delta\rho = -\chi^R_{\rho\rho}\phi_e$ in Sec. 13.2 from the linear response to the potential $\varepsilon_0 q^2 \phi_e(\mathbf{q},\omega) = \rho_e(\mathbf{q},\omega)$ induced by the external charge ρ_e. This led to

$$\boxed{\frac{1}{\varepsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega)\right).} \tag{40.28}$$

where $V_{\mathbf{q}} = e^2/\left(\varepsilon_0 q^2\right)$. But we can also obtain the induced charge $\delta\rho = -\chi^{irr,R}_{\rho\rho}(\mathbf{q},\omega)\,\phi(\mathbf{q},\omega)$ from the linear response to the total self-consistent potential, as we did in the previous section. In that case, Eq.(40.15) for the total potential can be written as

$$\left[q^2 + \frac{1}{\varepsilon_0}\chi^{irr,R}_{\rho\rho}(\mathbf{q},\omega)\right]\phi(\mathbf{q},\omega) = \frac{1}{\varepsilon_0}\rho_e(\mathbf{q},\omega) \tag{40.29}$$

so that we have the alternative expression for $\varepsilon^L(\mathbf{q},\omega)$, namely

$$\boxed{\frac{1}{\varepsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\frac{1}{1+V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)}.} \tag{40.30}$$

Equating the two expressions Eq.(40.28) and Eq.(40.30) for the longitudinal dielectric constant imposes a relation between the susceptibility to an external potential and the irreducible susceptibility, namely

$$\frac{1}{1 + V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)} = \left(1 - V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega)\right) \tag{40.31}$$

which leads, after a little algebra, to

$$\chi^R_{nn}(\mathbf{q},\omega) = \frac{\chi^{irr,R}_{nn}(\mathbf{q},\omega)}{1 + V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)}. \tag{40.32}$$

Classical electrodynamics thus imposes the above relation between the two different kinds of responses. We will see in Chapter 51 on Hedin's equations, how we can preserve this structure in general. In the random phase approximation (RPA) that I will discuss in the next chapter, the above relation will be satisfied with $\chi^{irr,R}_{nn}(\mathbf{q},\omega)$ replaced by $\chi^{0,R}_{nn}(\mathbf{q},\omega)$, the non-interacting density-density correlation function. In general, the definition $\Pi^R_{nn}(\mathbf{q},\omega) \equiv -\chi^{irr,R}_{nn}(\mathbf{q},\omega)$ is used for the so-called irreducible polarization $\Pi^R_{nn}(\mathbf{q},\omega)$.

Remark 276 *Note that because of the background,* $V_{\mathbf{q}=\mathbf{0}} = 0$. *On the other hand,* $\lim_{\mathbf{q}\to\mathbf{0}} V_{\mathbf{q}}$ *is a different object. So the limit* $\mathbf{q} \to 0$ *in the expression* $\lim_{\mathbf{q}\to 0} \lim_{\omega\to 0} \chi^R_{nn} = \lim_{\mathbf{q}\to 0} \lim_{\omega\to 0} \chi^{irr,R}_{nn}$, *must be taken as meaning that we take* $V_{\mathbf{q}=\mathbf{0}}$. *In other words, the thermodynamic sum rule* $\chi^R_{nn}(\mathbf{q}\to\mathbf{0},\omega=0) = (\partial n/\partial\mu)$ *has meaning only at charge neutrality, namely at* $V_{\mathbf{q}=\mathbf{0}} = 0$.

Remark 277 *Irreducibility with respect to the Coulomb interaction: If we write the last equation for the susceptibility in the form*

$$\begin{aligned}\chi^R_{nn}(\mathbf{q},\omega) &= \chi^{irr,R}_{nn}(\mathbf{q},\omega) - \chi^{irr,R}_{nn}(\mathbf{q},\omega)\, V_{\mathbf{q}} \chi^{irr,R}_{nn}(\mathbf{q},\omega) \\ &\quad + \chi^{irr,R}_{nn}(\mathbf{q},\omega)\, V_{\mathbf{q}} \chi^{irr,R}_{nn}(\mathbf{q},\omega)\, V_{\mathbf{q}} \chi^{irr,R}_{nn}(\mathbf{q},\omega) + \dots \end{aligned} \tag{40.33}$$

we can anticipate that the irreducible susceptibility will be defined by the set of all diagrams that cannot be cut in two by cutting a line representing a Coulomb interaction.

40.4 Plasma oscillations

Plasma oscillations are the density oscillations of a free electron gas. The physics of this is that because the system wants to stay neutral everywhere, electrostatic forces will want to bring back spontaneous electronic density fluctuations towards the uniform state but, because of the electron inertia, there is overshooting. Hence oscillations arise at a particular natural frequency, the so-called plasma frequency. In other words, it suffices to add inertia to our previous considerations to see the result come out.

We give a very simple minded macroscopic description valid only in the limit of very long wave length oscillations. Suppose there is a drift current

$$\mathbf{j} = -en\mathbf{v} \tag{40.34}$$

Taking the time derivative and using Newton's equations,

$$\frac{\partial \mathbf{j}}{\partial t} = -en\frac{\partial \mathbf{v}}{\partial t} = -\frac{en}{m}(-e\mathbf{E}) \tag{40.35}$$

Note that in Newton's equation we should use the total time derivative instead of the partial, but since we assume a uniform density ($\mathbf{q} = \mathbf{0}$) the total and partial derivative are identical. We are in a position where one more time derivative

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = \frac{ne^2}{m}\frac{\partial \mathbf{E}}{\partial t} \tag{40.36}$$

and an appeal to the *longitudinal* part of Maxwell's fourth equation

$$0 = \mu_0 \mathbf{j} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{40.37}$$

should give us the desired result, namely

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = -\frac{ne^2}{\varepsilon_0 m}\mathbf{j} \tag{40.38}$$

This equation has an oscillatory solution at a frequency ω_p

$$\boxed{\omega_p^2 \equiv \tfrac{ne^2}{\varepsilon_0 m}} \tag{40.39}$$

the so-called plasma frequency. Since we know that the longitudinal dielectric constant vanishes at a collective mode, this gives us another expected limit of this function

$$\boxed{\lim_{\omega\to\omega_p} \varepsilon^L(\mathbf{q}=\mathbf{0},\omega) = \lim_{\omega\to\omega_p} a(\omega-\omega_p)} \tag{40.40}$$

where a is an unknown, for the time being, positive constant. The sign is determined from the fact that the dielectric constant must return to a positive value equal to unity at very large frequency.

Alternate derivation: An alternate derivation that is more easily extended to films or wires takes the divergence of Eq.(40.35) and then uses current conservation with Maxwell's first equation to obtain

$$\frac{\partial \nabla\cdot\mathbf{j}}{\partial t} = -\frac{en}{m}(-e\nabla\cdot\mathbf{E}) \tag{40.41}$$

$$-\frac{\partial^2\rho}{\partial t^2} = \frac{e^2 n}{\varepsilon_0 m}\rho \tag{40.42}$$

which immediately leads to the desired expression for the plasma frequency. Note that writing $\nabla\cdot\mathbf{E} = -\nabla^2\phi = \rho/\varepsilon_0$ is equivalent to using the unscreened potential. This is correct at large frequency where screening cannot occur. This will come out automatically from the $\mathbf{q}$ and ω dependence of dielectric constant.

Remark 278 *Two dimensional case: Screening being different in for two dimensional films, as we have just seen, plasma oscillations will be different. In fact, the plasma frequency vanishes at zero wave vector. Indeed, current conservation for the surface quantities reads,*

$$\frac{\partial \rho_s}{\partial t} + \nabla_s\cdot\mathbf{j}_s = 0. \tag{40.43}$$

Taking the two-dimensional divergence of Newton's equation Eq.(40.35) on both sides, we obtain

$$\frac{\partial \nabla_s\cdot\mathbf{j}_s}{\partial t}\delta(z) = \frac{e^2 n_s}{m}\delta(z)\nabla_s\cdot\mathbf{E} \tag{40.44}$$

so that Fourier transforming and using charge conservation, we obtain

$$-\frac{\partial^2\rho_s(q_{||})}{\partial t^2} = \frac{e^2 n_s}{m} i\mathbf{q}_{||}\cdot\mathbf{E}(\mathbf{q}_{||}, z=0). \tag{40.45}$$

We can express the electric field in terms of the surface density to close the system of equations,

$$\mathbf{E}(\mathbf{q}_{||}, z=0) = -\mathbf{i}\mathbf{q}_{||}\phi(\mathbf{q}_{||}, z=0) = -\mathbf{i}\mathbf{q}_{||}\frac{\rho_s}{2\varepsilon_0 q_{||}} \tag{40.46}$$

where we used the unscreened Poisson equation for a film (two-dimensional material). This leads to

$$\frac{\partial^2\rho_s(q_{||})}{\partial t^2} = -\frac{e^2 n_s}{2\varepsilon_0 m} q_{||}\rho_s \tag{40.47}$$

which means that the plasma frequency is

$$\omega_p^2 = \frac{e^2 n_s}{2\varepsilon_0 m} q_{||} \tag{40.48}$$

that vanishes as $q_{||}$ does. It is important to note again that in the derivation we used the unscreened potential. The order of limits is important. We have assumed

that the frequency is too large for the other electrons to screen the charge displacement. In the end that frequency, ω_p, vanishes so we have to be careful. A full treatment of the momentum and frequency dependence of the dielectric function, as we will do in the next section, is necessary. In closing, note that the appeal to the longitudinal part of Maxwell's fourth equation, done in the very first derivation, is not so trivial in less than three dimension.

41. DENSITY RESPONSE IN THE PRESENCE OF INTERACTIONS

Now that we know what to expect, let us see what he complete calculation gives. As usual, you can follow the tracks of Fenyman or of Schwinger, in the end we have the same integrals to do.

41.1 Density-density correlations, RPA

As before we derive the relevant equation the Feynman way and the Schwinger way.

41.1.1 *The Feynman way

We are now ready to start our diagrammatic analysis. Fig.(41-1) shows all charge susceptibility diagrams to first order in the interaction. The four diagrams on the second line take into account self-energy effects on the single-particle properties. We will worry about this later. Of the two diagrams on the first line, the first one clearly dominates. Indeed, the dotted line leads to a factor $e^2/\left(\varepsilon_0 q^2\right)$ that diverges at small wave vectors. On the other hand, the contribution from the other diagram is proportional to

$$-2\int\frac{d^3k}{\left(2\pi\right)^3}T\sum_{ik_n}\int\frac{d^3k'}{\left(2\pi\right)^3}T\sum_{ik'_n}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k},ik_n\right)\times$$
$$\frac{e^2}{\varepsilon_0\left|\mathbf{k}-\mathbf{k}'\right|^2}\mathcal{G}^0_\sigma\left(\mathbf{k}'+\mathbf{q},ik'_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k}',ik'_n\right) \tag{41.1}$$

which is a convergent integral with no singularity at $q=0$.

Remark 279 *For a very short range potential, namely a wave-vector independent potential, the situation would have been completely different since the contribution of the last diagram would have been simply minus half of the contribution of the first one, the only differences being the additional fermion loop in the first one that leads to a sign difference and a factor of two for spin. We will come back on this in our study of the Hubbard model.*

Let us thus concentrate on the most important contribution at long wave lengths namely the first diagram. In addition to being divergent as $q\to 0$, it has additional pathologies. Indeed, it has double poles at the particle-hole excitations of the non-interacting problem while the Lehmann representation shows us that it should not. This problem sounds familiar. We have encountered it with the single-particle Green's function. The problem is thus solved in an analogous manner, by summing an infinite subset of diagrams. This subset of diagrams is

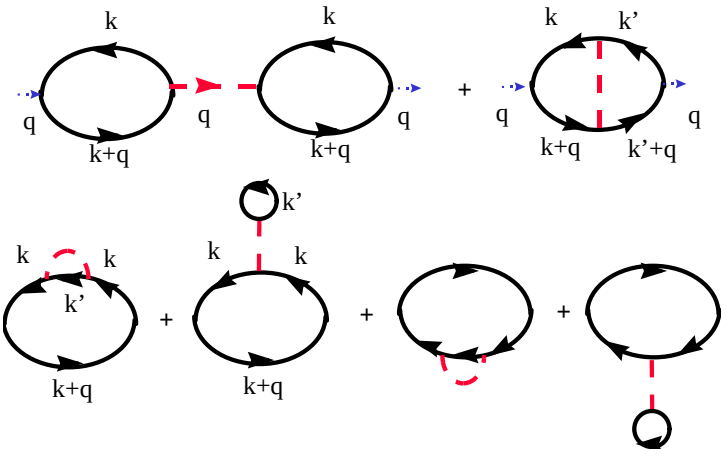


Figure 41-1 Charge susceptibility diagrams to first order in the interaction

illustrated in Fig.(41-2). It is the famous random phase approximation (RPA). One also meets the terminology *ring diagrams* (in the context of free energy calculations) or, more often, one also meets the name bubble diagrams. The full susceptibility is represented by adding a triangle to one of the external vertices. That triangle represents the so-called dressed three point vertex. The reason for this name will come out more clearly later. The full series, represented schematically on the first two lines of the figure, may be summed to infinity by writing down the equation on the last line. This equation looks like a particle-hole version of the Dyson equation. The undressed bubble plays the role of an irreducible susceptibility. It is irreducible with respect to cutting one interaction line.

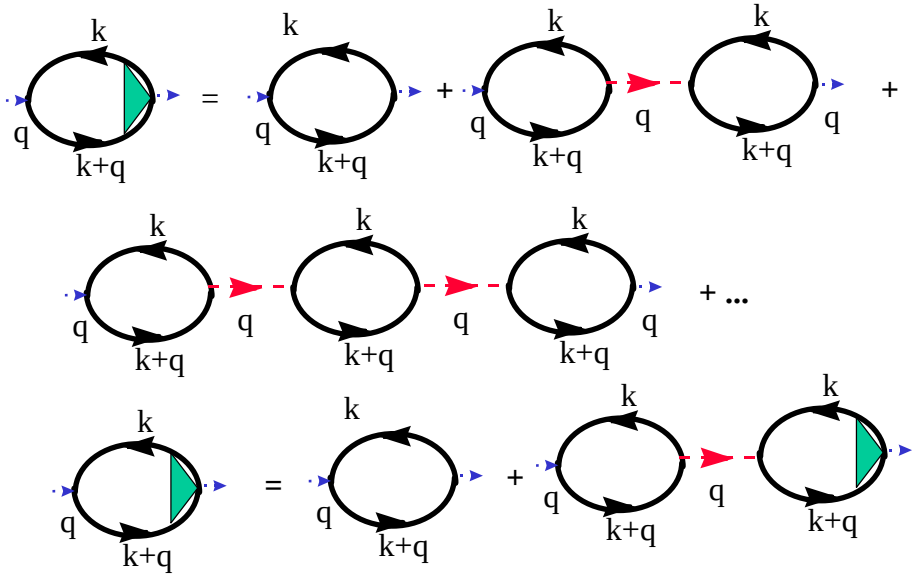


Figure 41-2 Bubble diagrams. Random phase approximation.

From our calculation of the susceptibility for non-interacting electrons we know that Feynman's rules apply for the diagrams on Fig.(41-2). Each bubble is associated with a factor $\chi^0_{nn}(\mathbf{q}, iq_n)$, a quantity defined in such a way that it contains the minus sign associated with the fermion loop. The dashed interaction lines each

lead to a factor $-V_{\mathbf{q}} = -e^2/\left(\varepsilon_0 q^2\right)$, the minus sign being associated with the fact that one more $V_{\mathbf{q}}$ means one higher order in perturbation theory (remember the $(-1)^n$ rule). The sum over bubbles, represented by the last line on Fig.(41-2) is easy to do since it is just a geometric series. The result is.

$$\boxed{\chi_{nn}(\mathbf{q}, iq_n) = \frac{\chi^0_{nn}(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}} \quad ; \quad V_{\mathbf{q}} = \frac{e^2}{\varepsilon_0 q^2} \tag{41.2}$$

41.1.2 The Schwinger way

We keep following our first step approach that gave us the Hartree-Fock approximation and corresponding susceptibility. Returning to our expression for the susceptibility in terms a functional derivative Eq.(90.15), namely

$$-\sum_{\sigma_1,\sigma_2} \frac{\delta \mathcal{G}\left(1,1^+\right)}{\delta\phi\left(2^+,2\right)} = \chi_{nn}\left(1-2\right) \tag{41.3}$$

and Fourier transforming, we obtain in the case where the irreducible vertex is obtained from functional derivatives of the Hartree-Fock self-energy the set of diagrams in Fig. 37-7. In the middle diagram on the right-hand side of the equality, there is a sum over wave vectors k' because three of the original coordinates of the functional derivative at the bottom of the diagram were different. This means there are two independent momenta, contrary to the last diagram in the figure. One of the independent momenta can be taken as q by momentum conservation while the other one, k', must be integrated over. The contribution from that middle diagram is not singular at small wave vector because the Coulomb potential is integrated over. By contrast, the last diagram has a $1/q^2$ from the interaction potential, which is divergent. We thus keep only that last term. The integral equation, illustrated in Fig. 41-3, then takes an algebraic form

$$\chi_{nn}(q) = \chi^0_{nn}(q) - \chi^0_{nn}(q)V_{\mathbf{q}}\chi_{nn}(q). \tag{41.4}$$

To figure out the sign from the figure, recall that the green triangle stands for $\frac{\delta\mathcal{G}\left(1,1^+\right)}{\delta\phi(2^+,2)}$, while there is a minus sign in the equation for the susceptibility Eq. (41.3). Since the integral equation (41.4) for $\chi_{nn}(q)$ has become an algebraic equation in Fourier-Matsubara space, it is easy to solve. We find,

$$\chi_{nn}(q) = \frac{\chi^0_{nn}(q)}{1+V_{\mathbf{q}}\chi^0_{nn}(q)} = \frac{1}{\chi^0_{nn}(q)^{-1}+V_{\mathbf{q}}}. \tag{41.5}$$

This is the so-called Random Phase Approximation, or RPA. The last form of the equality highlights the fact that the irreducible vertex, here $V_{\mathbf{q}}$, plays the role of an irreducible self-energy in the particle-hole channel. The analytical continuation will be trivial.

Note that we have written $\chi^0_{nn}(q)$ for the bubble diagram, i.e. the first term on the right-hand side of the equation in Fig. 37-7 even though everything we have up to now in the Schwinger formalism are dressed Green's functions. The reason is that neglecting the middle diagram on the right-hand side of the equality is like neglecting the contribution from the Fock, or exchange self-energy in Fig. 37-6. The only term left then is is the Hartree term that we argued should vanish because of the neutralizing background. Hence, the Green's functions are bare ones and the corresponding susceptibility is the Linhard function.

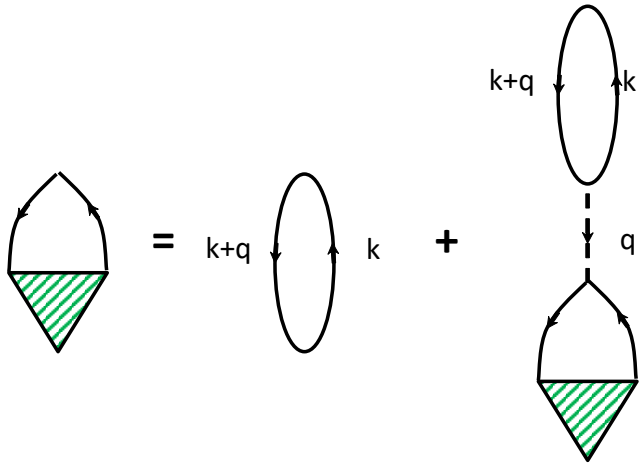


Figure 41-3 Fourier transform of $\frac{\delta \mathcal{G}(1,1^+)}{\delta \phi(2^+,2)}$ with a momentum q flowing top to bottom that is used to compute the density-density correlation function in the RPA approximation.

Remark 280 *The integral equation (41.4) for χ_{nn} shows very well that the irreducible vertex $V_{\mathbf{q}}$ here plays the role of a self-energy for the particle-hole response function. Compare that equation with $\mathcal{G} = \mathcal{G}^0 + \mathcal{G}^0 \Sigma \mathcal{G}$. Alternatively, compare $\mathcal{G}^{-1} = \mathcal{G}^{0-1} - \Sigma$ and the equation for the RPA susceptibility Eq. (41.5) $\chi_{nn}^{-1} = \chi_{nn}^{0-1} - V_{\mathbf{q}}$.*

Remark 281 *Equivalence to an infinite set of bubble diagrams: The integral equation for the susceptibility has turned into an algebraic equation in 41.4. By recursively replacing $\chi_{nn}(q)$ on the right-hand side of that equation by higher and higher order approximations in powers of $V_{\mathbf{q}}$ we obtain*

$$\begin{aligned} \chi_{nn}^{(1)}(q) &= \chi_{nn}^0(q) - \chi_{nn}^0(q) V_{\mathbf{q}} \chi_{nn}^0(q) \\ \chi_{nn}^{(2)}(q) &= \chi_{nn}^0(q) - \chi_{nn}^0(q) V_{\mathbf{q}} \chi_{nn}^0(q) \qquad (41.6) \\ &\quad + \chi_{nn}^0(q) V_{\mathbf{q}} \chi_{nn}^0(q) V_{\mathbf{q}} \chi_{nn}^0(q) + \ldots \qquad (41.7) \end{aligned}$$

etc. By solving the algebraic equation then, it is as if we had summed an infinite series which diagrammatically would look, if we turn it sideways, like Fig. 41-2. The analogy with the self-energy in the case of the Green's function is again clear.

Remark 282 *A direct expansion in powers of $V_{\mathbf{q}}$ without resumming would have been disatrous. Already the first term $\chi_{nn}^0(q) V_{\mathbf{q}} \chi_{nn}^0(q)$ diverges as $1/\mathbf{q}^2$ as $\mathbf{q}$ vanishes, and the following term as $1/\mathbf{q}^4$ etc. Doing perturbation theory with the Feynman formalism immediately leads to the questions of why are there divergences and why should we do infinite resummation to get rid of them. The reason why is clearer in the Schwinger formalism. Self-consistency is built in naturally in the formalism.*

41.2 Explicit form for the dielectric constant and special cases

Using our previous results for the imaginary part of the susceptibility for non-interacting particles, the real part can be found from taking the Hilbert transform. From this we obtain the explicit expression for the real and imaginary parts of the dielectric function in three dimensions at zero temperature. Recall that longitudinal dielectric constant and charge susceptibility are related by Eq. (13.15), namely

$$\frac{1}{\epsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - \frac{e^2}{\varepsilon_0 q^2}\chi^R_{nn}(\mathbf{q},\omega)\right) = \frac{1}{\varepsilon_0\left(1 + V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega)\right)} \tag{41.8}$$

or,

$$\boxed{\epsilon^L(\mathbf{q},\omega) = \varepsilon_0\left(1 + V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega)\right).} \tag{41.9}$$

For positive frequencies, one finds

$$\mathrm{Re}\left[\frac{\epsilon^L(\mathbf{q},\omega)}{\varepsilon_0}\right] \equiv \frac{\epsilon^L_1(\mathbf{q},\omega)}{\varepsilon_0} \tag{41.10}$$

$$\begin{aligned} &= 1 + \frac{q^2_{TF}}{q^2}\left\{\frac{1}{2} + \frac{k_F}{4q}\left[\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right)\ln\left|\frac{\omega - v_Fq - \varepsilon_q}{\omega + v_Fq - \varepsilon_q}\right|\right.\right. \\ &\left.\left. + \left(1 - \frac{(\omega+\varepsilon_q)^2}{q^2v_F^2}\right)\ln\left|\frac{\omega + v_Fq + \varepsilon_q}{\omega - v_Fq + \varepsilon_q}\right|\right]\right\} \end{aligned} \tag{41.11}$$

$$\mathrm{Im}\left[\epsilon^L(\mathbf{q},\omega)\right] \equiv \epsilon^L_2(\mathbf{q},\omega) \tag{41.12}$$

$$= \left\{\begin{array}{lll} \frac{\pi}{2}\frac{\omega}{v_Fq}\frac{q^2_{TF}}{q^2} \;; & \omega \le v_Fq - \varepsilon_q & \\ \frac{\pi k_F}{4q}\frac{q^2_{TF}}{q^2}\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right); & v_Fq - \varepsilon_q \le \omega \le \varepsilon_q + v_Fq & \left.\right\} \quad q < 2k_F \\ 0 \;; & \omega \ge \varepsilon_q + v_Fq & \\ \frac{\pi k_F}{4q}\frac{q^2_{TF}}{q^2}\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right); & \varepsilon_q - v_Fq \le \omega \le \varepsilon_q + v_Fq & \left.\right\} \quad q > 2k_F \end{array}\right. .$$

I agree this is not obvious. The integral is done at length in Fetter and Walecka [73]. We will see below that we can find the interesting limiting cases for the integrals entering the calculation of the Lindhard function rather easily, except for the logarithm. That logarithm is important for Friedel's oscillations. It comes basically from the Hilbert transform of the Heaviside θ function. Recall in our geometric arguments with Fermi spheres that discontinuities in the slope of the non-interacting charge susceptibility occur when $q = 2k_F$.

We now analyze these results to extract five important physical ingredients: a) There is a particle-hole continuum but the poles are simply shifted from their old positions instead of becoming poles of high-order. b) There is screening at low frequency. c) There are Friedel oscillations in space. d) There are plasma oscillations in time. e) At long wave lengths the plasma oscillations exhaust the $f-$sum rule.

41.2.1 Particle-hole continuum

Let us first think of a finite system with $2M$ discrete poles in $\chi^{0R}_{nn}(\mathbf{q},\omega)$ to see that these have been shifted. The number of simple poles is even because the function is odd. The spectral representation tells us, using the fact that, $\chi''_{nn}(\mathbf{q},\omega')$ is odd

$$\begin{aligned}\chi^{0R}_{nn}(\mathbf{q},\omega) &= \int \frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-\omega-i\eta} = \int \frac{d\omega'}{\pi}\frac{\omega'\chi''_{nn}(\mathbf{q},\omega')}{(\omega')^2-(\omega+i\eta)^2} \\ &= \sum_{i=1}^{M}\frac{A_i}{u_i^2-(\omega+i\eta)^2} = \frac{B\prod_{i=1}^{(M)-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M}\left(u_i^2-(\omega+i\eta)^2\right)} \end{aligned} \tag{41.13}$$

where A_i is positive because $\omega'\chi''_{nn}(\mathbf{q},\omega')$ is positive, as required by positivity of dissipation, and u_i are positions of the delta functions in $\omega'\chi''_{nn}(\mathbf{q},\omega')$. The parameters A_i and u_i then are respectively the residue and the location of each pole in $\chi^{0R}_{nn}(\mathbf{q},\omega)$. We have combined the sum of fractions on a common denominator so that the numerator of the last expression has one less power of $(\omega+i\eta)^2$. We do not need to specify the values of B and v_i. Using this expression for the non-interacting susceptibility in the result Eq.(41.2) for the RPA susceptibility we find,

$$\chi^{R}_{nn}(\mathbf{q},\omega) = \frac{B\prod_{i=1}^{M-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M}\left(u_i^2-(\omega+i\eta)^2\right)+V_{\mathbf{q}}B\prod_{i=1}^{M-1}\left((\omega+i\eta)^2-v_i^2\right)} \tag{41.14}$$

The denominator can be rewritten as a polynomial of the same order as the non-interacting susceptibility, namely of order M in $(\omega+i\eta)^2$, but the zeros of this polynomial, corresponding to the poles of the retarded susceptibility, have shifted.

To find out the location of the poles of the charge excitations, at least qualitatively, it suffices to look for the domain where the imaginary part is non vanishing. Using our RPA result Eq.(41.2) and simple algebra

$$\mathrm{Im}\left(\frac{x+iy}{1+x+iy}\right) = \frac{y}{(1+x)^2+y^2} \tag{41.15}$$

we find the following result for the imaginary part

$$\mathrm{Im}\,\chi^{R}_{nn}(\mathbf{q},\omega) = \frac{\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)}{\left(1+V_{\mathbf{q}}\,\mathrm{Re}\,\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2+\left(V_{\mathbf{q}}\,\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2}. \tag{41.16}$$

In a finite system, as above, $\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$ would be proportional to a delta function whenever there is a pole in the non-interacting susceptibility. The square of this delta function that appears in the denominator cancels the corresponding delta function in the numerator, which is another (less clear) way of saying what we have just shown in full generality above, namely that in the interacting system the poles are different from those of the non-interacting system. The new poles are a solution of

$$\frac{1}{V_{\mathbf{q}}}+\mathrm{Re}\,\chi^{0R}_{nn}(\mathbf{q},\omega) = \frac{1}{V_{\mathbf{q}}}+\sum_{i=1}^{M}\frac{A_i}{u_i^2-\omega^2} \tag{41.17}$$

$$= \frac{1}{V_{\mathbf{q}}}+\sum_{i=1}^{M}\frac{A_i}{2u_i}\left(\frac{1}{u_i-\omega}+\frac{1}{u_i+\omega}\right)=0 \tag{41.18}$$

The solution of this equation may in principle be found graphically as illustrated in Fig.(41-4). I have taken the simple case $2M = 6$ for clarity. In reality, $M \to \infty$ and the separation between each discrete pole of $\mathrm{Re}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$ is inversely proportional to a power of the size of the system $1/\mathcal{V}$. The delta functions of the non-interacting susceptibility are on the real axis at the intersection of the vertical asymptotes of the poles of $\mathrm{Re}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$. Each delta function of the non-interacting $\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$ leads to a pole in $\mathrm{Re}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$. The new delta functions of the interacting $\mathrm{Im}\,\chi^{R}_{nn}(\mathbf{q},\omega)$ are the solution of the above equation. They are the intersection of the horizontal line $1/V_{\mathbf{q}}$ and of the lines that behave as $1/(u_i - \omega)$ near every vertical asymptote. Clearly, except for the last two symmetrically located solutions at large frequency, all the new solutions are very close to those of the non-interacting system. And they are at a location where the ininteracting $\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$ vanishes so that the interacting $\mathrm{Im}\,\chi^{R}_{nn}(\mathbf{q},\omega)$ Eq. (41.16) does look as a set of delta functions displaced from the original positions of the non-interacting $\mathrm{Im}\,\chi^{0R}_{nn}(\mathbf{q},\omega)$.

In summary then, the particle-hole continuum is basically at the same place as it was in the non-interacting system, even though the residues may have changed. The two solutions at large frequency correspond to plasma oscillations, as we will see later. They are well separated from the particle-hole continuum for small q where $1/V_{\mathbf{q}}$ is very small. However, at large wave vector it is quite possible to find that the high frequency poles become very close again to the particle-hole continuum.

Remark 283 *Note that the number of poles in the interacting system is the same as the number of poles in the non-interacting one. In the situation illustrated in Fig(41-4), there are six non-interacting poles and six interacting ones. If $V_{\mathbf{q}}$ were negative and sufficiently large, we would loose two solutions. These missing solutions still exist as a pair of complex conjugate imaginary frequencies. One of these frequencies then is on the wrong half-plane. This indicates an instability towards another phase. This is a phase transition. The $\omega = 0$ value of the susceptiblity would be negative, another way to know that the system becomes unstable. I will discuss this in more detail when we get to phase transitions.*

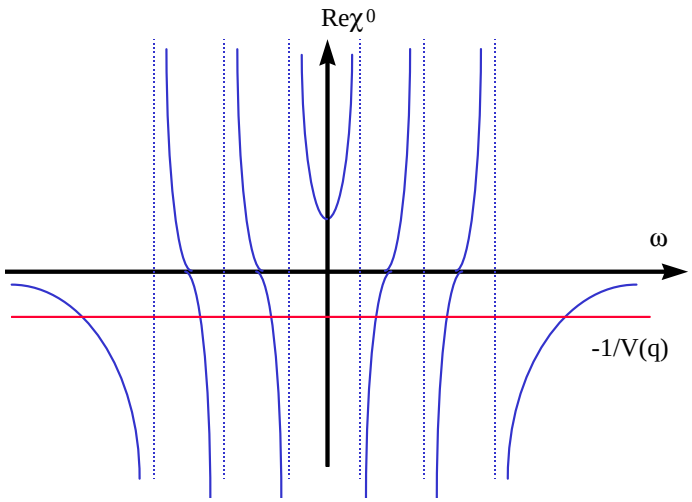


Figure 41-4 Graphical solution for the poles of the charge susceptibility in the interacting system.

Since $\mathrm{Im}\left(\epsilon^{L}(\mathbf{q},\omega)/\varepsilon_0\right)^{-1} = 1 + V_{\mathbf{q}}\,\mathrm{Im}\,\chi^{R}_{nn}(\mathbf{q},\omega)$ the zeros of the dielectric constant are at the same location as the poles of $\chi^{R}_{nn}(\mathbf{q},\omega)$ and, from what we just

said, these poles are located basically in the same $(\omega, \mathbf{q})$ domain as the particle-hole continuum of the non-interacting system, except for possibly a pair of poles. This situation is illustrated schematically in Fig.(41-5), that generalizes Fig.(39-6)

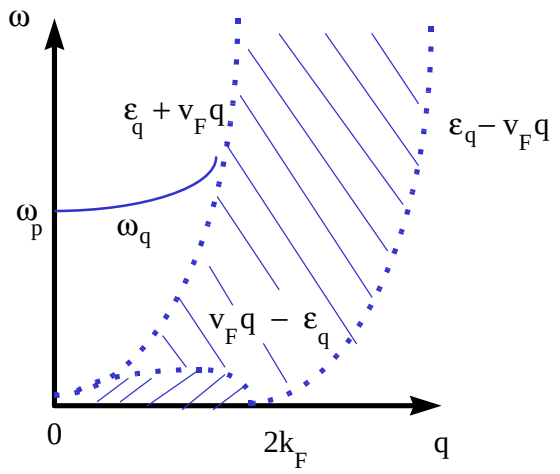


Figure 41-5 Schematic representation of the domain of frequency and wave vector where there are poles in the charge susceptibility, or zeros in the longitudinal dielectric function. In addition to the particle-hole continuum, there is a plasma pole.

41.2.2 Screening

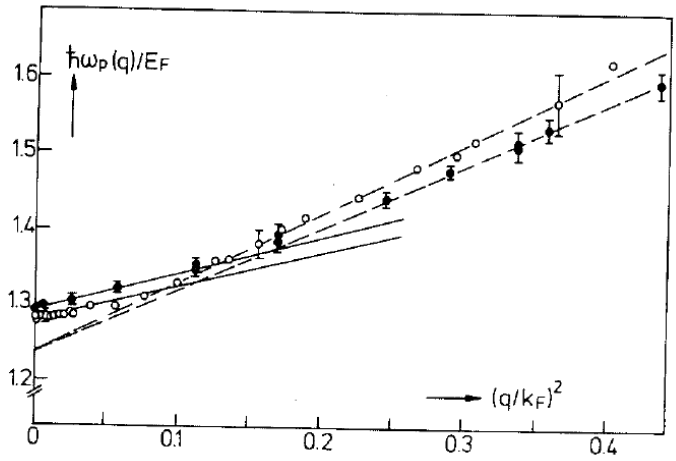
At zero frequency, namely for a static charge perturbation, the imaginary part of the dielectric constant vanishes, as shown by Eq.(41.12), while the real part Eq.(41.10) becomes

$$\frac{\varepsilon_1^L(\mathbf{q},0)}{\varepsilon_0} = 1 + \frac{q_{TF}^2}{q^2}\left[\frac{1}{2} + \frac{k_F}{2q}\left(1 - \frac{q^2}{(2k_F)^2}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right|\right] \tag{41.19}$$

In the long wave length limit, we recover our Thomas Fermi result Eq.(40.18). This limit can also be obtained directly by approximating the integral defining Lindhard function Eq.(39.25) that enters the RPA dielectric function Eqs.(41.9)

$$\begin{aligned}
\lim_{\mathbf{q}\to 0}\varepsilon_1^L(\mathbf{q},0) &= \lim_{\mathbf{q}\to 0}\left[1 - 2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}}\right] && (41.20)\\
&= \left[1 - 2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{\partial f(\zeta_{\mathbf{k}})}{\partial\zeta_{\mathbf{k}}}\right] && (41.21)\\
&= 1 + V_{\mathbf{q}}\frac{\partial}{\partial\mu}\left[2\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\right] && (41.22)\\
&= 1 + \frac{e^2}{\varepsilon_0 q^2}\frac{\partial n}{\partial\mu} && (41.23)\\
&= 1 + \frac{q_{TF}^2}{q^2} && (41.24)
\end{aligned}$$

Fig. 28



Plasmon dispersion curves for Al. Open circles from Kloos (1973), full circles from Petri and Otto (1975), dashed lines indicate their quadratic fit to the experimental data, solid line indicate their hquadratic fit by the present author to obtain α_{exp} (after Sturm 1978 d).

The definition of q_{TF} is in Eq.(40.16). The corresponding potential

$$V_{eff}(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3}\frac{e^2}{\varepsilon_0}\frac{1}{q^2+q_{TF}^2}e^{i\mathbf{q}\cdot\mathbf{r}} \propto \frac{e^2}{\varepsilon_0 r}e^{-rq_{TF}} \tag{41.25}$$

is the screened Coulomb interaction.

Remark 284 *The expression* $\varepsilon_1^L(\mathbf{q},0) = \varepsilon_0\left(1+V_{\mathbf{q}}\chi_{nn}^0(\mathbf{q},0)\right)$ *would be replaced by* $\varepsilon_1^L(\mathbf{q},0) = \varepsilon_0\left(1-V_{\mathbf{q}}\Pi_{nn}^{R(1)}(\mathbf{q},0)\right)$ *in the general case, with* $-\Pi_{nn}^{R(1)}(\mathbf{q},0)$ *the irreducible polarization. This is made clearer in Chap.(51). That quantity,* $\Pi_{nn}^{R(1)}(\mathbf{q},0)$*, is the sum of all the diagrams that cannot be cut in two by eliminating one interaction line. In general then,* $\partial n/\partial\mu$ *in Eq.(41.23) would be different from the non-interacting result. This is relevant in effective models such as the Hubbard model.*

41.2.3 Friedel oscillations

If instead of using the limiting Thomas-Fermi form for small wave vectors one does a more careful evaluation[15] of the Fourier transform of $\varepsilon_1(\mathbf{q},0)$ Eq.(41.19), one finds

$$\lim_{r\to\infty} V_{eff}(r) \propto \frac{\cos(2k_F r)}{r^3} \tag{41.26}$$

These are so-called Friedel oscillations. Returning to Fig. (39-5) you will recall that in Fourier space there are discontinuity in slopes at $q = 2k_F$. Friedel oscillations are the real-space manifestation of these discontinuity in slope. In other words they come from the real-space version of the logarithm at $q = 2k_F$. They manifest

themselves physically in several ways. For example they broaden NMR lines and they give rise to an effective interaction $J\mathbf{S}_1\cdot\mathbf{S}_2$ between magnetic impurities whose amplitude J oscillates in sign. This is the so-called RKKY interaction. The change in sign of J with distance is a manifestation of Friedel's oscillations. The Friedel oscillations originate in the sharpness of the Fermi surface. At finite temperature, where the Fermi surface broadens, they are damped as $e^{-k_F r(\Delta/E_F)}$ where Δ is of order T. Another way to write this last result is $e^{-r/\xi_{th}}$ where the thermal de Broglie wavelength is of order v_F/T in our units. Restoring physical units, that length is defined by setting the thermal energy uncertainty k_BT equal to $v_F\hbar\Delta k$ and identifying the spread in wave vector around k_F as $\Delta k \sim \xi_{th}^{-1}$. We will encounter this length in other contexts as well.

41.2.4 Plasmons and Landau Damping

We have already suggested in Fig.(41-4) that at small wave numbers, a large frequency pole far from the particle-hole continuum appears. Let us look at this parameter range. Taking v_Fq/ω as a small parameter, the imaginary part of the dielectric constant Eq.(41.12) is infinitesimal at the plasmon pole but vanishes everywhere else in its vicinity. On the other hand the limiting form of the real part of the dielectric constant may be obtained directly by expanding Eqs.(41.9) and (39.25). Indeed, when the frequency is large and outside the particle-hole continuum, we can write

$$\lim_{\mathbf{q}\ll\mathbf{k}_F}\lim_{\omega\gg\varepsilon_q+\mathbf{v}_Fq}\frac{\varepsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0}=\lim_{\mathbf{q}\to0}\lim_{\omega\gg\varepsilon_q+\mathbf{v}_Fq}\left[1-2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}\right] \tag{41.27}$$

$$=\lim_{\mathbf{q}\ll\mathbf{k}_F}\left[1+2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2}(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})\right] \tag{41.28}$$

$$=\lim_{\mathbf{q}\ll\mathbf{k}_F}\left[1+\frac{4V_{\mathbf{q}}}{\omega^2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})\right] \tag{41.29}$$

To obtain the last expression we did the change of variables $\mathbf{k}\to-\mathbf{k}-\mathbf{q}$ and used $\zeta_{\mathbf{k}+\mathbf{q}}=\zeta_{-\mathbf{k}-\mathbf{q}}$. The term linear in $\mathbf{q}$ vanishes when the angular integral is done and we are left with

$$\lim_{\mathbf{q}\ll\mathbf{k}_F}\lim_{\omega\gg\varepsilon_q+\mathbf{v}_Fq}\frac{\varepsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0}=1-\frac{2V_{\mathbf{q}}n}{\omega^2}\frac{q^2}{2m} \tag{41.30}$$

$$=1-\frac{\omega_p^2}{\omega^2} \tag{41.31}$$

with the value of $\omega_p^2=\frac{ne^2}{\varepsilon_0 m}$ defined in Eq.(40.39). One can continue the above approach to higher order or proceed directly with a tedious Taylor series expansion of the real part Eq.(41.10) in powers of v_Fq/ω to obtain

$$\lim_{\omega\gg\varepsilon_q+\mathbf{v}_Fq}\frac{\varepsilon_1^L(\mathbf{q}\to0,\omega)}{\varepsilon_0}=1-\frac{\omega_p^2}{\omega^2}-\frac{3}{5}\frac{\omega_p^2}{\omega^2}\frac{(v_Fq)^2}{\omega^2}+\ldots \tag{41.32}$$

Several physical remarks follow directly from this result

- Even at long wave lengths $(q \to 0)$, the interaction becomes unscreened at sufficiently high frequency. More specifically,

$$\frac{\varepsilon_1^L(\mathbf{q} \to 0, \omega \gg \omega_p)}{\varepsilon_0} \to 1 \tag{41.33}$$

- The collective plasma oscillation that we expected does show up. Indeed, $\varepsilon_1(\mathbf{q} \to 0, \omega) = 0$ when

$$0 = \omega^2 - \omega_p^2 - \frac{3}{5}\frac{\omega_p^2}{\omega^2}(v_F q)^2 + \ldots \tag{41.34}$$

$$\omega^2 \approx \omega_p^2 + \frac{3}{5}(v_F q)^2 + \ldots \tag{41.35}$$

Letting the right-had side be called ω_q, we have in the vicinity of this solution $\omega \approx \omega_q$

$$\frac{\varepsilon_1^L(\mathbf{q} \to 0, \omega)}{\varepsilon_0} \approx 1 - \frac{\omega_q^2}{\omega^2} \approx \frac{2}{\omega_q}(\omega - \omega_q) \tag{41.36}$$

which is precisely the form we had obtained from macroscopic considerations. We now know that the unknown constant we had at this time in Eq.(40.40) has the value $a = 2/\omega_q$.

Fig.(41-6) shows a plot of both the real and the imaginary parts of the dielectric constant for small wave vector $(q \ll q_{TF})$. We see that the dielectric constant is real and very large at zero frequency, representing screening, whereas the vanishing of the real part at large frequency leads to the plasma oscillations, the so-called plasmon. Given the scale of the figure, it is hard to see the limiting behavior $\varepsilon_1(\mathbf{q}, \infty) \to 1$ but the zero crossing is illustrated by the maximum in $\mathrm{Im}(1/\varepsilon)$. There is another zero crossing of ε_1 but it occurs in the particle-hole continuum where ε_2 is large. Hence this is an overdamped mode.

When q is sufficiently large that the plasmon enters the particle-hole continuum, damping becomes very large. This mechanism for damping is known as Landau damping.

41.2.5 $f-$sum rule

We have not checked yet whether the $f-$sum rule is satisfied. Let us first recall that it takes the form,

$$2\int_0^\infty \frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{nq^2}{m}. \tag{41.37}$$

Using our relation between dielectric constant and density fluctuations Eq.(39.2) $\varepsilon_0/\epsilon^L(\mathbf{q},\omega) = 1 - V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega)$ we obtain the corresponding sum rule for the longitudinal dielectric constant

$$\int_0^\infty \frac{d\omega}{2\pi}\omega\,\mathrm{Im}\left[\frac{\varepsilon_0}{\varepsilon^L(\mathbf{q} \to 0, \omega)}\right] = -V_{\mathbf{q}}\frac{nq^2}{4m} \tag{41.38}$$

$$= -\frac{ne^2}{4m\varepsilon_0} = -\frac{\omega_p^2}{4} \tag{41.39}$$

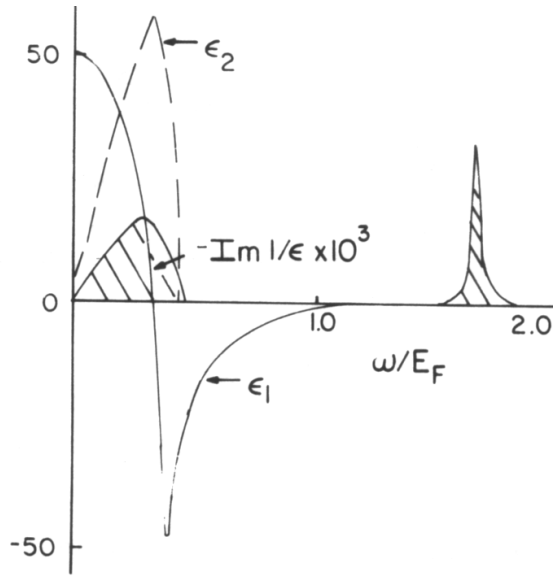


Figure 41-6 Real and imaginary parts of the dielectric constant and $\mathrm{Im}\,(1/\varepsilon)$ as a function of frequency, calculated for $r_s = 3$ and $q = 0.2k_F$. Shaded plots correspond to $\mathrm{Im}\,(1/\varepsilon)$. Taken from Mahan *op. cit.* p.430

Let us obtain the plasmon contribution to this sum rule by using the approximate form Eq.(41.36)

$$\int_0^\infty \frac{d\omega}{2\pi}\omega\,\mathrm{Im}\left[\frac{1}{\frac{2}{\omega_q}(\omega-\omega_q)+i\eta}\right] = -\pi\int_0^\infty \frac{d\omega}{2\pi}\omega\left|\frac{\omega_q}{2}\right|\delta(\omega-\omega_q) \quad (41.40)$$

$$= -\frac{\omega_q^2}{4} \quad (41.41)$$

This means that at $q = 0$, the plasmon exhaust the $f-$sum rule. Nothing else is necessary to satisfy this sum rule. On the other hand, for $q \neq 0$, one can check that the particle-hole continuum gives a contribution

$$-\frac{\omega_p^2}{4}+\frac{\omega_q^2}{4} = \frac{3}{20}(v_F q)^2 \quad (41.42)$$

as necessary to satisfy the $f-$sum rule.

Remark 285 *One of the key general problems in many-body theory is to devise approximations that satisfy conservation laws in general and the $f-$sum rule in particular. The RPA is such an approximation. This is non-trivial. It is a consequence of the fact that RPA is consistent with charge conservation. We will discuss this problem in more details later.*

42. SINGLE-PARTICLE PROPERTIES AND HARTREE-FOCK

We have already mentioned several times our strategy. First we will show the failure of Hartree-Fock and try to understand the reason for it by returning to consistency relations between self-energy and density fluctuations. Having cured the problem by using the screened interaction in the calculation, we will discuss the physical interpretation of the result, including a derivation of the Fermi liquid scattering rate that we discussed in the previous Part in the context of photoemission experiments.

It is useful to derive the result from the variational principle as well as directly from a Green's function point of view. Since Hartree-Fock is sometimes actually quite good, it is advisable to develop a deep understanding of this approach.

42.1 *Variational approach

In Hartree-Fock theory, we give ourselves a trial one-particle Hamiltonian and use the variational principle to find the parameters. In the electron gas case the true non-interacting part of the Hamiltonian is

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \frac{k^2}{2m} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{42.1}$$

where the spin-sum is represented by a sum over σ. The interacting part, written in Fourier space, takes the form

$$H - H_0 = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \sum_{\mathbf{q}} c^+_{\mathbf{k},\sigma} c^+_{\mathbf{k}',\sigma'} V_{\mathbf{q}} c_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} \tag{42.2}$$

with $V_{\mathbf{q}}$ the Fourier transform of the Coulomb potential

$$V_{\mathbf{q}} = \frac{e^2}{4\pi\varepsilon_0 q^2}. \tag{42.3}$$

Electroneutrality leads to $V_{\mathbf{q}=\mathbf{0}} = 0$ as before. The form of the interaction with all the proper indices is not difficult to understand when we consider the diagrammatic representation in Fig.(42-1). All that is needed is the conservation of momentum coming from integrals over all space and translational invariance. The factor of $1/\mathcal{V}$ in front comes from a factor $\mathcal{V}^{-1/2}$ for each change of variable from real-space to momentum space, $\left(\mathcal{V}^{-1/2}\right)^4$, and one overall factor of volume $\mathcal{V}$ from translational invariance which is used to eliminate one of the momentum sums through momentum conservation. Although there are several ways of labeling the momenta, the above one is convenient. In this notation $\mathbf{q}$ is often referred to as the "transfer variable" while $\mathbf{k}$ and $\mathbf{k}'$ are the band variables.

To apply the variational principle, one takes

$$\boxed{\widetilde{H}_0 = \textstyle\sum_{\mathbf{k},\sigma} \widetilde{\epsilon}_{\mathbf{k}} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}} \tag{42.4}$$

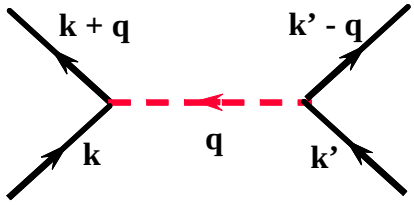


Figure 42-1 Momentum conservation for the Coulomb interaction.

with the variational parameter $\widetilde{\epsilon}_{\mathbf{k}}$. Using the Feynman variational principle, also known as Bogoliubov's inequality, Eq.(33.74), we minimize the right-hand side of

$$\boxed{-T\ln Z \leq -T\ln Z_0 + \left\langle H-\widetilde{H}_0\right\rangle_0.} \tag{42.5}$$

The partition function for $\widetilde{H}_0 - \mu N$ is computed as usual for non-interacting electrons

$$-T\ln Z_0 = -T\ln\prod_{\mathbf{k},\sigma}\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right) = -T\sum_{\mathbf{k},\sigma}\ln\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right). \tag{42.6}$$

Then the quantity $\left\langle H-\widetilde{H}_0\right\rangle_0$ is easily evaluated as sums of products of pairs of Green's functions since the average is taken in the case where there are no interactions, i.e. $\widetilde{H}_0$ is quadratic in creation-annihilation operators. This can be derived from the functional derivative approach and is the content of Wick's theorem. Here we use it directly to obtain,

$$\left\langle H-\widetilde{H}_0\right\rangle_0 = \sum_{\mathbf{k},\sigma}\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right)\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0 \tag{42.7}$$

$$+\frac{1}{2\mathcal{V}}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'}\sum_{\mathbf{q}}V_{\mathbf{q}}\left[\left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k}'-\mathbf{q},\sigma'}\right\rangle_0\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k}+\mathbf{q},\sigma}\right\rangle_0 - \left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k}+\mathbf{q},\sigma}\right\rangle_0\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k}'-\mathbf{q},\sigma'}\right\rangle_0\right]. \tag{42.8}$$

which may be simplified by using

$$\left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k},\sigma}\right\rangle_0 = \delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0 \equiv \delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}f\left(\widetilde{\zeta}_{\mathbf{k}}\right) = \frac{1}{e^{\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}+1} \tag{42.9}$$

to obtain

$$\left\langle H-\widetilde{H}_0\right\rangle_0 = \sum_{\mathbf{k},\sigma}\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right)f\left(\widetilde{\zeta}_{\mathbf{k}}\right) - 2\frac{1}{2\mathcal{V}}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}V_{\mathbf{k}'-\mathbf{k}}f\left(\widetilde{\zeta}_{\mathbf{k}'}\right)f\left(\widetilde{\zeta}_{\mathbf{k}}\right) \tag{42.10}$$

where the overall factor of 2 comes from what is left of the spin sums. We have dropped the term that leads to $V_{\mathbf{q}=\mathbf{0}}$ as usual because of the neutralizing background.

We can now determine our variational parameter $\widetilde{\epsilon}_{\mathbf{k}}$ by minimizing with respect to it:

$$\frac{\partial}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left[-T\sum_{\mathbf{k},\sigma}\ln\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right)\right] = \frac{2e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}}{\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right)} = 2f\left(\widetilde{\zeta}_{\mathbf{k}}\right) \tag{42.11}$$

$$\frac{\partial}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left\langle H-\widetilde{H}_0\right\rangle_0 = -2f\left(\widetilde{\zeta}_{\mathbf{k}}\right) + \frac{\partial f\left(\widetilde{\zeta}_{\mathbf{k}}\right)}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left[2\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right) - \frac{2}{\mathcal{V}}\sum_{\mathbf{k}'}V_{\mathbf{k}'-\mathbf{k}}f\left(\widetilde{\zeta}_{\mathbf{k}'}\right)\right]. \tag{42.12}$$

Setting the sum of the last two equations to zero, we see that the coefficient of the square bracket must vanish. Using $V_{\mathbf{q}} = V_{-\mathbf{q}}$ we then have

$$\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} V_{\mathbf{k}'-\mathbf{k}} f\left(\widetilde{\zeta}_{\mathbf{k}'}\right) = \epsilon_{\mathbf{k}} - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} V_{\mathbf{k}-\mathbf{k}'} f\left(\widetilde{\zeta}_{\mathbf{k}'}\right) \tag{42.13}$$

$$\boxed{\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 |\mathbf{k}-\mathbf{k}'|^2} \frac{1}{e^{\beta(\widetilde{\epsilon}_{\mathbf{k}'}-\mu)}+1}} \tag{42.14}$$

As usual the chemical potential is determined by fixing the number of particles. Before we evaluate this integral let us obtain this same result from the Green's function point of view.

In principle we should check that the extremum point that we found by taking the first derivative is a minimum. An alternate derivation of the Hartree-Fock equations may be found in Appendix C.

42.2 Hartree-Fock from the point of view of Green's functions

The above equation Eq.(42.15) may be obtained directly from the Schwinger or Feynman approaches. First, recall that the Hartree term disappears because it involves $V_{\mathbf{q}=0} = 0$ that vanishes because of the neutralizing background.

Remark 286 *The Hartree term vanishes in the translationally invariant case. Note that to obtain the first term of the irreducible vertex entering the RPA equation, Fig.(37-3), the Hartree term in the self-energy does not vanish. It is because we cannot assume translational invariance during the process where we take functional derivvatives. Indeed, while we are doing that, there is a source field that breaks that symmetry.*

Keeping only the Fock term in the self-energy we get a minus sign when we work directly in the Schwinger approach. In the Feynman approach, the minus sign is there because we compute to first order and there is no fermion loop. Furthermore, we have the $e^{ik'_n\eta}$ convergence factor with $\eta = 0^+$ in the Feynman approach. In the Schwinger approach, it comes form the $+$ in $V(1-3)\mathcal{G}^0(1,3^+)$ in Eq.(36.34) and from the $\delta(\tau_1 - \tau_3)$ in the potential energy. Ultimately, this order at equal time comes from the fact that in the potential energy, creation operators are to the left. Assuming that the Green's function that appears in the diagram is a dressed Green's function, as appears naturally in the Schwinger approach, we obtain (for the Schwinger approach see Eq. (37.25))

$$\boxed{\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{e^2}{\varepsilon_0 |\mathbf{k}-\mathbf{k}'|^2} \frac{1}{ik'_n - (\epsilon_{\mathbf{k}'}-\mu) - \Sigma^{(1)}(\mathbf{k}')} e^{ik'_n\eta}}. \tag{42.15}$$

Since the potential is frequency independent, notice that the sum over ik'_n is easily performed and that $\Sigma^{(1)}(\mathbf{k})$ is independent of external frequency ik_n. Defining the new pole of the Green's function $\widetilde{\epsilon}_{\mathbf{k}}$ by

$$\widetilde{\epsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}), \tag{42.16}$$

before we do the sum over ik'_n, it is easy to see that we recover the Hartree-Fock result Eq. (42.14).

From the point of view of non-interacting Green's functions, it looks as if the perturbation expansion for the full Green's function, illustrated by a thick arrow in Fig.(42-2), was written in terms of a perturbation series that involves the full Green's function itself. Iterating shows that in this approximation we have a self-energy that resums the infinite subset of diagrams illustrated on the bottom part of this same figure. In the Feynman approach, one commonly says that all the "rainbow" diagrams have been summed. In principle this Hartree-Fock Green's

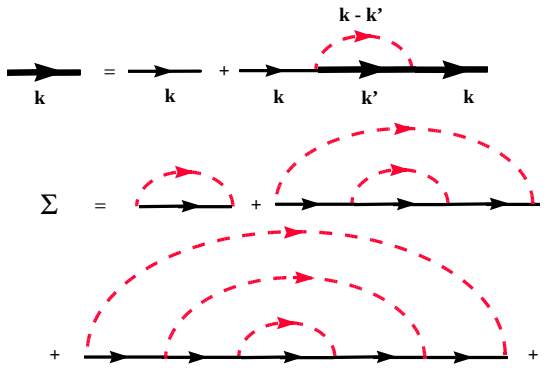


Figure 42-2 Hartree-Fock as a self-consistent approximation for the Green's function. This self-consistent approximation is equivalent to a self-energy that sums all the rainbow diagrams illustrated on the bottom part of the figure. The thick line is the full Green's function.

function may be used in further perturbative calculations. We just have to be careful not to double-count the diagrams we have already included.

42.3 Hartree-Fock from the point of view of renormalized perturbation theory and effective medium theories

We want to do perturbation theory but using this time for the Hamiltonian

$$H = \widetilde{H}_0 + \left(H_0 - \widetilde{H}_0 + V \right) \tag{42.17}$$

That is a trick that I will use repeatedly when we study broken symmetries and phase transitions. That is not the case here, but it is a nice and easy warmup. The unperturbed Hamiltonian is now $\widetilde{H}_0$ and we assume that it takes the same form as Eq.(42.4) above. In addition to the usual perturbation V, there is now a translationally invariant one-body potential $H_0 - \widetilde{H}_0$. One determines the self-energy in such a way that $\widetilde{H}_0$ becomes the best "effective medium" in the sense that to first order in $\left(H_0 - \widetilde{H}_0 + V \right)$ the self-energy calculated in this effective medium vanishes completely. This is illustrated in Fig.(42-3). This kind of approach is also known as renormalized perturbation theory [25].

The so-called Hartree diagram (or tadpole diagram) with one loop does not contribute because it is proportional to $V_{\mathbf{q}=0} = 0$. The Hartree term is in a sense the classical contribution coming from the interaction of the electron with the

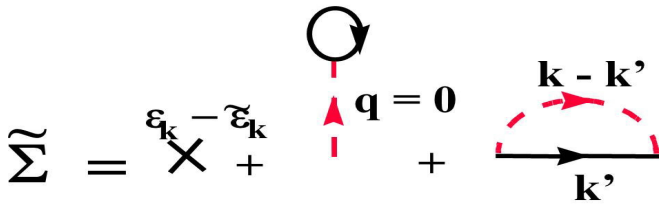


Figure 42-3 Effective medium point of view for the Hartree-Fock approximation. In this figure, the propagators are evaluated with the effective medium $\tilde{H}_0$.The Hartree term is known as the tadpole diagram and the Fock term as the sunrise diagram.

average charge density. Because of electroneutrality here it vanishes. The last diagram on the right of the figure is the Fock term that comes from exchange and is a quantum effect. Algebraically, Fig.(42-3) gives

$$\widetilde{\Sigma} = \epsilon_{\mathbf{k}} - \widetilde{\epsilon}_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) = 0 \tag{42.18}$$

Using the expression for the exchange, or Fock, diagram $\Sigma^{(1)}(\mathbf{k})$ we obtain for $\Sigma^{(1)}(\mathbf{k})$

$$\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{e^2}{\varepsilon_0 \left|\mathbf{k}-\mathbf{k}'\right|^2} \widetilde{\mathcal{G}}^0(\mathbf{k}', ik'_n)\, e^{ik'_n \eta} \tag{42.19}$$

that we can evaluate using our formula for Matsubara sums. Substituting back into Eq.(42.18) we get precisely our Hartree-Fock result Eq.(42.14) obtained from the variational principle. Performing the summation over Matsubara frequencies and using Eq.(42.18) to relate $\widetilde{\epsilon}_{\mathbf{k}}$ to $\Sigma^{(1)}(\mathbf{k})$, this expression is found identical to our earlier variational result Eq.(42.14). Using that same equation Eq.(42.18) for $\widetilde{\epsilon}_{\mathbf{k}}$, we can remove all reference to $\widetilde{\epsilon}_{\mathbf{k}}$ and write the above equation in the same form as Eq. (42.15) for the self-energy that we found directly from the Schwinger approach.

Remark 287 *In all higher order diagrams, if a Green's function is dressed by a rainbow diagram in the Feynman formalism, these diagrams are removed and the Green's function is judt replaced by the dressed Green's function that I just discussed. That is a special case of a skeleton expansion.*

42.4 The pathologies of the Hartree-Fock approximation for the electron gas.

To evaluate our expression for the Hartree-Fock self-energy $\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k})$ Eq.(42.14) we need the chemical potential. As usual in the grand-canonical ensemble, the chemical potential is determined by requiring that we have the correct

density. Let us suppose then that we have a density n. Then

$$n = 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} T\sum_{ik_n} \widetilde{\mathcal{G}}^0(\mathbf{k}, ik_n)\, e^{ik_n\eta} \tag{42.20}$$

$$= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\beta\left(\epsilon_{\mathbf{k}}+\Sigma^{(1)}(\mathbf{k})-\mu\right)}+1} \tag{42.21}$$

Let us focus on the zero temperature case. Then the Fermi function is a step function and the last integral reduces to

$$n = 2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\theta\left(k_F - |\mathbf{k}|\right) \tag{42.22}$$

where the chemical potential is given by

$$\epsilon_{\mathbf{k}_F} + \Sigma^{(1)}(\mathbf{k}_F) - \mu = 0 \tag{42.23}$$

The equation Eq.(42.22) that gives us n tells us that k_F is precisely the same as in the non-interacting case. This is an elementary example of a much more general theorem due to Luttinger that we will discuss in a later chapter. This theorem says that the volume enclosed by the Fermi surface is independent of interactions. Clearly, if μ_0 is the value of the chemical potential in the non-interacting system, then $\Sigma^{(1)}(\mathbf{k}_F) - \mu = -\mu_0$.

The integral to do for the Hartree-Fock self-energy is thus, at zero temperature

$$\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^2}{\varepsilon_0\left|\mathbf{k}-\mathbf{k}'\right|^2}\theta\left(k_F - |\mathbf{k}'|\right) \tag{42.24}$$

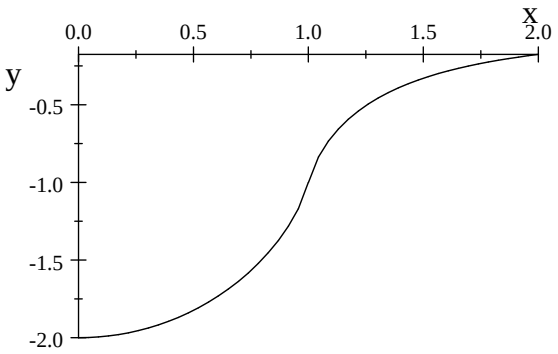
$$= -\frac{e^2}{\varepsilon_0 8\pi^3}\int_0^{k_F}(k')^2\,dk'\int_{-1}^{1}\frac{2\pi d(\cos\theta)}{k^2+(k')^2-2kk'\cos\theta} \tag{42.25}$$

$$= -\frac{e^2}{4\pi^2\varepsilon_0}\int_0^{k_F} k'\frac{1}{-2k}\ln\left(\left|\frac{(k'-k)^2}{(k+k')^2}\right|\right)dk' \tag{42.26}$$

We evaluated the integral as a principal part integral because we have argued that the potential should have no $q=0$ component which means $\left|\mathbf{k}-\mathbf{k}'\right|^2 \neq 0$. Pursuing the calculation, we have

$$\Sigma^{(1)}(\mathbf{k}) = -\frac{e^2}{4\pi^2\varepsilon_0}k_F\left[1+\frac{1-y^2}{2y}\ln\left(\left|\frac{1+y}{1-y}\right|\right)\right] \quad ; \quad y \equiv \frac{k}{k_F} \tag{42.27}$$

The function $\Sigma^{(1)}(\mathbf{k}) / \left(\frac{e^2}{4\pi^2\varepsilon_0}k_F\right)$ is plotted in Fig.(42.4).



Plot of the Hartree-Fock self-energy at zero temperature.

$\Sigma^{(1)}(k/k_F) / \left(\frac{e^2}{4\pi^2\varepsilon_0}k_F\right)$

Since $\lim_{x\to 0} x \ln x = 0$, we have that

$$\Sigma^{(1)}(\mathbf{k}_F) = -\frac{e^2}{4\pi^2\varepsilon_0} k_F \tag{42.28}$$

The ratio of this term to the zeroth order term, namely the kinetic energy $k_F^2/2m$ is of order r_s

$$\propto \frac{me^2 k_F}{k_F^2 \varepsilon_0} \propto \frac{1}{k_F a_0} \propto r_s \tag{42.29}$$

as can be seen using the definitions Eqs.(40.2)(40.5).

Up to here everything seems to be consistent, except if we start to ask about the effective mass. The plot of the self-energy suggests that there is an anomaly in the slope at $y = 1$ (or $k = k_F$). This reflects itself in the effective mass. Indeed, using the general formula found in the previous chapter, Eq.(31.33)

$$\frac{m}{m^*} = \lim_{\mathbf{k}\to\mathbf{k}_F} \frac{1 + \frac{\partial}{\partial\zeta_{\mathbf{k}}} \mathrm{Re}\,\Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial\omega} \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\big|_{\omega = E_{\mathbf{k}} - \mu}} = 1 + \frac{dk}{d\zeta_{\mathbf{k}}} \frac{\partial\Sigma^{(1)}(\mathbf{k})}{\partial k}\bigg|_{k=k_F} \tag{42.30}$$

we have

$$\frac{\partial\Sigma^{(1)}(\mathbf{k})}{\partial k}\bigg|_{k=k_F} \propto k_F \left(\frac{dy}{dk}\right)_{y=1} \frac{d\left[1 + \frac{1-y^2}{2y} \ln\left(\left|\frac{1+y}{1-y}\right|\right)\right]}{dy}\bigg|_{y=1} . \tag{42.31}$$

The problem comes from $\ln(1-y)$. Let us concentrate on the contributions proportional to this term

$$\begin{aligned} \frac{d}{dy}\left[\left(\frac{1}{2y} - \frac{y}{2}\right)\ln(1-y)\right] &= \left(-\frac{1}{2y^2} - \frac{1}{2}\right)\ln(1-y) \\ &\quad - \left(\frac{1}{2y} - \frac{y}{2}\right)\frac{1}{1-y} \end{aligned} \tag{42.32}$$

As $y \to 1$ we obtain a singularity from $\ln(0) = -\infty$. This corresponds to the unphysical result $m^* = 0$. An effective mass smaller than the bare mass is possible but rather unusual. This is seen for example in three dimension for very small r_s (table 8.7 in Giuliani-Vignale [82]). However, in general, interactions will make quasiparticles look heavier. The result $m^* = 0$ obtained here is as close to ridiculous as one can imagine.

The physical reason for the failure of Hartree-Fock is the following. It is correct to let the electron have exchange interaction of the type included in rainbow diagrams do, but it is incorrect to neglect the fact that the other electrons in the background will also react to screen this interaction. We discuss this in more details below.

43. *MORE FORMAL MATTERS: CONSISTENCY RELATIONS BETWEEN SINGLE-PARTICLE SELF-ENERGY, COLLECTIVE MODES, POTENTIAL ENERGY AND FREE ENERGY

To cure the above pathology, it will be useful to relate self-energy to density fluctuations. This is in a sense already done if you followed the Schwinger approach. You need to read this Chapter if you followed the Feynman approach. Otherwise part of its main message has already been mentioned in earlier sections and the considerations on the free energy will come later.

We have found an expression for the density fluctuations that appears correct since it has all the correct Physics. It was a non-trivial task since we had to sum an infinite subset of diagrams. We will see that it is also difficult to obtain the correct expression for the self-energy without a bit of physical hindsight. We might have thought that the variational principle would have given us a good starting point but we will see that in this particular case it is a disaster. The following theorems will help us to understand why this is so and will suggest how to go around the difficulty.

We thus go back to some formalism again to show that there is a general relation between self-energy and charge fluctuations. We will have a good approximation for the self-energy only if it is consistent with our good approximation for the density fluctuations. We also take this opportunity to show how to obtain the self-energy since just a few additional lines will suffice.

43.1 *Consistency between self-energy and density fluctuations

43.1.1 *Equations of motion for the Feynmay way

You do not need to read this section if you have followed the source field approach. You can skip to the next subsection. We start from the equations of motion for the Green's function. We need first those for the field operators.

$$\frac{\partial \psi(1)}{\partial \tau_1} = -[\psi(1), K] \tag{43.1}$$

Using $[A,BC]=\{A,B\}C-B\{A,C\}$ and Eq.(38.1) for K we have

$$\begin{aligned}\frac{\partial\psi_{\sigma_1}(\mathbf{x}_1,\tau_1)}{\partial\tau_1} &= \frac{\nabla_1^2}{2m}\psi_{\sigma_1}(\mathbf{x}_1,\tau_1)+\mu\psi_{\sigma_1}(\mathbf{x}_1,\tau_1) \\ &-\sum_{\sigma_{1'}}\int d\mathbf{x}_{1'}v(\mathbf{x}_1-\mathbf{x}_{1'})\psi^\dagger_{\sigma_{1'}}(\mathbf{x}_{1'},\tau_1)\psi_{\sigma_{1'}}(\mathbf{x}_{1'},\tau_1)\psi_{\sigma_1}(\mathbf{x}_1,\tau_1)\end{aligned} \tag{43.2}$$

Remark 288 *We assume that the potential has no $q=0$ component because of the compensating effect of the positive background. The argument for the neutralizing background is as follows. If we had kept it, the above equation would have had an extra term*

$$+n\left[\int d\mathbf{x}_{1'}v(\mathbf{x}_1-\mathbf{x}_{1'})\right]\psi_{\sigma_1}(\mathbf{x}_1,\tau_1) \tag{43.3}$$

The $\mathbf{q}=\mathbf{0}$ contribution of the potential in the above equation of motion gives on the other hand a contribution

$$-\left[\int d\mathbf{x}_{1'}v(\mathbf{x}_1-\mathbf{x}_{1'})\right]\left[\frac{1}{\mathcal{V}}\int d\mathbf{x}_{1'}\sum_{\sigma_{1'}}\psi^\dagger_{\sigma_{1'}}(\mathbf{x}_{1'},\tau_1)\psi_{\sigma_{1'}}(\mathbf{x}_{1'},\tau_1)\right]\psi_{\sigma_1}(\mathbf{x}_1,\tau_1) \tag{43.4}$$

While the quantity in bracket is an operator and not a number, its deviations from n vanish like $\mathcal{V}^{-1/2}$ in the thermodynamic limit, even in the grand-canonical ensemble. Hence, to an excellent degree of approximation we may say that the only effect of the neutralizing background is to remove the $q=0$ component of the Coulomb potential. The result that we are about to derive would be different in other models, such as the Hubbard model, where the $q=0$ component of the interaction potential is far from negligible.

Reintroducing our time-dependent potential Eq.(38.7) the above result can be written in the shorthand notation

$$\frac{\partial\psi(1)}{\partial\tau_1}=\frac{\nabla_1^2}{2m}\psi(1)+\mu\psi(1)-\int_{1'}\psi^\dagger(1')\,V(1-1')\,\psi(1')\,\psi(1) \tag{43.5}$$

From this, we can easily find the equation of motion for the Green's function

$$\mathcal{G}(1,2)=-\left\langle T_\tau\left[\psi(1)\,\psi^+(2)\right]\right\rangle \tag{43.6}$$

namely,

$$\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\mathcal{G}(1,2)=-\delta(1-2)+\left\langle T_\tau\left[\int_{1'}\psi^\dagger(1'^+)\,V(1-1')\,\psi(1')\,\psi(1)\,\psi^\dagger(2)\right]\right\rangle \tag{43.7}$$

where as usual the delta function comes from the action of the time derivative on the θ functions implicit in the time ordered product. The right-hand side is not far from what we want. The last term on the right-hand side can be related to the product of the self-energy with the Green's function since, comparing the equation of motion for the Green's function with Dyson's equation

$$\mathcal{G}_0^{-1}\mathcal{G}=1+\Sigma\mathcal{G} \tag{43.8}$$

we have that

$$\boxed{\int_{1''}\Sigma(1,1'')\,\mathcal{G}(1'',2)=-\left\langle T_\tau\left[\int_{1'}\psi^\dagger(1'^+)\,V(1'-1)\,\psi(1')\,\psi(1)\,\psi^\dagger(2)\right]\right\rangle} \tag{43.9}$$

which, in all generality, can be taken as a *definition* of the self-energy.

The last equation (43.9) has been derived also in Eq.(36.13) in a different notation if you followed the functional derivative approach. In this section we keep the integral on space-time coordinates explicitly. If you have read the first remark in Sec. 36.2 the first few equations below are nothing new.

In the limit $2 \rightarrow 1^+$ where

$$1^+ \equiv \left(\mathbf{x}_1, \tau_1 + 0^+; \sigma_1\right) \tag{43.10}$$

the term on the right-hand side of Eq.(43.9) is

$$\left\langle T_\tau \left[\int_{1'} \psi^\dagger \left(1^+\right) \psi^\dagger \left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle$$

where we have written explicitly the integral. Note that we have placed $\psi^\dagger(2) \rightarrow \psi^\dagger\left(1^+\right)$ to the far left of the three fermion operators $\psi^\dagger\left(1'\right)\psi\left(1'\right)\psi\left(1\right)$ because the potential is instantaneous and these three fermion operators are all at the same time and in the given order. Recalling the definition of the average potential energy

$$2\left\langle V\right\rangle = \sum_{\sigma_1} \int d^3\mathbf{x}_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger \left(1^+\right) \psi^\dagger \left(1'\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle \tag{43.11}$$

we directly get from Eq.(43.9) above a relation between self-energy and potential energy

$$\sum_{\sigma_1} \int d^3\mathbf{x}_1 \int_{1'} \Sigma\left(1,1'\right) \mathcal{G}\left(1',1^+\right) = 2\left\langle V\right\rangle \tag{43.12}$$

We have the freedom to drop the time-ordered product when we recall that the operators are all at the same time and in the indicated order. Using time-translational invariance the last result may also be written

$$\boxed{\int_1 \int_{1'} \Sigma\left(1,1'\right) \mathcal{G}\left(1',1^+\right) = 2\left\langle V\right\rangle \beta = \int_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger \left(1^+\right) \psi^\dagger \left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle} \tag{43.13}$$

Remark 289 *The 1^+ on the left-hand side is absolutely necessary for this expression to make sense. Indeed, taken from the point of view of Matsubara frequencies, one knows that the self-energy goes to a constant at infinite frequency while the Green's function does not decay fast enough to converge without ambiguity. On the right-hand side of the above equation, all operators are at the same time, in the order explicitly given.*

The right-hand side of the last equation is in turn related to the density-density correlation function. To see this, it suffices to return to space spin and time indices and to recall that the potential is instantaneous and spin independent so that

$$2\left\langle V\right\rangle \beta = \int_{1'} \int_{1} \left\langle \psi^\dagger \left(1^+\right) \psi^\dagger \left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right\rangle \tag{43.14}$$

$$\begin{aligned} = & -\beta \sum_{\sigma_1,\sigma_{1'}} \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle \psi^\dagger_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \psi_{\sigma_1}\left(\mathbf{x}_1\right) \right\rangle \delta_{\sigma_1,\sigma_{1'}} \delta\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \\ & +\beta \sum_{\sigma_1,\sigma_{1'}} \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle \psi^\dagger_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) \psi_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \psi^\dagger_{\sigma_1}\left(\mathbf{x}_1\right) \psi_{\sigma_1}\left(\mathbf{x}_1\right) \right\rangle \\ = & -n\mathcal{V}\beta v\left(0\right) + \beta \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle n\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) n\left(\mathbf{x}_1\right) \right\rangle \end{aligned} \tag{43.15}$$

where in the last equation we have used

$$\int d^3\mathbf{x}_1 \sum_{\sigma_1} \left\langle \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\,\psi_{\sigma_1}(\mathbf{x}_1)\right\rangle = N = n\mathcal{V} \tag{43.16}$$

Going to Fourier space, we have

$$\int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle n(\mathbf{x}_{1'})\, v(\mathbf{x}_{1'}-\mathbf{x}_1)\, n(\mathbf{x}_1)\right\rangle \tag{43.17}$$

$$= \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 v(\mathbf{x}_{1'}-\mathbf{x}_1)\,\chi_{nn}(\mathbf{x}_{1'},0;\mathbf{x}_1 0) \tag{43.18}$$

$$= \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[\lim_{\tau\to 0} \mathcal{V}\chi_{nn}(\mathbf{q},\tau)\right] \tag{43.19}$$

We did not have to take into account the disconnected piece that appears in Eq.(43.17) but not in $\chi_{nn}(\mathbf{q},\tau)$ because this disconnected piece contributes only at $\mathbf{q}=0$ and we have argued that $V_{\mathbf{q}=0}=0$. Note that there is no jump in $\chi_{nn}(\mathbf{q},\tau)$ at $\tau=0$ contrary to the case of the single-particle Green's function. Substituting back into Eq.(43.15) we have

$$2\langle V\rangle\beta = \int_{1'}\int_1 \left\langle \psi^\dagger(1^+)\,\psi^\dagger(1'^+)\; V(1'-1)\,\psi(1')\,\psi(1)\right\rangle = \tag{43.20}$$

$$\begin{aligned} &= \beta\mathcal{V}\left[-nv(0) + \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} T\sum_{iq_n} \chi_{nn}(\mathbf{q},iq_n)\right] \\ &= \beta\mathcal{V}\left[\int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) - n\right]\right] \end{aligned}$$

Substituting the above Eq.(43.20) into the consistency relation between self-energy and potential energy Eq.(43.13) and then using invariance under time and space translations as well as spin rotation symmetry to replace $\int_1$ by $2\beta\mathcal{V}$, this gives the following relation between self-energy and density fluctuations

$$\int_{1'} \Sigma(1,1')\,\mathcal{G}(1',1^+) = \tag{43.21}$$

$$T\sum_{ik_n}\int \frac{d^3k}{(2\pi)^3}\Sigma(\mathbf{k},ik_n)\,G(\mathbf{k},ik_n)\,e^{ik_n\eta} \tag{43.22}$$

$$= \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) - n\right]. \tag{43.23}$$

This plays the role of a sum-rule relating single-particle properties, such as the self-energy and Green function, to a two-particle quantity, the density-density correlation function or potential energy.

Remark 290 *In short range models, we need to restore the $v_{\mathbf{q}=\mathbf{0}}$ component and the disconnected piece has to be treated carefully. Also, the spin fluctuations will come in. This subject is for the chapter on the Hubbard model.*

44. SECOND STEP OF THE APPROXIMATION: GW CURING HARTREE-FOCK THEORY

In this Section, we present the solution to the failure of Hartree-Fock that was found by Gell-Man and Brueckner[17]. In brief, in the first step of the calculation we obtained collective modes with bare Green's functions. We saw that just trying to do Hartree-Fock at the single-particle level was a disaster. Now we want to improve our calculation of the single-particle properties. The Physics is that the interaction appearing in Hartree-Fock theory should be screened. Or equivalently, the self-energy that we find should be consistent with the density fluctuations found earlier since $\Sigma\mathcal{G}$ is simply related to density fluctuations. The resulting expresssion that we will find is also known as the GW approximation. We will come back on this nomenclature in Chapter 49.

The first subsection should be read if you follow the Feynman way. Otherwise, skip to the next subsection.

44.1 *An approximation for $\sum$ that is consistent with the Physics of screening

For Feynman afficionados, we have seen in a previous Chapter, more specifically Eq.(43.21), that the self-energy is related to density fluctuations. More specifically, if we multiply the self-energy by the Green's function and take the trace, we should have the same thing basically as we would by multiplying the density-density correlation function by the potential and taking the trace. This is illustrated schematically for the Hartree-Fock approximation by the diagram of Fig.(44-1). The diagram on the left is built from the rainbow self-energy of Fig.(42-2) by multiplying it by a dressed Green's function. The one on the right is obtained by taking a single bubble with dressed propagators and multiplying by a potential. The change of integration variables $\mathbf{k}-\mathbf{k}'=-\mathbf{q}$ shows trivially that the diagrams are identical. The extra term that appears on the right-hand side of the relation between self-energy and density Eq.(43.21) is due to the fact that one forces the Green's functions to correspond to a given time order in the self-energy calculation that is different from the one appearing naturally on the right-hand side.

Remark 291 *Equality (43.21) for the Hartree-Fock approximation. Let us check just the sums over Matsubara frequencies on both sides of Eq.(43.21) to see that they are identical. First, the sum on the left hand-side.*

$$T\sum_{ik_n} T\sum_{ik'_n} \frac{e^{ik_n\eta}}{ik_n-\zeta_{\mathbf{k}}}\frac{e^{ik'_n\eta}}{ik'_n-\zeta_{\mathbf{k}'}} = f\left(\zeta_{\mathbf{k}}\right) f\left(\zeta_{\mathbf{k}'}\right) \tag{44.1}$$

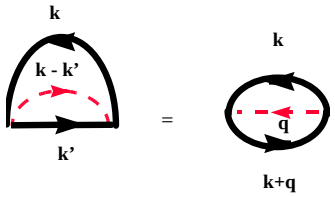


Figure 44-1 Approximation for the density fluctuations that corresponds to the Hartree-Fock self-energy.

While the sum on the right-hand side is

$$T\sum_{ik_n} T\sum_{iq_n} \frac{1}{ik_n - \zeta_{\mathbf{k}}} \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}'}} \tag{44.2}$$

$$= T\sum_{ik_n} T\sum_{q_n} \left[\frac{1}{ik_n - \zeta_{\mathbf{k}}} - \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}'}}\right] \frac{1}{iq_n - \zeta_{\mathbf{k}'} + \zeta_{\mathbf{k}}} \tag{44.3}$$

$$= T\sum_{q_n} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})}{iq_n - \zeta_{\mathbf{k}'} + \zeta_{\mathbf{k}}} = -\left[f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})\right] n_B(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}}) \tag{44.4}$$

where we used, with n_B the Bose function

$$T\sum_{q_n} \frac{1}{iq_n - a} = -n_B(a) \quad or \quad -n_B(a) - 1 \tag{44.5}$$

The result of the sum depends on the convergence factor but the -1 in the second possibility does not contribute once the sum over wave vectors are done. We are thus left only with

$$\begin{aligned} -\left[f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})\right] n_B(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}}) &= -\frac{e^{\beta\zeta_{\mathbf{k}'}} - e^{\beta\zeta_{\mathbf{k}}}}{(e^{\beta\zeta_{\mathbf{k}'}} + 1)(e^{\beta\zeta_{\mathbf{k}}} + 1)} \frac{1}{e^{\beta(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}})} - 1} \\ &= -\frac{e^{\beta\zeta_{\mathbf{k}}}}{(e^{\beta\zeta_{\mathbf{k}'}} + 1)(e^{\beta\zeta_{\mathbf{k}}} + 1)} \qquad (44.6) \\ &= -(1 - f(\zeta_{\mathbf{k}}))\, f(\zeta_{\mathbf{k}'}) \qquad (44.7) \end{aligned}$$

Eq.(44.1) and the last equation are not strictly equal and that is why it is necessary to subtract n in Eq.(44.1).

Fig.(44-1) shows that the Hartree-Fock approximation corresponds to a very poor approximation for the density fluctuations, namely one that has no screening, and no plasma oscillation. Knowing that the RPA approximation for the density has all the correct properties, it is clear that we should use for the self-energy the expression appearing in Fig.(44-2). Indeed, in such a case, multiplying Σ by $\mathcal{G}^0$ gives a a result, illustrated in Fig.(44-3) that does correspond to multiplying the RPA expression for the density Fig.(41-2) by $V_{\mathbf{q}}$ and summing over $\mathbf{q}$. These are the ring diagrams.

Using Feynman's rules, the corresponding analytical expression is

$$\begin{aligned} \Sigma_{RPA}(\mathbf{k}, ik_n) &= \qquad (44.8) \\ &\quad -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{iq_n} \frac{V_{\mathbf{q}}}{1 + V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q}, iq_n)} \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \\ &= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{iq_n} \frac{V_{\mathbf{q}}}{\varepsilon(\mathbf{q}, iq_n)} \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \end{aligned}$$

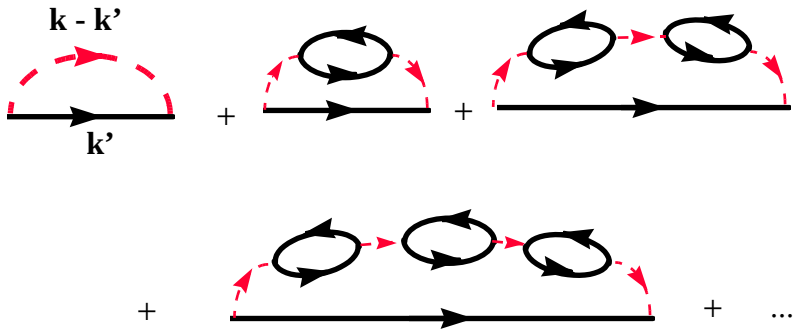


Figure 44-2 Diagrammatic expression for the self-energy in the RPA approximation.

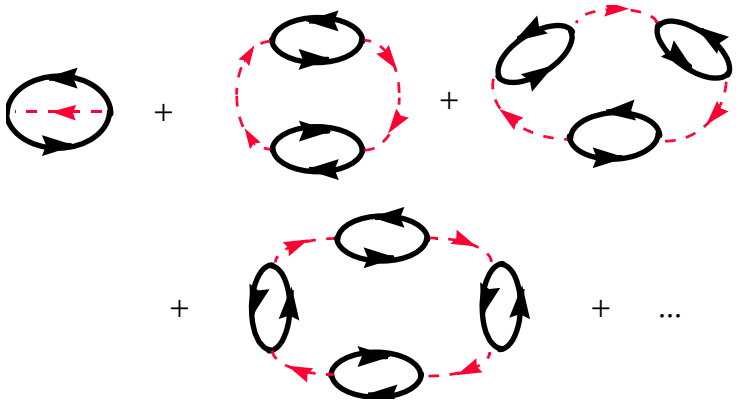


Figure 44-3 Ring diagrams for $\Sigma\mathcal{G}$ in the RPA approximation. The same diagrams are used for the free energy calculation.

Comparing with the Hartree-Fock approximation Eq.(42.15) the differences here are that a) we do not have self-consistency, b) more importantly, the interaction is screened. This is illustrated diagrammatically in Fig.(44-4) which is analogous

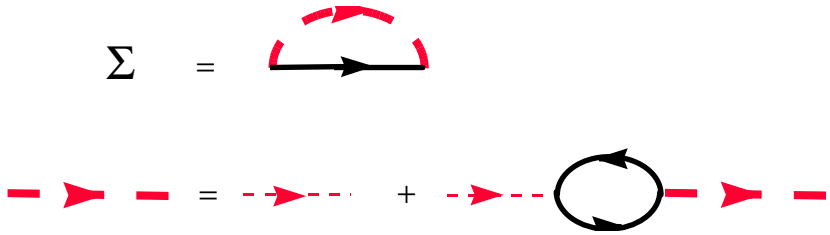


Figure 44-4 RPA self-energy written in terms of the screened interaction.

to the diagram for the Hartree-Fock approximation Fig.(42-2) but with a screened interaction and only the first rainbow diagram, without self-consistency.

Remark 292 *If, instead of summing the whole series in Fig.(44-2) we had stopped at any finite order, we would have had to deal with divergent integrals. Indeed, consider expanding the RPA susceptibility to first order in Eq.(44.8). This corresponds to the diagram with one bubble. The corresponding expression is*

$$\int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{iq_n} V_{\mathbf{q}}^2 \chi_{nn}^0 (\mathbf{q}, iq_n) \mathcal{G}^0 (\mathbf{k}+\mathbf{q}, ik_n + iq_n)$$

which is divergent since $V_{\mathbf{q}}^2$ is proportional to q^{-4} while the integral over q is in three dimensions only. Higher order bubbles are worse.

44.2 Self-energy and screening, GW the Schwinger way

We have derived in Eq.(36.13) an expression for the product $\Sigma\mathcal{G}$. When $\phi = 0$ and $2 = 1^+$, this equation reduces to

$$\boxed{\Sigma (1,\overline{2})_\phi \mathcal{G} (\overline{2}, 1^+)_\phi = V (1-\overline{2}) \left\langle T_\tau \left[\psi^\dagger \left(\overline{2^+} \right) \psi (\overline{2}) \psi^\dagger (1^+) \psi (1) \right] \right\rangle .} \quad (44.9)$$

It shows that we should have an approximation for the self-energy that, when multiplied by $\mathcal{G}$, gives the density-density correlation function. That is a very general result, or sum-rule, is a sort of consistency relation between one- and two-particle properties. It is equivalent to Eq.(43.23). This is a very important property that we will use also later in the context of non-perturbative treatments of the Hubbard model.

To obtain an approximation for the self-energy Σ that is consistent with the density-density correlation function that we just evaluated in the RPA approximation, we return to the general expression for the self-energy Eq.(36.34) and the corresponding pictorial representation Eq.(36-2). We replace the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$ by the one shown in Fig. 41-3 that we used to compute the density-density correlation function illustrated in Fig. 37-7. Note however that, as we did before, we keep only the terms where $V_{\mathbf{q}}$ carries a momentum $\mathbf{q}$. We neglect the next to

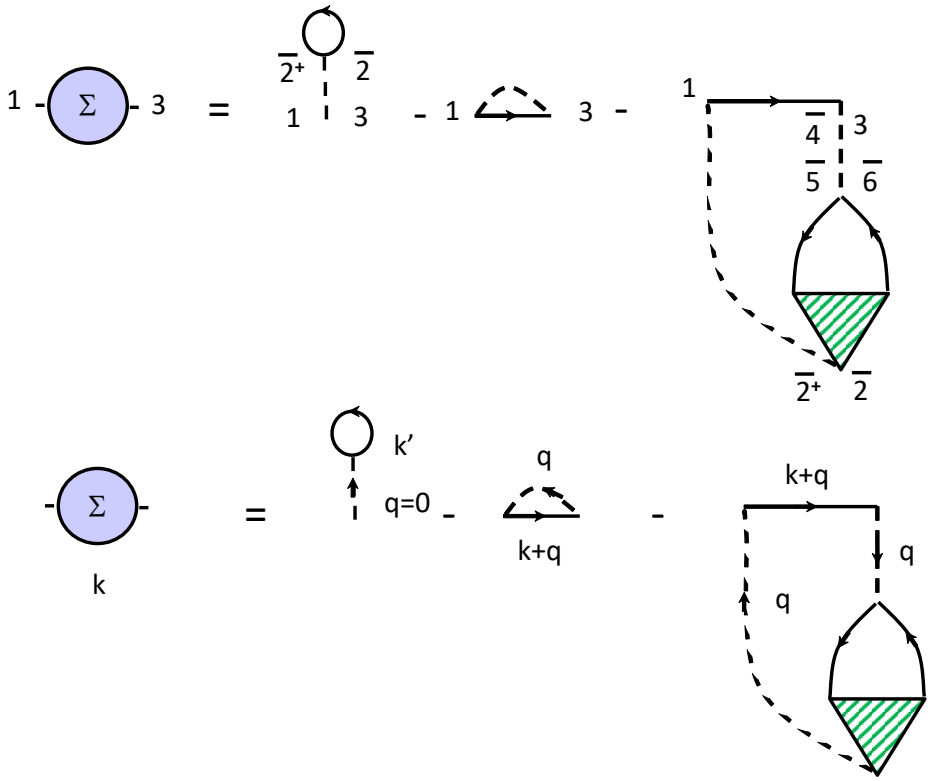


Figure 44-5 Coordinate (top) and momentum space (bottom) expressions for the self-energy at the second step of the approximation. The result, when multiplied by $\mathcal{G}$, is compatible with the density-density correlation function calculated in the RPA approximation.

last diagram in Fig.37-7. The other way to justify why we keep only these terms is that they are the most divergent diagrams. Their sum to infinity is however finite. We also know that by summing all diagrams to infinity, we are calculating the two-particle equivalent of a self-energy, shifting poles of the non-interacting density-density correlation function, as we should.

The final result is illustrated in Fig. 44-5. We just need to replace the functional derivative of the Green function appearing at the bottom right by the RPA series illustrated in Fig. 41-3. Recalling that the Hartree term vanishes, the final result is equivalent, when looked at sideways, to the series of bubble diagrams illustrated in Fig. 44-2,

The algebraic expression for this second level of approximation for the self-energy can be read off the figure. It takes the explicit form

$$\begin{aligned}\Sigma_{RPA}\left(\mathbf{k},ik_n\right) &= \Sigma^{(2)}\left(\mathbf{k},ik_n\right) \\ &= -\int \frac{d^3\mathbf{q}}{\left(2\pi\right)^3} T\sum_{iq_n} V_{\mathbf{q}}\left[1-\frac{V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\right]\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\end{aligned} \tag{44.10}$$

where the first term comes from the Fock contribution. The minus sign in the second term comes from the fact that the bubble with vertex is related to $\delta\mathcal{G}/\delta\phi$ that is minus the charge susceptibility. The two terms can be combined into the

single expression

$$\Sigma^{(2)}(\mathbf{k},ik_n) = -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{iq_n} \frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)} \mathcal{G}^0(\mathbf{k}+\mathbf{q},ik_n+iq_n). \quad (44.11)$$

Using our result for the longitudinal dielectric constant that follows from the density fluctuations in the RPA approximation Eq. (41.9), the last result can be written as

$$\Sigma^{(2)}(\mathbf{k},ik_n) = -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{iq_n} \frac{V_{\mathbf{q}}}{\varepsilon_L(\mathbf{q},iq_n)/\varepsilon_0} \mathcal{G}^0(\mathbf{k}+\mathbf{q},ik_n+iq_n) \quad (44.12)$$

which has the very interesting interpretation that the effective interaction entering the Fock term should be the screened one instead of the bare one. The two are equal only at very high frequency. The screened potential

$$\frac{V_{\mathbf{q}}}{\varepsilon_L(\mathbf{q},iq_n)/\varepsilon_0} = \frac{e^2}{\varepsilon_L(\mathbf{q},iq_n)\,q^2}$$

is often denoted W which means that the integrand is $W\mathcal{G}^0$, hence the name GW approximation. We will discuss this further in Chapter 51 on Hedin's equations.

Remark 293 *We can check that the relation between $\Sigma\mathcal{G}$ Eq.(44.9) and density fluctuations is satisfied by noticing that when we integrate this equation over 1, it is equivalent to computing a trace. That trace can be computed in any basis, in particular in the $\mathbf{k}$ basis. Diagrammatically, from Fig. 44-5, it is clear that multiplying by $\mathcal{G}^0$ and summing over $\mathbf{k}$ (i.e. taking the trace), we obtain the series of bubble diagrams for the density fluctuations, multiplied by the potential. That corresponds to the total potential energy. Hence, one recovers the sum-rule relating single and two-particle properties Eq.(43.23). Algebraically, we start from Eq.(44.11) just above and compute*

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} T\sum_{ik_n} \Sigma^{(2)}(\mathbf{k},ik_n)\,\mathcal{G}^0(\mathbf{k},ik_n)\,e^{-ik_n0^-} =$$

$$-\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{iq_n} \frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)} \int \frac{d^3\mathbf{k}}{(2\pi)^3} T\sum_{ik_n} \mathcal{G}^0(\mathbf{k}+\mathbf{q},ik_n+iq_n)\,\mathcal{G}^0(\mathbf{k},ik_n)\,e^{-ik_n0^-}$$

The convergence factor $e^{-ik_n0^-}$ is necessary to enforce $\Sigma(1,\overline{2})\,G(\overline{2},1^+)$ and obtain the potential energy to the right. It is not obvious from the right-hand side that we need the convergence factor until one realizes that there is a sum over k_n and q_n and only two Green's functions $\mathcal{G}^0(\mathbf{k}+\mathbf{q},ik_n+iq_n)\,\mathcal{G}^0(\mathbf{k},ik_n)$ that survive at very large frequency, giving a result that is formally divergent. Hence we should not invert the order of summation over k_n and q_n as we did. That can cost the constant term that appears in Eq.(43.23).

45. PHYSICS IN SINGLE-PARTICLE PROPERTIES

In this Chapter, we interpret the results of calculations based on formulas of the previous Chapter, and compare with experiments. In particular, after a look at the overall picture, we will recover theoretically the Fermi liquid regime, and compare with experiment.

45.1 Single-particle spectral weight

The real-part and the absolute value of the imaginary part of the RPA self-energy at zero temperature are plotted in Fig.(45-1) as a function of frequency for three different wave vectors. In the Hartree-Fock approximation, the self-energy was completely frequency independent. The result here is quite different. The screened interation contains the plasmons and has a drastic effect on single-particle properties. There are several points worth mentioning.

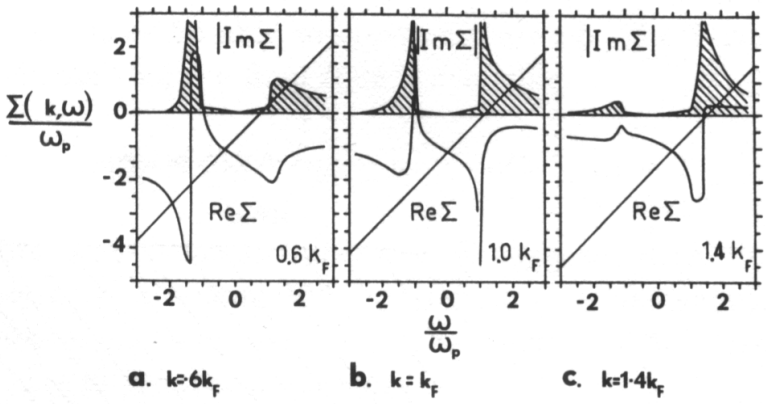


Figure 45-1 Real and imaginary part of the RPA self-energy for three wave vectors, in units of the plasma frequency. The chemical potential is included in ReΣ. The straight line that appears on the plots is $\omega - \varepsilon_{\mathbf{k}}$. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7,** 117 (1968). $r_s = 5$?

- $\mathrm{Im}\,\Sigma\,(\mathbf{k},\omega = 0) = 0$ for all wave vectors. This is true only at zero temperature. This property will play a key role in the derivation of Luttinger's theorem later. It will be proven within our approximation in Sec. (45.2) below.

- The straight line that appears on the plots is $\omega - \varepsilon_{\mathbf{k}}$. The intersection of this straight line with $\mathrm{Re}\,\Sigma$, which is defined on the figure to contain the chemical

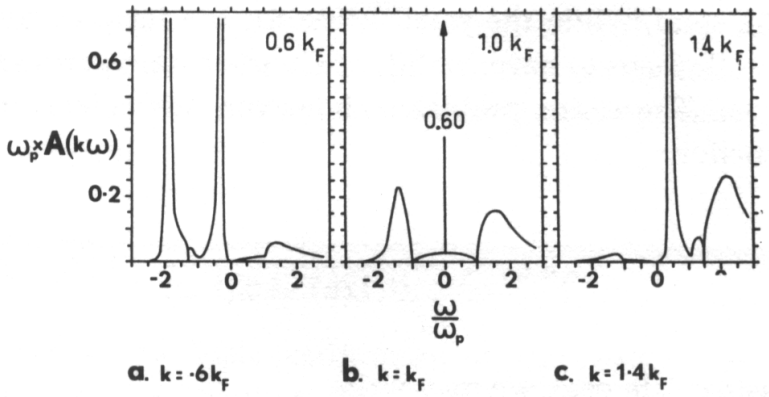


Figure 45-2 RPA spectral weight, in units of the inverse plasma frequency. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7,** 117 (1968).

potential, corresponds (in our notation) to the solution of the equation

$$\omega - \varepsilon_{\mathbf{k}} = \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega) - \mu \tag{45.1}$$

As we argued in the previous chapter Eq.(31.20), this determines the position of maxima in the spectral weight,

$$A(\mathbf{k},\omega) = -2\,\mathrm{Im}\,G^R(\mathbf{k},\omega) \tag{45.2}$$

$$= \frac{-2\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{\left(\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\sum^R(\mathbf{k},\omega)\right)^2 + \left(\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2} \tag{45.3}$$

maxima that we identify as quasiparticles. Let us look at the solutions near $\omega = 0$. These correspond to a peak in the spectral weight Fig.(45-2). At the Fermi wave vector, the peak is located precisely where the imaginary part of the self-energy vanishes, hence the peak is a delta function. On the other hand, away from $\mathbf{k} = \mathbf{k}_F$, the maximum is located in a region where the imaginary part is not too large, hence the quasiparticle has a finite lifetime. Recall that to have the quasiparticle shape described in the previous chapter Eq.(31.25),

$$A(\mathbf{k},\omega) \approx 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + (\Gamma_{\mathbf{k}}(\omega))^2}\right] + inc \tag{45.4}$$

it is necessary that at the crossing point, the slope of $\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$ be negative because it is necessary that

$$Z_{\mathbf{k}} = \frac{1}{1 - \frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\big|_{\omega = E_{\mathbf{k}} - \mu}} \geq 0 \tag{45.5}$$

if the previous formula is to make sense. The value of $Z_{\mathbf{k}_F}$, namely 0.6, is indicated on this plot.

- Note that in Fig. 45-1 there is a threshold-like feature at $\omega_p = \pm 1$ where $\mathrm{Im}\,\Sigma^R$ becomes large. This is when the one-particle excitations can emit or absorb real plasmons. This is discussed further below.

- From the previous discussion, we see that the two maxima away from $\omega = 0$ at $k = k_F$ do not correspond to quasiparticle solutions. The weight near the maxima away from $\omega = 0$ come from scattering rates $\mathrm{Im}\,\Sigma^R$ that are large, but not too large compared with the value of $\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$. At the threshold where $\mathrm{Im}\,\Sigma^R$ is really large, the spectral weight in fact vanishes because of the denominator in the general expression for the spectral weight Eq.(45.2). Note that the maxima away from $\omega = 0$ at $k = k_F$ are near the value of ω where the quasiparticle condition Eq. (45.1) is almost satisfied.
- For the figure on the right, $k = 1.4k_F$, the peak nearest $\omega = 0$ corresponds to a quasiparticle solution. Note however that for wave vectors so far from the Fermi surface, the width of the peak starts to be quite a bit larger. The maxima further away all occur in regions where $\mathrm{Im}\,\Sigma^R$ is large and the quasiparticle condition Eq. (45.1) is almost satisfied.
- For $k = 0.6k_F$, there seems to be an additional quasiparticle solution, namely a solution where $\frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma^R$ is negative and $\mathrm{Im}\,\Sigma^R$ is not too large, located at an energy ω_p below the main quasiparticle energy. Since the free-electron band is bounded from below, $\mathrm{Im}\,\Sigma^R$ vanishes at sufficiently negative frequency, allowing a new solution to develop when interactions are sufficiently strong. This solution looks like a bound state.

45.2 Simplifying the expression for Σ''

In this section, we write the imaginary part of the self-energy in a form that is easy to interpret physically. The evaluation in the Fermi-liquid limit is given in the following section. Here we want to first show that the imaginary part of the self-energy defined by

$$\Sigma^R(\mathbf{k},\omega) = \Sigma'(\mathbf{k},\omega) + i\Sigma''(\mathbf{k},\omega) \tag{45.6}$$

may be written in the form

$$\boxed{\Sigma''(\mathbf{k},\omega) = -\frac{m}{2|k|}\int\frac{d^2q_\perp}{(2\pi)^2}\int\frac{d\omega'}{\pi}\left[n_B(\omega') + f(\omega+\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}(q_\perp, q_\parallel, \omega')} \tag{45.7}$$

where $q_\parallel$ is the solution of the equation

$$\frac{|k|}{m}q_\parallel + \frac{q_\parallel^2}{2m} = \left[\omega + \omega' - \left(\frac{k^2}{2m} - \mu + \frac{q_\perp^2}{2m}\right)\right] \tag{45.8}$$

Proof: It is preferable to first rewrite the RPA expression Eq.(44.8) in the following form

$$\Sigma_{RPA}(\mathbf{k},ik_n) = -\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}V_{\mathbf{q}}\left[1 - \frac{V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}\right]\mathcal{G}^0(\mathbf{k}+\mathbf{q}, ik_n+iq_n) \tag{45.9}$$

$$= \Sigma_{HF}(\mathbf{k}) + \int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}\left[V_{\mathbf{q}}\chi^{RPA}_{nn}(\mathbf{q},iq_n)\,V_{\mathbf{q}}\right]\mathcal{G}^0(\mathbf{k}+\mathbf{q}, ik_n+iq_n) \tag{45.10}$$

The first term at $T = 0$ is the Hartree-Fock contribution, as we can see from Eq.(42.24). In other words, whether we use $\mathcal{G}^0$ or the dressed $\tilde{\mathcal{G}}^0$ in

the Hartree-Fock calculation we obtain the same result at zero temperature. The important points here however are that (i) it is the only contribution that survives at infinite frequency and (ii) the imaginary part comes only from the second term. That second term contains a quantity in square brackets that looks like two interaction vertices, $V_{\mathbf{q}}$ coupling to a density propagator $\chi_{nn}^{RPA}(\mathbf{q},iq_n)$. When we consider interactions with other types of excitations, including with phonons, this form will reoccur and will be more easily susceptible to generalizations. To find the imaginary part, let us concentrate on this last expression and use the spectral representation for χ_{nn}^{RPA}. We then have

$$\Sigma_{RPA}(\mathbf{k},ik_n)-\Sigma_{HF}(\mathbf{k}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\int \frac{d\omega'}{\pi} T\sum_{iq_n}\left[V_{\mathbf{q}}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-iq_n}V_{\mathbf{q}}\right]\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}. \tag{45.11}$$

To do the sum over bosonic Matsubara frequencies first, we do the partial fraction decomposition as usual

$$-T\sum_{iq_n}\frac{1}{iq_n-\omega'}\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{45.12}$$

$$= -T\sum_{iq_n}\left[\frac{1}{iq_n-\omega'}-\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{45.13}$$

$$= \left[n_B(\omega')+f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{45.14}$$

We do not need a convergence factor since the terms of the original sum decrease in $1/(iq_n)^2$. However, since we have splitted the sum in two terms which do not individually converge, we need to use the same convergence factor for both sums individually. Whichever convergence factor is used, the result is the same. Note that for any ik_n, the sum ik_n+iq_n is a fermionic Matsubara frequency when iq_n is a bosonic one. That is why we obtained a Fermi distribution in the last term. Substituting back into our expression for the self-energy, the analytic continuation $ik_n \to \omega+i\eta$ can be done and we obtain

$$\Sigma^R(\mathbf{k},\omega)-\Sigma_{HF}(\mathbf{k}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\int \frac{d\omega'}{\pi}\left[n_B(\omega')+f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\frac{V_{\mathbf{q}}\chi''_{nn}(\mathbf{q},\omega')V_{\mathbf{q}}}{\omega+i\eta+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}}. \tag{45.15}$$

The imaginary part is thus

$$\Sigma''(\mathbf{k},\omega) = -\pi\int \frac{d^3\mathbf{q}}{(2\pi)^3}\int \frac{d\omega'}{\pi}\left[n_B(\omega')+f(\omega+\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}(\mathbf{q},\omega')\,\delta\left(\omega+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}\right) \tag{45.16}$$

Defining $q_{||}$ by the direction parallel to the wave vector $\mathbf{k}$ and calling $q_\perp$ the other directions, the integral over $q_{||}$ can be performed, giving the condition in Eq.(45.8). We then obtain, assuming that we are in a region of frequency where the delta function has a solution, the desired result Eq.(45.7)

Remark 294 *Order of summation and analytic continuation: In Eq.(45.11), we cannot perform the analytical continuation $ik_n \to \omega+i\eta$ before we have performed the sum over iq_n because, except for $iq_n=0$, this would necessitate going through the poles at $\omega=-iq_n+\zeta_{\mathbf{k}+\mathbf{q}}$. In addition, recall that we want the high-frequency behavior to be $1/ik_n$ before we do the analytic continuation, but until we have done the sum over iq_n we cannot say that we have that asymptotic behavior since iq_n extends to infinity.*

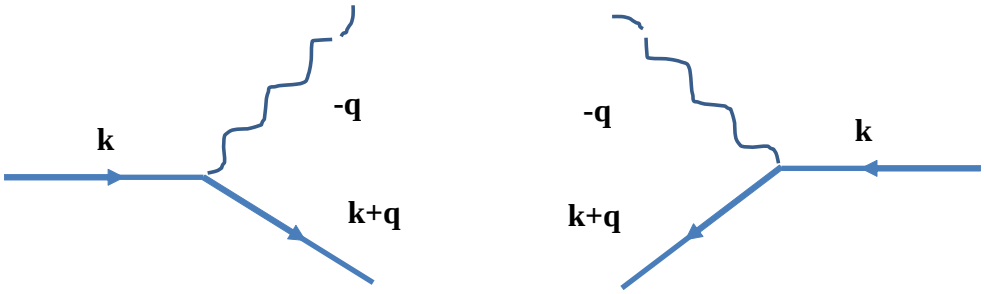


Figure 45-3 Schematic representation of the processes contained in the imaginary part of the self-energy. On the left, an electron in with momentum and frequency $\mathbf{k}$,ω decays into another a quasiparticle $\mathbf{k}+\mathbf{q}$,$\zeta_{\mathbf{k}+\mathbf{q}}$ plus a particle-hole excitation $-\mathbf{q}, \omega - \zeta_{\mathbf{k}+\mathbf{q}}$ that can be a plasmon, depending on the conditions on wave-vector and frequency. On the right, the analogous process for a hole.

In the zero temperature limit, $f(\omega+\omega') = \theta(-\omega-\omega')$ and $n_B(\omega') = -\theta(-\omega')$ so that if we take $\omega > 0$ then the integral over ω' extends over the interval $-\omega < \omega' < 0$ where $n_B(\omega') + f(\omega+\omega')$ takes the value -1. At low temperature, the contributions to Σ'' Eq.(45.7) will come mostly from this same frequency interval since this is where the combination $n_B(\omega') + f(\omega+\omega') \neq 0$. This immediately allows us to understand why the imaginary part of the self-energy in Fig.(45-1) above starts to be large when the frequency becomes of the order of the plasma frequency. This is only when ω is that large that the contributions from $\omega' \approx \omega_p$ in χ''_{nn} can start to contribute. This is where the quasiparticles can start to absorb or emit plasmons.

Remark 295 *Vanishing of Σ'' at zero temperature: Our general formula for the imaginary part Eq.(45.7) tells us that at zero temperature $\Sigma''(\mathbf{k}, \omega = 0) = 0$ for **all** wave vectors, as we have seen in Fig.(45-1). Mathematically, this is so because $\lim_{T\to 0}[n_B(\omega') + f(\omega')] = 0$ for all ω'. Physically, it is because phase space vanishes when we sit right at the chemical potential $(\omega = 0)$.*

45.3 Physical processes contained in Σ''

It is easier to interpret the physical meaning of the imaginary part by concentrating on the case $\omega > 0$ and then performing a change of variables $\omega' \to -\omega'$. Then the integration window at $T = 0$ becomes $-\omega < -\omega' < 0$, or $\omega > \omega' > 0$. Using

$$n_B(-\omega') = -(1 + n_B(\omega')) \tag{45.17}$$

and $\chi''_{nn}(\mathbf{q}, -\omega') = -\chi''_{nn}(\mathbf{q}, \omega') = -\chi''_{nn}(-\mathbf{q}, \omega')$, the imaginary part of the self-energy becomes

$$\begin{aligned}
\Sigma''(\mathbf{k}, \omega) &= -\pi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[(1 + n_B(\omega')) - f(\omega - \omega')\right] V_{\mathbf{q}}^2 \chi''_{nn}(\mathbf{q}, \omega') \, \delta\left(\omega - \omega' - \zeta_{\mathbf{k}+\mathbf{q}}\right) \\
&= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} V_{\mathbf{q}}^2 \chi''_{nn}\left(-\mathbf{q}, \omega - \zeta_{\mathbf{k}+\mathbf{q}}\right) \\
&\quad \left[\left(1 + n_B\left(\omega - \zeta_{\mathbf{k}+\mathbf{q}}\right)\right)\left(1 - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right) + n_B\left(\omega - \zeta_{\mathbf{k}+\mathbf{q}}\right) f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]
\end{aligned}$$

The first term $\left(1+n_B\left(\omega-\zeta_{\mathbf{k}+\mathbf{q}}\right)\right)\left(1-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right)$ represents the decay of a particle of energy ω and wave vector $\mathbf{k}$ into an empty particle state of energy $\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $\mathbf{k}+\mathbf{q}$, plus a bosonic excitation (particle-hole continuum or plasmon) of energy $\omega-\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $-\mathbf{q}$. The second term $n_B\left(\omega-\zeta_{\mathbf{k}+\mathbf{q}}\right)f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)$ represents the case where the incident state is a hole of energy ω and wave vector $\mathbf{k}$ that decays into another hole of energy $\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $\mathbf{k}+\mathbf{q}$ by absorbing a boson of energy $\omega-\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $-\mathbf{q}$. The latter is in some sense the first process but time reversed. This is illustrated in Fig.(45-3). "Scattering-in" terms that represent repopulation of the state $\mathbf{k}$ occur in transport equations, or two-body response functions, not here.

45.4 Fermi liquid results

Perhaps the best known characteristic of a Fermi liquid is that at frequencies and temperatures much smaller than the Fermi energy, $\Sigma''^R\left(\mathbf{k}_F,\omega;T=0\right)\propto\omega^2$ and $\Sigma''^R\left(\mathbf{k}_F,\omega=0;T\right)\propto T^2$. To recover this result, valid far from phase transitions, we start from the above expression Eq.(45.7) for Σ'' but we evaluate it at $\mathbf{k}=\mathbf{k}_F$ and use $v_F\equiv k_F/m$ so that

$$\boxed{\Sigma''\left(\mathbf{k}_F,\omega\right)=-\tfrac{1}{2v_F}\int\tfrac{d^2q_\perp}{(2\pi)^2}\int\tfrac{d\omega'}{\pi}\left[n_B\left(\omega'\right)+f\left(\omega+\omega'\right)\right]V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp,q_\parallel,\omega'\right)} \tag{45.18}$$

where $q_\parallel$ is obtained from the solution of

$$v_Fq_\parallel+\frac{q_\parallel^2}{2m}=\left[\omega+\omega'-\frac{q_\perp^2}{2m}\right]. \tag{45.19}$$

The key to understanding the Fermi liquid regime is in the relative width in frequency of $\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ *vs* the width of the combined Bose and Fermi functions. In general, the function $n_B\left(\omega'\right)+f\left(\omega+\omega'\right)$ depends on ω' on a scale $\max\left(\omega,T\right)$ while far from a phase transition, $\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ depends on frequency only on the scale of the Fermi energy. We can assume that it is independent of frequency at low frequency.

Proof: As we can see from the explicit expression for the imaginary part of χ''_{nn} Eq.(41.16), and using the fact that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},0)=0$,

$$\lim_{\omega\to0}\operatorname{Im}\chi^R_{nn}(\mathbf{q},\omega)/\omega=\lim_{\omega\to0}\frac{\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega}{\left(1+V_{\mathbf{q}}\operatorname{Re}\chi^{0R}_{nn}(\mathbf{q},0)\right)^2} \tag{45.20}$$

it suffices that the Lindhard function $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ has the property that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega$ is independent of frequency at low frequency. As expected from the fact that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is odd in frequency, it turns out that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is indeed linear in frequency at low frequency, which proves our point. The linearity can be explicitly checked from our previous results Eqs.(41.12) and (41.9).

Hence, at low frequency, we can assume that $\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ is independent of frequency in the frequency range over which $n\left(\omega'\right)+f\left(\omega+\omega'\right)$ differs from zero. Also, $V_{\mathbf{q}}^2\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ depends on wave vector over a scale that is of order q_F as we can see from Fig.(41-5). Hence, we can neglect the ω and ω' dependence of the

solution for $q_{\|}$ in Eq.(45.19) when we substitute it in our expression for Σ''. One then finds

$$\boxed{\Sigma''(\mathbf{k}_F,\omega) \simeq -\frac{A(\mathbf{k}_F)}{2v_F}\int \frac{d\omega'}{\pi}\left[n(\omega')+f(\omega+\omega')\right]\omega' = -\frac{A(\mathbf{k}_F)}{4v_F}\left[\omega^2+(\pi T)^2\right]} \tag{45.21}$$

where the substitution $x = e^{\beta\omega}$ allowed the integral to be done exactly [18] and where

$$A(\mathbf{k}_F) \equiv \int \frac{d^2q_\perp}{(2\pi)^2}\lim_{\omega'\to 0}\frac{V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp, q_{\|}(q_\perp,v_F);\omega'\right)}{\omega'}. \tag{45.22}$$

The presence of $V_{\mathbf{q}}^2$ does not give rise to problems in the integral over $q_\perp$ near $q=0$ because in this region the contribution is canceled by $V_{\mathbf{q}}^2$ that appears in the denominator of the RPA susceptibility Eq.(45.20). The above result Eq.(45.21) for Σ'' is the well known Fermi liquid result.

Remark 296 *Note that the ω^2 dependence in the $T=0$ limit is easy to obtain since in that limit,*

$$\int d\omega'\left[n(\omega')+f(\omega+\omega')\right]\omega' = -\int_{-\omega}^{0} d\omega'\omega' = \frac{\omega^2}{2}. \tag{45.23}$$

Remark 297 *There are known corrections to the Fermi liquid self-energy that come from the non-analytic ω'/v_Fq behavior of $\chi''_{nn}(\mathbf{q},\omega')$ near $\mathbf{q}=\mathbf{0}$. In three dimensions[19] this non-analyticity leads to subdominant $\omega^3\ln\omega$ corrections, while in two dimensions it leads to the dominant $\omega^2\ln\omega$ behavior.[20][21]*

Remark 298 *Relevance of screened interaction to low-frequency Physics near the Fermi surface: It can clearly be seen from the above derivation that it is the low-frequency limit of the screened interaction that gives rise to the damping near the Fermi surface. This is a key result. If we are interested in properties near the Fermi surface, screened interactions suffice. This should be kept in mind when we discuss the Hubbard model later.*

Remark 299 *Important result $\Sigma''(\mathbf{k},0)=0$ at zero temperature for all wave vectors. Although the above result was obtained for $\mathbf{k}=\mathbf{k}_F$, the result $\Sigma''(\mathbf{k},0)=0$ is valid for all wave vectors. Indeed the only change is on the relation between $q_{||}$ and frequency. Eq. (45.19) will be replaced by $\frac{kq_{\|}}{m}+\frac{q_{\|}^2}{2m} = \left[\omega+\omega'-\frac{q_\perp^2}{2m}-\frac{k^2}{2m}+\mu\right]$ and once again, the dependence on ω can be neglected. When ω becomes of the order of the Fermi energy, all of the above fails.*

We now just quote without proof some of the results of further calculations of Fermi liquid parameters. The solution of the quasiparticle equation Eq.(45.1) gives

$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - 0.17r_s(\ln r_s+0.2)\frac{k_Fk}{2m} + cst \tag{45.24}$$

The effective mass appearing in this expression is now obviously finite and given by

$$m^* = \frac{m}{1-0.08r_s(\ln r_s+0.2)} \tag{45.25}$$

If we evaluate the scattering rate for $\omega = E_{\mathbf{k}}-\mu$ we find

$$\Gamma_{\mathbf{k}}(E_{\mathbf{k}}-\mu) = 0.25r_s^{1/2}\frac{(k-k_F)^2}{2m} \tag{45.26}$$

Quinn and Ferrell[22] write the following physically appealing form

$$\Gamma_{\mathbf{k}}\left(\zeta_{\mathbf{k}}\right) Z_{\mathbf{k}}^{-1}=\frac{\sqrt{3}\pi^2}{128}\omega_p\left(\frac{\zeta_{\mathbf{k}}}{E_F}\right)^2 \tag{45.27}$$

The scattering rate is proportional to the plasma frequency, but reduced by an important phase space factor. The more general results, beyond leading order in r_s can be found in Eqs.(8.92-8.93) of Giuliani and Vignale "Quantum theory of the electron liquid".

Fig.(45-4) gives the value of the Σ' and Σ'' evaluated at the frequency corresponding to the quasiparticle position. The important point is that the real-part of the self-energy is weakly wave vector dependent up to about $k=2k_F$. The imaginary part on the other hand vanishes as expected on the Fermi surface, while away from it remains relatively small on the scale of the Fermi energy. This justifies *a posteriori* the success of the free electron picture of solids. Note however that states far from the Fermi surface do have a lifetime, contrary to the predictions of band structure calculations.

Remark 300 *These results on the figure were obtained in the zero-temperature formalism where by construction the imaginary part of the calculated Green's function is equal to the imaginary part of the retarded self-energy above the Fermi surface and to the imaginary part of the advanced self-energy below the Fermi surface. This explains the sign change on the figure.*

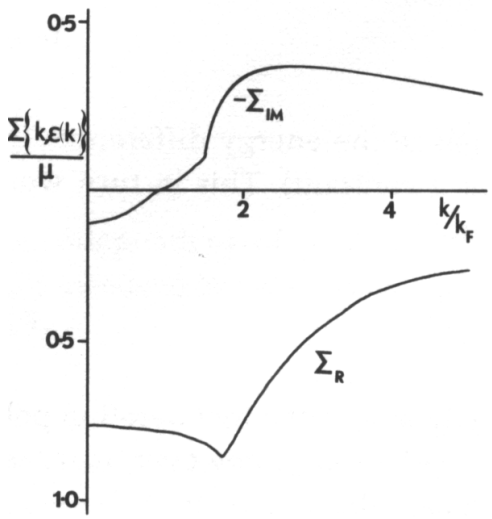


Figure 45-4 Real and imaginary parts of the self-energy of the causal Green's function in the zero-temperature formalism. From L. Hedin and S. Lundqvist, *Solid State Physics* **23,** 1 (1969).

45.5 Comparison with experiments

We are finally ready to compare the predictions of this formalism to experiments. The results shown in the present section are taken from Ref.[24].

The first quantity that comes to mind to compare with experiment is the effective mass. This quantity can in principle be obtained from cyclotron resonance or from specific heat measurements. It turns out however that the theoretical prediction for m^*/m differs from unity by only about 10%. But what makes comparisons with experiment for this quantity very difficult is that there are two other contributions to the effective mass in real materials. First there are band structure effects. These are small in sodium but large in lithium and many other metals. The second additional contribution to the effective mass comes from electron-phonon interactions. We will see in the next chapter that these effects can be quite large. So we need to wait.

A striking prediction of many body theory is that the size of the jump in momentum distribution at the Fermi level at zero temperature should be quite different from unity. Fig.(45-5) illustrates the prediction for sodium at $r_s = 3.97$. The following Table of expected jumps is from Hedin[8].

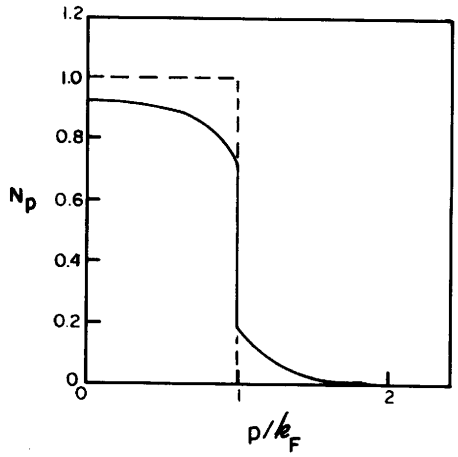


Figure 45-5 Momentum density in the RPA approximation for an electron gas with $r_s = 3.97$. From E. Daniel and S.H. Vosko, Phys. Rev. **120**, 2041 (1960).

r_s	Z_{RPA}
0	1
1	0.859
2	0.768
3	0.700
4	0.646
5	0.602
6	0.568

(45.28)

Unfortunately even through photoemission we do not have access directly to this jump in three dimensional materials, as we discussed in the previous chapter. Another probe that gives indirect access to this jump is Compton scattering. In Compton scattering, a photon scatters off an electron, leaving with a different energy an momentum along with an electron in a new momentum state. This is really as if photons scattered-off electrons as billiard balls, conserving energy and momentum. Photons are scattered inelastically from all the electrons in the solid. The contribution from conduction electrons can be extracted by subtraction. In the so-called "sudden approximation", the cross section for photon scattering is

proportional to

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int d^3\mathbf{k} n_{\mathbf{k}} \delta\left(\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}\right) \tag{45.29}$$

where ω is the energy and $\mathbf{q}$ the wave vector transferred by the photon and $n_{\mathbf{k}} = \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$. We do not need $(1 - n_{\mathbf{k}+\mathbf{q}})$ to insure that the final electron state is empty because the energy transfer is so large, as we see in the experimental results, that we are sure the state will be empty. Changing to polar coordinates, we see that

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int k^2 dk d\left(\cos\theta\right) n_{\mathbf{k}} \delta\left(\omega - \varepsilon_{\mathbf{q}} - \frac{kq}{m}\cos\theta\right) \tag{45.30}$$

$$\propto \int k dk \frac{m}{q} n_k \theta\left(k - |Q|\right) \tag{45.31}$$

where

$$Q \equiv \frac{m}{q}\left(\varepsilon_q - \omega\right) \tag{45.32}$$

In terms of Q, we have

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \frac{1}{q}\int_{|Q|}^{\infty} n_k k dk \tag{45.33}$$

For free electrons, this gives

$$\frac{d^2\sigma}{d\omega d\Omega} \propto J\left(Q\right) \propto \frac{1}{2q}\left(k_F^2 - Q^2\right)\theta\left(k_F - Q\right). \tag{45.34}$$

In this case then, the slope is discontinuous at $k_F = Q$ as illustrated on the left of Fig.(45-6). In the interacting case, the change in slope at k_F remains theoretically related to Z. Also, one expects a signal above k_F as illustrated on the left of the figure. Experimental results for sodium, $r_s = 3.96$, are given on the right of the figure along with the theoretical prediction. This metal is the one closest to the free electron model. The experimentalists have verified that Q is a good scaling variable, in other words that the cross section depends mainly on Q. Also, the existence of a tail above k_F is confirmed. However, the agreement with theory is not excellent.

The experimental results for the mean free path are more satisfactory. Let the mean free path $\ell_{\mathbf{k}}$ be defined by

$$\frac{1}{\ell_{\mathbf{k}}} = \frac{\Gamma_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1}{\tau_{\mathbf{k}} v_{\mathbf{k}}} = -\frac{2}{v_{\mathbf{k}}}\operatorname{Im}\Sigma\left(\mathbf{k},\zeta_{\mathbf{k}}\right) \tag{45.35}$$

Remark 301 *The factor of* 2 *is not so easy to explain here, except to say that if we look at a density perturbation, the scattering rate is twice that appearing in the single-particle Green functions.*

Remark 302 *Compton scattering was one of the key experiments that helped convince people that light could behave as if it was made up of particles: photons.*

Fig.(45-7) presents the results of experiments on aluminum, $r_s = 2.07$. If one takes into account only scattering by plasmons one obtains the dashed line. The full RPA formula, including the contribution from the particle-hole continuum, was obtained numerically by Lundqvist for $r_s = 2$ and is in excellent agreement with experiment.

The cross section for inelastic electron scattering, that is proportional to $\operatorname{Im}\left(1/\varepsilon^L\right)$, is shown in Fig. (45-8) for aluminum. The plasma resonance at low momentum transfer is visible around 15 eV for the larger nanoparticles. You can even see the

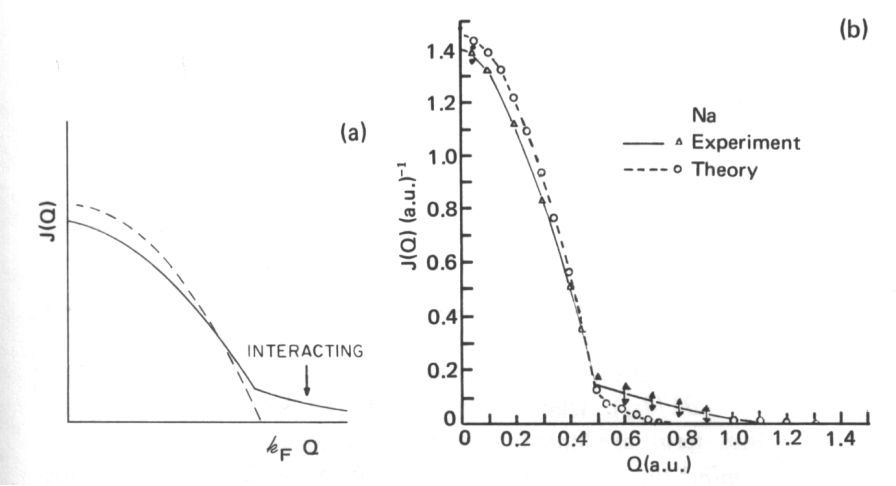


Figure 45-6 a) Dashed line shows the momentum distribution in Compton scattering for the non-interacting case while the solid line is for an interacting system. b) Experimental results in metallic sodium compared with theory, $r_s = 3.96$. Eisenberger *et al.* Phys. Rev. B **6**, 3671 (1972).

two plasmon peak around 30 eV. The resonance is much larger than the particle-hole continuum, as we saw in the theoretical plot of Fig.(41-6). The small peak at small frequency is a surface plasmon. In Ref. [227] you can find an analysis of the width of the plasmon. It comes, in particular, from the decay of the plasmon in other conduction-electron bands.

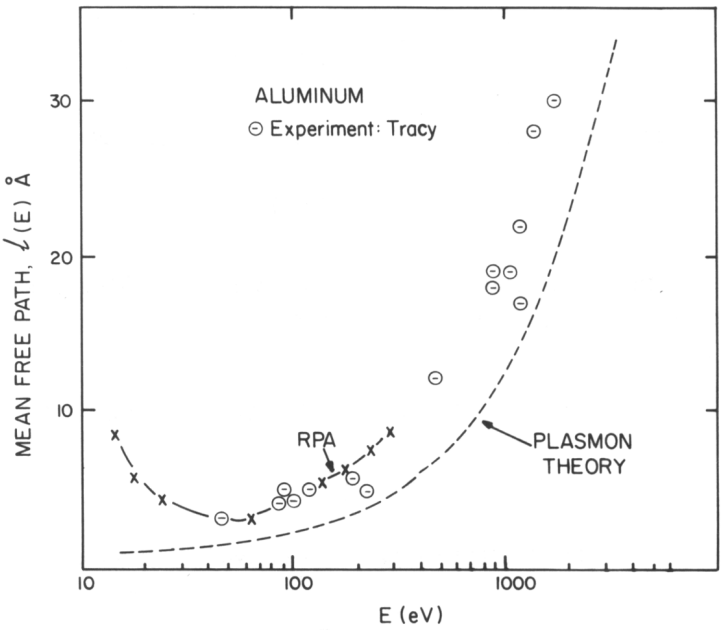


Figure 45-7 Mean free path of electrons in aluminum $(r_s = 2.07)$ as a function of energy above the Fermi surface. Circles are experimental results of J.C. Tracy, J. Vac. Sci. Technol. **11**, 280 (1974). The dashed line with symbols X was obtained with RPA for $r_s = 2$ by B.I. Lundqvist Phys. Status Solidi B **63**, 453 (1974).

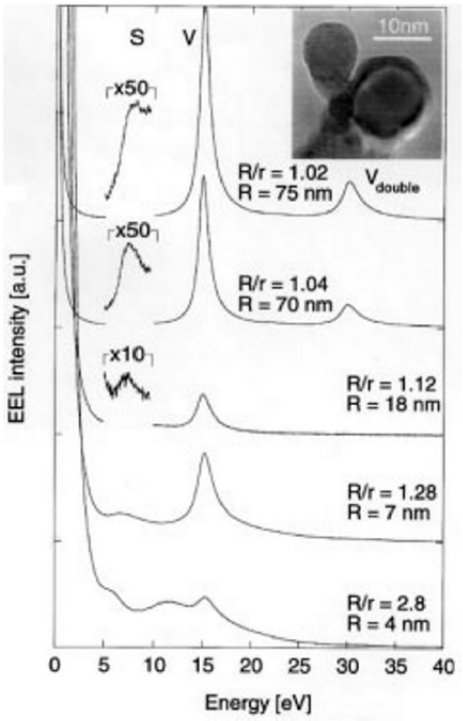


Fig. 1. EEL spectra of Al nanospheres with different radii R and ratio R/r. R is the radius of the sphere consisting of the Al core and the oxide shell, and r is the radius of the Al core only. V indicates the volume plasmon loss, V_{double} the corresponding double loss and S the surface plasmon loss. *Inset:* TEM micrograph of a typical Al nanosphere. The oxide layer and the Al core can be distinguished

Figure 45-8 The top curve shows the plasmon around 15 eV for aluminum. Two plasmons can also be emitted, as you can see around 30 eV. As the nanoparticles become smaller, the spectrum deviates from the bulk result. Z. Phys. D **40**, 425–428 (1997)

46. FREE-ENERGY CALCULATIONS

The diagram rules for the free energy are more complicated than for the Green's function. For those that have followed the Feynman track, we have seen in the previous chapter the form of the linked-cluster theorem for the free-energy. It is given by a sum of connected diagrams. However, in doing the Wick contractions for a term of order n, there will be $(n-1)!$ identical diagrams instead of $n!$. This means that there will be an additional $1/n$ in front of diagrams of order n, by contrast with what happened for Green's functions. This makes infinite resummations a bit more difficult (but not undoable!).

There is an alternate way of obtaining the free energy without devising new diagram rules. It uses integration over the coupling constant. We discuss this in full generality in the next section. Then we apply the result to RPA.

46.1 Free energy and consistency between one and two-particle quantities

I first start with a general theorem to compute the free energy and show that it can be obtained either directly from the density fluctuations or from the self-energy and the Green's function, which we know already are related.

This trick is apparently due to Pauli [16]. The proof is simple. First, notice that

$$-\frac{1}{\beta}\frac{\partial \ln Z}{\partial \lambda} = -\frac{1}{\beta}\frac{1}{Z}\frac{\partial Tr\left[e^{-\beta(H_0+\lambda V-\mu N)}\right]}{\partial \lambda} = \frac{1}{Z}Tr\left[e^{-\beta(H_0+\lambda V-\mu N)}V\right] = \frac{1}{\lambda}\left\langle \lambda V\right\rangle_\lambda . \tag{46.1}$$

To differentiate the operator, $e^{-\beta(H_0+\lambda V-\mu N)}$, we have used its definition as a power series and then taken the derivative with respect to λ. Even if the operator V does not commute with H_0, the cyclic property of the trace allows one to always put V on the right-hand side so that in the end, the derivative worked out just as with ordinary number. (Alternatively, one can do the proof in the interaction representation). The subscript λ in $\left\langle \lambda V\right\rangle_\lambda$ is to remind ourselves that the trace is taken for a Hamiltonian with coupling constant λ.

The free energy we are interested in is for $\lambda = 1$, so

$$\boxed{\Omega = -T\ln Z = -T\ln Z_0 + \int_0^1 \frac{d\lambda}{\lambda}\left\langle \lambda V\right\rangle_\lambda .} \tag{46.2}$$

From a diagrammatic point of view, the role of the integral over λ is to regive the factor of $1/n$ for each order in perturbation theory.

Remark 303 *Recall that the free energy in this grand-canonical ensemble is related to the pressure.*

$$\Omega = -P\mathcal{V}. \tag{46.3}$$

The expectation value of the potential energy may be obtained by writing down directly a diagrammatic expansion, or by using what we already know, namely the density correlations. Indeed we have shown in a previous section, Eq.(43.20), how the potential energy may be obtained from density correlations,

$$\begin{aligned}\Omega &= -T\ln Z = -T\ln Z_0 \\ &+\frac{\mathcal{V}}{2}\int_0^1\frac{d\lambda}{\lambda}\left\langle\lambda\int\frac{d^3q}{(2\pi)^3}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}\left(\mathbf{q},iq_n\right)-n\right]\right\rangle_\lambda .\end{aligned} \tag{46.4}$$

Using our previous relation between self-energy and potential energy, Eq.(43.13) the coupling-constant integration in Eq.(46.2) may also be done with

$$\Omega = -T\ln Z_0 + \frac{T}{2}\int_0^1\frac{d\lambda}{\lambda}\int d1\int d1"\,\Sigma_\lambda\left(1,1"\right)\mathcal{G}_\lambda\left(1",1^+\right). \tag{46.5}$$

where the subscript λ reminds oneself that the interaction Hamiltonian must be multiplied by a coupling constant λ.

46.2 Free energy for the Coulomb gas in the RPA approximation

We use our coupling-constant integration formula Eq.(46.2). In the zero temperature limit, there will be no contribution from entropy and we will obtain the ground state energy in the RPA approximation

$$\begin{aligned}E_{Tot}^{RPA}\left(T=0\right)-\mu N &= \lim_{T\to0}\Omega = \lim_{T\to0}\left\{-T\ln\left[\prod_{\mathbf{k},\boldsymbol{\sigma}}\left(1+e^{-\beta\zeta_{\mathbf{k}}}\right)\right]\right. \\ &\left.+\frac{\mathcal{V}}{2}\int_0^1\frac{d\lambda}{\lambda}\lambda\int\frac{d^3q}{(2\pi)^3}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}^{\lambda}\left(\mathbf{q},iq_n\right)-n\right]\right\}\end{aligned} \tag{46.6}$$

We have for the sum over Matsubara frequencies

$$T\sum_{iq_n}\chi_{nn}\left(\mathbf{q},iq_n\right) = T\sum_{iq_n}\int\frac{d\omega'}{\pi}\frac{\chi_{nn}''\left(\mathbf{q},\omega'\right)}{\omega'-iq_n} \tag{46.7}$$

$$= \int\frac{d\omega'}{\pi}n_B\left(\omega'\right)\chi_{nn}''\left(\mathbf{q},\omega'\right) \tag{46.8}$$

In the zero temperature limit,

$$\lim_{T\to0}\int\frac{d\omega'}{\pi}n_B\left(\omega'\right)\chi_{nn}''\left(\mathbf{q},\omega'\right) = -\int_{-\infty}^0\frac{d\omega'}{\pi}\chi_{nn}''\left(\mathbf{q},\omega'\right) \tag{46.9}$$

$$= \int_0^\infty\frac{d\omega'}{\pi}\chi_{nn}''\left(\mathbf{q},-\omega'\right) \tag{46.10}$$

$$= -\int_0^\infty\frac{d\omega'}{\pi}\chi_{nn}''\left(\mathbf{q},\omega'\right) \tag{46.11}$$

so that the expression for the ground state energy becomes

$$\begin{aligned} & \frac{E_{Tot}^{RPA}\left(T=0\right)-\mu N}{\mathcal{V}} \\ = \; & 2\int_{k<k_F}\frac{d^3k}{\left(2\pi\right)^3}\left(\frac{k^2}{2m}-\mu\right) \\ & +\frac{\mathcal{V}}{2}\int\frac{d^3q}{\left(2\pi\right)^3}\int_0^1\frac{d\lambda}{\lambda}\lambda V_{\mathbf{q}}\left[-\operatorname{Im}\int_0^\infty\frac{d\omega'}{\pi}\frac{\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)}{1+\lambda V_{\mathbf{q}}\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)}-n\right] \end{aligned} \tag{46.12}$$

Note that we have replaced everywhere $V_{\mathbf{q}}$ by $\lambda V_{\mathbf{q}}$ as prescribed in the coupling constant integration trick.

Remark 304 *Role of the coupling constant integration from the point of view of diagrams: By expanding the RPA expression, we see that what this coupling constant integration trick does, is give a factor* $1/n$ *in front of the corresponding term of order* n *in the interaction. As mentioned earlier, if we had developed Feynman rules directly for the free energy instead of using the coupling constant trick, we would have written down closed loop diagrams such as those of Fig.(44-3) and modified Feynman's rules to add the rule that there is a factor* $1/n$ *for every topologically different diagram of order* n*.*

The coupling constant integration is easy to perform

$$\begin{aligned} & \int_0^1\frac{d\lambda}{\lambda}\lambda V_{\mathbf{q}}\left[-\operatorname{Im}\int_0^\infty\frac{d\omega'}{\pi}\frac{\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)}{1+\lambda V_{\mathbf{q}}\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)}-n\right] \\ = \; & -V_{\mathbf{q}}n-\int_0^\infty\frac{d\omega'}{\pi}\operatorname{Im}\left\{\ln\left[1+V_{\mathbf{q}}\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)\right]\right\} \end{aligned} \tag{46.13}$$

The rest of the calculation is tedious. One finds at zero temperature, [23]:

$$\frac{E_{Tot}^{RPA}\left(T=0\right)}{N}=\frac{2.21}{r_s^2}-\frac{0.916}{r_s}+0.0622\ln r_s-0.142+\mathcal{O}\left(r_s,r_s\ln r_s\right) \tag{46.14}$$

The first term is the kinetic energy, the second the contribution from the Fock (exchange) diagram while the rest is the so-called correlation energy, namely everything beyond Hartree-Fock.

47. LANDAU FERMI LIQUID FOR RESPONSE FUNCTIONS

^{3}He is an example of a fluid of fermions with short-range interactions. It inspired Landau to develop "Fermi liquid theory". Since we saw that interactions become short range in the Coulomb gas, in the end it can be considered as a Fermi liquid. In this Chapter, I define so-called "Landau Parameters" for thermodynamic quantities and show how they appear in a few quantities. I neglect the imaginary part of the self-energy. This assumes that we are at very low temperature. The imaginary part of the self-energy comes in calculation of transport quantities, such as resistivity, thermal conductivity etc.

Landau Fermi liquid theory is based on the existence of quasiparticles, so I will assume that the Green's function take a quasiparticle form

$$\mathcal{G}\left(\mathbf{k},ik_n\right) \tilde{} \frac{Z_{\mathbf{k}_F}}{\left(ik_n+\mu-E_{\mathbf{k}}\right)} \tag{47.1}$$

where $Z_{\mathbf{k}}$ is evaluated at the Fermi level since contributions come mostly from there.

47.0.1 Compressibility

Assume that I want the compressibility.

48. *EXPANSION IN TERMS OF DRESSED OR BARE GREEN'S FUNCTIONS: SKELETON DIAGRAMS

In this brief chapter, I try to discuss the delicate question of perturbation theory in terms of dressed or bare Green's functions. self-consistency. To be completed...

48.1 The expansion in terms of bare Green's functions can be derived using the Schwinger approach

49. *GENERAL CONSIDERATIONS ON PERTURBATION THEORY AND ASYMPTOTIC EXPANSIONS

It is striking that in the end the RPA results, such as those for the ground state energy Eq.(46.14), the effective mass Eq.(45.25) or the scattering rate Eq.(45.26) are non-analytic in r_s near $r_s = 0$. This often occurs in perturbation theory. In fact, the perturbation expansion is at best an asymptotic expansion since for attractive potential at zero temperature the ground state is a superconductor and not a Fermi liquid. In other words, $r_s = 0$ is a point of non-analyticity since for $r_s < 0$ there is symmetry breaking. The following simple example taken from Ref.[27] is instructive of the nature of asymptotic expansions.

Suppose we want to evaluate the following integral

$$Z(g) = \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2} - \frac{g}{4}x^4} \tag{49.1}$$

This is an example where the integral does not exist for $g < 0$ but where we will try nevertheless to expand in powers of g around $g = 0$. If we do this then,

$$Z(g) = \sum_{n=0}^{\infty} g^n Z_n \tag{49.2}$$

where

$$Z_n = \frac{(-1)^n}{4^n n!} \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} x^{4n} \tag{49.3}$$

$$= \frac{(-1)^n}{4^n n!} \frac{(4n-1)!!}{2^n} \tag{49.4}$$

with

$$(4n-1)!! \equiv (4n-1)(4n-3)(4n-5)\ldots 1 \tag{49.5}$$

$$= \frac{(4n)!}{(4n)(4n-2)(4n-4)\ldots 2} \tag{49.6}$$

$$= \frac{(4n)!}{2^n (2n)!} \tag{49.7}$$

hence,

$$Z_n = \frac{(-1)^n}{16^n n!} \frac{(4n)!}{(2n)!} \tag{49.8}$$

Using Stirling's formula,

$$n! \approx \sqrt{2\pi} n^{n+1/2} e^{-n}$$

we are left with

$$Z_n \propto \frac{1}{\sqrt{n\pi}} \left(\frac{-4n}{e}\right)^n \tag{49.9}$$

The value of each successive term in the power series is illustrated in Fig.(49-1). Clearly, whatever the value of g, if n is sufficiently large, the higher order terms

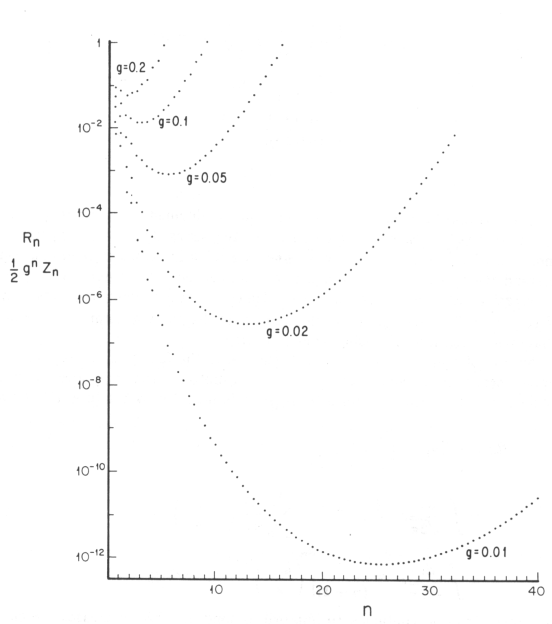


Figure 49-1 Asymptotic expansion of $Z(g)$ for different values of g. The residual error $R_n is$ plotted for the half-integer values. From J.W. Negele and H. Orland, *op. cit.* p.56

start to be larger than the low order ones. This is a characteristic of an asymptotic series.

We can even evaluate the error done when the series is stopped at order n. Let this error be

$$R_n = \left| Z(g) - \sum_{m=0}^{n} g^m Z_m \right| \tag{49.10}$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| e^{-\frac{g}{4}x^4} - \sum_{m=0}^{n} \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \tag{49.11}$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| \sum_{m=n+1}^{\infty} \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \tag{49.12}$$

The series in the absolute value is an alternating series and it converges. Hence, an upper bound for this series is the value of the first term, as may be seen from the fact that

$$a_{n+1} - (a_{n+2} - a_{n+3}) - (a_{n+4} - a_{n+5}) - \ldots \leq a_{n+1} \tag{49.13}$$

Hence,

$$R_n \leq g^{n+1} |Z_{n+1}| \tag{49.14}$$

We also plot the error in Fig.(49-1). Clearly, the error starts to grow eventually.

Despite this terrible behavior of asymptotic expansions they can be quite useful in practice. For example, for $g = 0.01$, the precision is 10^{-10} after 25 terms. This may be estimated by noting from Eq.(49.9) for the asymptotic value of Z_n that $g^n Z_n$ starts to grow when $4gn$ becomes of order unity. The minimum error is then estimated with our formula for R_n. Even quantum electrodynamics is an asymptotic expansion, but the expansion parameter is $\alpha = 1/137$. It is thus an

extremely good expansion parameter. Sometimes the asymptotic series may be resumed, at least partially as in RPA, or mathematical techniques, such as Borel summation, may be used to extract the non-analytic behavior.

50. *BEYOND RPA: SKELETON DIAGRAMS, VERTEX FUNCTIONS AND ASSOCIATED DIFFICULTIES.

It is quite difficult to go beyond RPA while preserving important physical properties, such as conservation laws, or the $f-$sum rule. We can illustrate this by the following simple example. The Lindhard function with bare Green's function satisfies conservation laws since it is the charge susceptibility of free electrons. Suppose that in the presence of interactions, we succeed in computing the exact one-body Green's function. Then, it is tempting to compute the density fluctuations using a bubble made up of the exact Green's functions that we just obtained. For one-body interactions, as for example in the impurity problem, this would be the exact result, as we saw in a previous chapter. However, in the case where two-body interactions are present, this becomes an approximation that violates charge conservation.

Before we reformulate perturbation theory in general terms at the end of this Chapter and in the next, we proceed to illustrate some of the problems that arise if we try to improve on simple perturbation theory or on RPA in naive ways.

50.1 *A dressed bubble diagram violates charge conservation

To see this, we will show that the following consequence of charge conservation is violated[29]

$$\chi_{nn}\left(\mathbf{q}=\mathbf{0},iq_n\right)=0 \quad ; \quad \text{if} \quad iq_n\neq 0. \tag{50.1}$$

To check that this last equation is a consequence of charge conservation, note that at $\mathbf{q}=\mathbf{0}$ the density operator is the number operator, an operator that commutes with the Hamiltonian. This means that $\chi_{nn}\left(\mathbf{q}=\mathbf{0},\tau\right)$ is independent of imaginary time, which implies that its only non-vanishing Matsubara frequency component is $q_n=0$. Using the spectral representation for the Green's function and inversion symmetry in the Brillouin zone, our single dressed bubble calculation for χ_{nn} on the other hand will give us the following expression

$$\tilde{\chi}_0\left(\mathbf{q},iq_n\right)=\frac{2}{N}\sum_{\mathbf{k}}\int\frac{d\omega}{2\pi}\int\frac{d\omega'}{2\pi}A\left(\mathbf{k},\omega\right)A\left(\mathbf{k}+\mathbf{q},\omega'\right)\frac{\left(\omega-\omega'\right)\left(f\left(\omega'\right)-f\left(\omega\right)\right)}{\left(\omega-\omega'\right)^2+q_n^2}. \tag{50.2}$$

When there are no interactions and $A\left(\mathbf{k},\omega\right)$ is a delta function, it is clear that our exact result Eq.(50.1) is satisfied since only $\omega=\omega'$ will contribute. Otherwise, the integrand is positive definite so the result is different from zero at $\mathbf{q}=\mathbf{0}$.

Another consequence of charge conservation is the $f-$sum rule. Indeed, recall that the $f-$sum rule is obtained from a frequency integral over $\omega\chi''_{nn}\left(\omega\right)$. This means that in real time it involves the derivative of the density, which is related to a current by charge conservation. One then has to evaluate an equal-time

commutator between current and density, which can be done exactly and gives the $f-$sum rule.

The $f-$sum rule manifests itself in the high frequency behavior of $\chi_{nn}(\mathbf{q},iq_n)$. This can be seen as follows. First, recall that $\chi''_{nn}(\omega)$ is odd by time-reversal symmetry. Then,

$$\chi_{nn}(\mathbf{q},iq_n)=\int\frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-iq_n}=\int\frac{d\omega'}{\pi}\frac{\omega'\chi''_{nn}(\mathbf{q},\omega')}{(\omega')^2+(q_n)^2} \tag{50.3}$$

so that the leading high-frequency behavior is given by the $f-$ sum rule:

$$\lim_{q_n\to\infty}q_n^2\chi_{nn}(\mathbf{q},iq_n)=\int\frac{d\omega'}{\pi}\omega'\chi''_{nn}(\mathbf{q},\omega'). \tag{50.4}$$

We just saw that if we replace $\chi_{nn}(\mathbf{q},iq_n)$ by the dressed bubble $\tilde{\chi}_0(\mathbf{q},iq_n)$ then $\tilde{\chi}_0(\mathbf{q}=\mathbf{0},iq_n)$ is different from zero so that the equation we just derived, Eq.(50.4), tells us that the $f-$sum rule is violated in this approximation.

50.2 *RPA with dressed bubble violates the $f-$sum rule and gives bad results

To see that knowing the exact one-body Green's function in an interacting system is not enough to know the density fluctuations, it suffices to return to Fig.(41-1). The diagrams on the bottom may be accounted for by using dressed propagators, but the diagrams on the first line cannot be. In the Schwinger approach, the diagrams on the first line come from iterating the integral equation in Fig. 37-7. They enter the general category of vertex corrections, namely diagrams that cannot be included by simply dressing propagators. The lesson we have just learned is that to satisfy conservation laws, the vertex corrections representing the dressed interaction between quasiparticles have to do some non-trivial things since the dressed bubble by itself does not satisfy the conservation law expressed in the form of Eq.(50.1).

We may think that taking partial care of the vertex corrections by summing the bubble diagrams in the first line of Fig.(41-1) as we did in RPA and just replacing the Green's functions by dressed ones would do the trick. This does not happen. Indeed, consider

$$\chi_{nn}(\mathbf{q},iq_n)=\frac{\tilde{\chi}_0(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\tilde{\chi}_0(\mathbf{q},iq_n)}. \tag{50.5}$$

Then we fall back on the violation of the $f-$ sum rule that we saw with the dressed bubble because

$$\lim_{q_n\to\infty}q_n^2\chi_{nn}(\mathbf{q},iq_n)=\lim_{q_n\to\infty}q_n^2\tilde{\chi}_0(\mathbf{q},iq_n). \tag{50.6}$$

To see another example of how apparently reasonable improvements over RPA may lead to miserable failures consider the following reasoning. We saw from RPA that there are quasiparticles near the Fermi surface. Also, the low-frequency and small momentum density fluctuations are determined mainly by quantities near the Fermi surface, as one can check from the Lindhard function. It would thus be tempting, in a next iteration, to compute the bubbles entering RPA with a renormalized propagator

$$\frac{Z_{\mathbf{k}}}{ik_n-E_{\mathbf{k}}+\mu} \tag{50.7}$$

In practice $Z_{\mathbf{k}}$ is in the range 0.5 to 0.7 which means that the dielectric constant might change from $1 - V_{\mathbf{q}}GG$ to $1 - \frac{1}{4}V_{\mathbf{q}}GG$ when $Z_{\mathbf{k}} = 0.5$ for example. That would spoil the agreement that we had with experiment. Again, dressing the bubble and doing nothing to the vertex is not a good idea. It is as if the vertex must compensate the $Z_{\mathbf{k}}$ appearing in the Green's functions.

50.3 *Two reformulations of perturbation theory

Another way to approach the problem of going beyond the simple perturbative approaches is to start from exact reformulations of perturbation theory. Other useful guides when one tries to push beyond the simplest perturbative approaches are conservation laws, known as Ward identities, as well as sum rules and other exact results such as the relation between $\Sigma\mathcal{G}$ and density fluctuations that we have introduced in the present chapter. We will come back on these general considerations in a later chapter. For the time being we give two ways to reformulate the diagrammatic expansion in a formally exact way. From the point of view of Feynman, this is a way to rearrange the infinite series of diagrams. But it you have followed the Schwinger way, this comes out rather naturally, especially in second case discussed below. I prove the first reorganisation of the perturbation series, due to Hedin, in Chap.(51).

The first reformulation is illustrated in Fig.(50-1). The propagators are fully dressed. The interaction line must also be dressed, as illustrated on the second line. The bubble appearing there is called the polarization propagator since it plays the role of the polarizability in the definition of the dielectric constant. It is defined as the set of all diagrams that cannot be cut in two pieces by cutting a single interaction line. The polarization propagator has a bubble with dressed propagators but this is not enough. We must also include some more vertex corrections. These vertex corrections, represented by the triangle, are illustrated by the first few terms of their diagrammatic expansion on the last line of the figure. A vertex correction (irreducible) of the type envisaged here cannot be cut in two pieces by cutting either a propagator or an interaction line, and it is attached to the outside world by three points, two of which are fermionic, and one of which is bosonic (*i.e.* attaching to an interaction line). Both in the polarization bubble and in the self-energy, only one of the vertices is dressed, otherwise that would lead to double counting as one can easily check by writing down the first few terms and returning to Feynman's rules (The Schwinger approach is in the next section). One can also check by writing down a few terms that vertex corrections on the Hartree diagrams are indistinguishable from self-energy effects so they are included in the dressed propagator. What is not so obvious from this diagrammatic (Feynman) approach, is what should be included in the vertex correction. The Schwinger approach teaches us that it can be obtained from the functional derivative of the self-energy when we drop the Hartree term. Chapter 51 on Hedin's equations will obtain these equations rather easily using the Schwinger approach.

We will see in a subsequent chapter that the theory for electron-phonon interactions may be written precisely in the form of Fig.(50-1) except for the fact that the interaction line becomes replaced by a phonon propagator. In addition a key theorem, that we shall prove, the so-called Migdal theorem, shows that for electron-phonon interactions vertex corrections may be neglected. The first two lines of Fig.(50-1) then form a closed set of equations. Migdal's theorem is behind the success of electron-phonon theories, in particular the theory of superconduc-

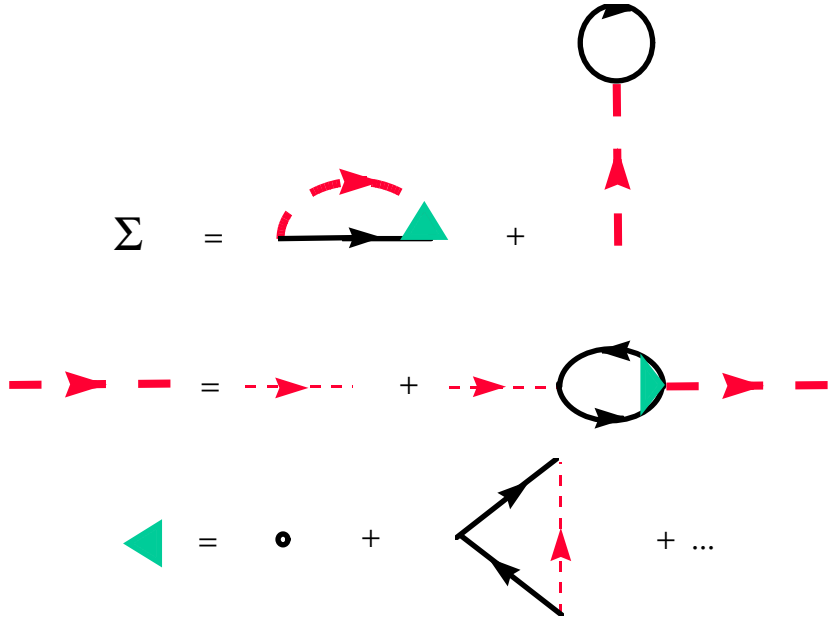


Figure 50-1 Exact resummation of the diagrammatic perturbation expansion. The dressed interaction on the second line involves the one-interaction irreducible polarisation propagator. The last line gives the first terms of the diagrammatic expansion for the vertex corrections.

tivity in its Eliashberg formulation.

For pure electron-electron interactions, vertex corrections may not be neglected. Non-diagrammatic ways of approaching the problem, such as that of Singwi[28], have proven more successful. We have already shown algebraically in the Schwinger approach that perturbation theory for electron-electron interactions may also be formulated in a way that is diagrammatically equivalent to Fig.(50-2). That is our second exact reformulation of perturbation theory[29] (there are others). For those that have followed the Feynman approach only, the triangle now represents the fully reducible vertex, namely diagrams that can be cut in two by cutting interaction lines or particle-particle pairs or particle-hole pairs in a different channel. (We will discuss the notion of channel in more details in a later chapter). The box on the other hand represents all terms that are irreducible with respect to cutting a particle-hole pair of lines in the chosen channel. To be complete we would need to give a diagrammatic expansion for the square box but, in practice, the way to make progress with this approach is to proceed non-perturbatively, namely to parametrize the box in such a way that it can later be determined by using sum rules and various other exact constraints of many-body theory, such as the Pauli exclusion principle and conservation laws. This will be discussed in Chapter 57 dealing with the two-particle self-consistent approach.

50.4 *Skeleton diagrams

The diagrams in Fig.(50-1) and Fig.(50-2) above are skelton diagrams. This means that the Green's functions that appear there do not have self-energy insertions.

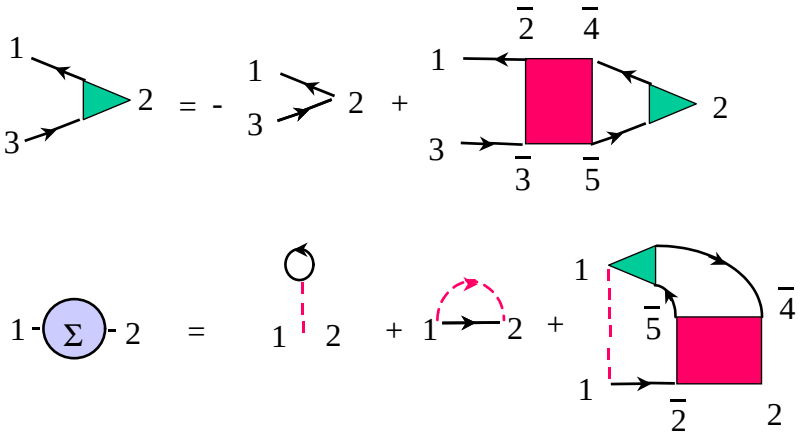


Figure 50-2 Exact representation of the full perturbation series. The triangle now represents the fully reducible vertex whereas the box represents all terms that are irreducible with respect to cutting a particle-hole pair of lines in the indicated channel.

In other words, we cannot cut two propagator lines and be left with two pieces, one of which looks like a self-energy diagram. In the jargon, we say that the diagrams are two-particle irreducible (2PI). Another way to say this is that the diagrams are built from dressed Green's functions. In the Schwinger approach, the diagrams come out this way directly. In the Feynman approach, one needs to do resummations to see these skeleton diagrams appear.

50.5 *Channels

We know that

$$\Sigma\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},3\right)=-V\left(1-\overline{2}\right)\left\langle T_{\tau}\psi^{\dagger}\left(\overline{2}^{+}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^{\dagger}\left(3\right)\right\rangle . \tag{50.8}$$

Up to now, we have expressed the four point function by associating the last two indices to the right, $\psi\left(1\right)\psi^{\dagger}\left(3\right)$, to a Green's function and differentiating with respect to a source field. More specifically, we have used

$$\frac{\delta\mathcal{G}\left(1,3\right)}{\delta\phi\left(2^{+},2\right)}. \tag{50.9}$$

Then we wrote an integral equation for this quantity that involves $\delta\Sigma/\delta\phi=\mathcal{G}\left(\delta\Sigma/\delta\mathcal{G}\;\delta\mathcal{G}/\delta\phi\right)\mathcal{G}$. A momentum $\mathbf{q}$ flowing through $\mathcal{G}\;\mathcal{G}$ became important in momentum space and allowd us to select out a series of important diagrams, the RPA ones. That is the longitudinal particle-hole channel, or sometimes called the Peierls channel.

We could have decided to take $\psi\left(2\right)\psi^{\dagger}\left(3\right)$ as the fields for the Green's function. Then, we would have needed

$$\frac{\delta\mathcal{G}\left(2,3\right)}{\delta\phi\left(2^{+},1\right)}. \tag{50.10}$$

Note this time that the spin indices in ϕ are no longer the same in general since σ_2 can be different from σ_1. In other words, the field ϕ does not conserve spin. No problem since in the end we will set $\phi=0$. When we work out

$\delta\Sigma/\delta\phi = \mathcal{G}\left(\delta\Sigma/\delta\mathcal{G}\ \delta\mathcal{G}/\delta\phi\right)\mathcal{G}$ keeping the same definitions of Fourier transforms, i.e. associating $\mathbf{q}$ to $1-2$, $\mathbf{k}$ to $1-3$ and $\mathbf{k}'$ to $2-3$ for example, the momentum that will be single out in $\mathcal{G}\ \mathcal{G}$ will be different from the $\mathbf{q}$ considered above. We call this the transverse particle-hole channel.

There is one last possibility as you have already guessed, the particle-particle, or Cooper channel. There we take for example $\psi\left(\overline{2}\right)\psi\left(1\right)$ as associated to a Green's function and we take a derivative with respect to a field η coupled to $\psi^{\dagger}\left(\overline{2}^{+}\right)\psi^{\dagger}\left(3\right)$ that breaks particle number conservation. The important functional derivative will be

$$\frac{\delta\mathcal{G}_{1,2}\left(2,1\right)}{\delta\eta\left(2^{+},3\right)}.$$

The subscripts to $\mathcal{G}_{1,2}$ remind us (in the Nambu notation that we will expand on later) that the Green's function no longer involves ψ and $\psi^{\dagger}$, but $\psi\psi$. Again, when we move to $\mathcal{G}\left(\delta\Sigma/\delta\mathcal{G}\ \delta\mathcal{G}/\delta\eta\right)\mathcal{G}$, a different momentum will enter $\mathcal{G}\ \mathcal{G}$ and will be important.

Depending on the details of the interaction, one channel or the other can be important. For a long-range Coulomb interaction, the longitudinal channel suffices. For the Hubbard on-site (momentum independent) interaction, both longitudinal and transverse channels are important, while for an attractive potential, it is the Cooper channel that counts.

50.6 *Crossing symmetry

The different channels discussed above are related since the four point function just gives a sign change if we interchange the indices of two creation or two destruction operators, namely

$$\left\langle T_{\tau}\psi^{\dagger}\left(\overline{2}^{+}\right)\psi\left(2\right)\psi\left(1\right)\psi^{\dagger}\left(3\right)\right\rangle = -\left\langle T_{\tau}\psi^{\dagger}\left(\overline{2}^{+}\right)\psi\left(1\right)\psi\left(2\right)\psi^{\dagger}\left(3\right)\right\rangle \tag{50.11}$$

and

$$\left\langle T_{\tau}\psi^{\dagger}\left(\overline{2}^{+}\right)\psi\left(2\right)\psi\left(1\right)\psi^{\dagger}\left(3\right)\right\rangle = -\left\langle T_{\tau}\psi^{\dagger}\left(3\right)\psi\left(2\right)\psi\left(1\right)\right\rangle \psi^{\dagger}\left(\overline{2}^{+}\right). \tag{50.12}$$

This is particularly relevant for the two particle-hole channels.

51. *HEDIN'S EQUATIONS

The idea of an effective screened interaction that is discussed in the previous section and that you can see in the second line of Fig.(50-1) is quite helpful in the Coulomb gas context. The Schwinger approach can be rewritten in such a way that the effective interaction appears explicitly. That will lead to Hedin's equations.[11] The diagrammatic Feynman arguments leading to the same result have been sketched in the previous section.

To proceed with the Schwinger derivation, we first identify two contributions to the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$ represented by the red box appearing in both Fig.(36-2) for the self-energy and in Fig.(36-1) for the four point function. The first contribution comes from the functional derivative of the Hartree term and the second contribution from the functional derivative of everything else. We then include the Hartree term in the non-interacting Green's function. Fig.(36-2) for the self-energy and Fig.(36-1) for the four point function then become as illustrated in Fig.(51-1). In the top row for the four point function, we have simply joined the points on the bottom and separated the red box for the irreducible vertex into two contributions, one from the functional derivative of the Hartree term, that is the last term, and one from the functional derivative of the rest of the self-energy (on the bottom line), represented by the blue textured box. The same replacement has been done for the irreducible vertex (red box) entering the self-energy. The blue textured box will contain diagrams that cannot be cut in two by cutting an interaction line.

We can now isolate the so-called fully reducible vertex, represented by the green triangle, by matrix multiplying both sides of the equation appearing on the first line of Fig.(51-1) by $\mathcal{G}^{-1}\left(4,\bar{1}\right)\mathcal{G}^{-1}\left(\bar{2},3\right)$ and relabeling. We then obtain the first line of Fig.(51-2). Note that the dot with the three places to attach is given algebraically by $\delta\left(1-3^{+}\right)\delta\left(2-3\right)$. We have also put back some variables of integration on the right-hand side because the triangle does not include the Green's functions anymore.

We see now that we can replace the equation for the self-energy appearing on the second line of Fig.(51-1) by the second line of Fig.(51-2). The latter expression for the self-energy in terms of the fully reducible vertex does not depend on our original separation of the irreducible vertex (red box) into two contribution. It is completely general.

We want to express the fully reducible vertex appearing in the expression for the self-energy in terms of Green's functions, effective interaction and irreducible vertex. To proceed further, we resort to algebra. You can think of each block in the first line of Fig.(51-2) as being a square matrix. Take for example the triangle. Call it $\Theta\left(2^{+},2;4,3\right)$. The pair $4,3$ is one matrix index and the pair $2^{+},2$ another matrix index. The two indices $2^{+},2$ happen to be equal, but we can consider the general case. Then, on the right hand side, reading from bottom to top, is like matrix multiplication from left to right. It is as if we rotated the diagrams by $\pi/2$ clockwise. We need to recall that it is and incoming Green's functions that attaches to 4 and and outgoing one that attaches to 3.

Let us call the blue irreducible vertex with the two attached Green's functions $\mathcal{GG}I$, and the bubble with the interaction $\mathcal{GG}V$. Then, the first line of Fig.(51-2) is the matrix equation

$$\Theta = 1 + \Theta\mathcal{GG}I + \Theta\mathcal{GG}V \tag{51.1}$$

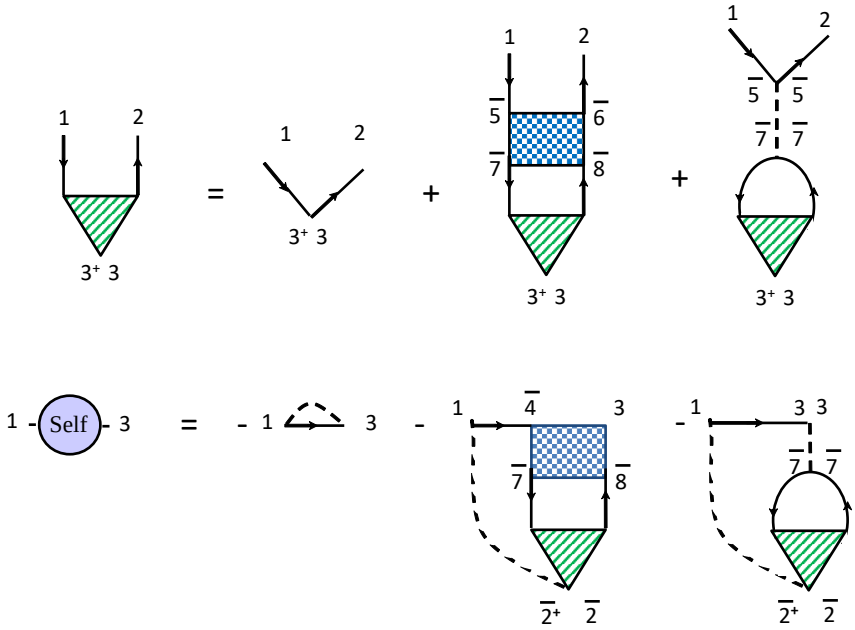


Figure 51-1 Rewriting our two equations for $\delta\mathcal{G}/\delta\phi$ and for Σ in such a way that the Hartree term has been absorbed in a redefinition of the chemical potential and the irreducible vertex that was the red box entering the equation for $\delta\mathcal{G}/\delta\phi$ has been separated in two parts: the last term of the top line that comes from $\delta\Sigma/\delta\mathcal{G}$ of the Hartree term in Σ and the blue box that represents the derivative of the rest of Σ that appears on the bottom line. The green triangle, as before, is the fully reducible vertex.

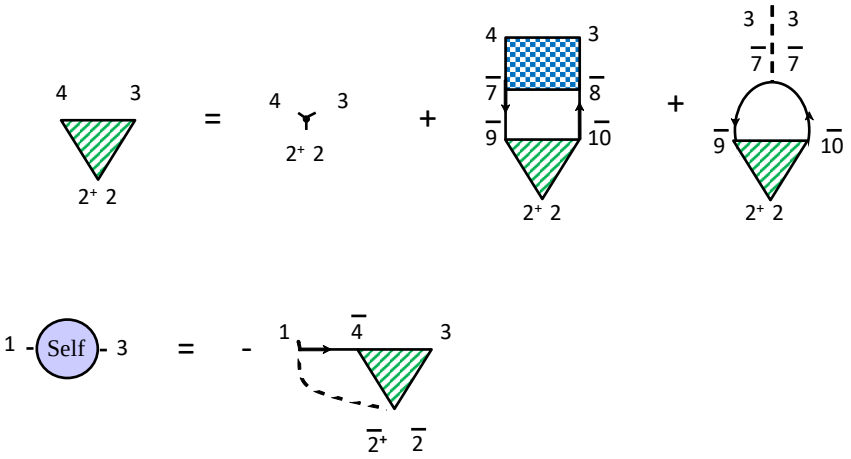


Figure 51-2 $\delta\mathcal{G}/\delta\phi$ has been separated in two parts: the last term of the top line that comes from $\delta\Sigma/\delta\mathcal{G}$ of the Hartree term in Σ and the blue box that represents the rest. That blue box appears both on the top and the bottom line. The top line is the same figure as the preceding one, but with the two external legs amputated. Comparing with the equation for the self-energy in the previous figure, we see that the self-energy can now be written entirely in terms of the green triangle, also known as fully reducible vertex.

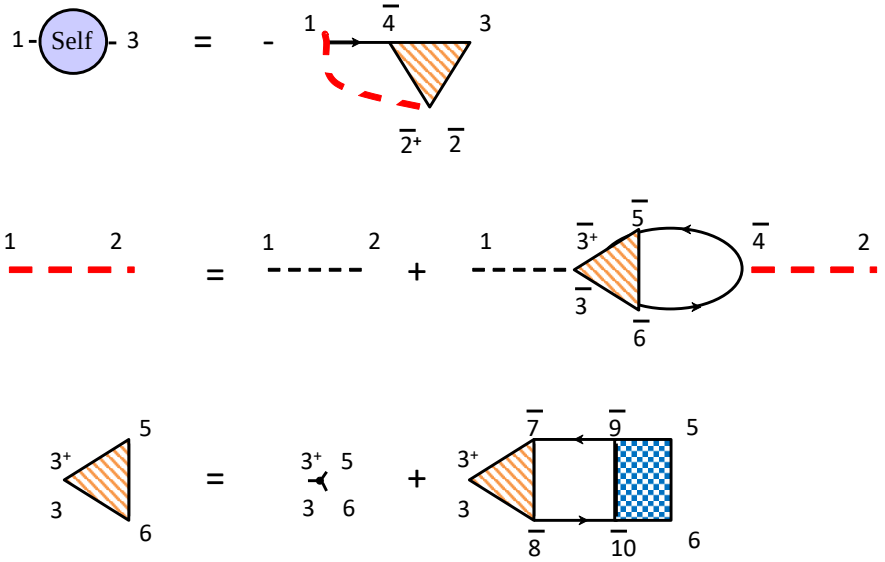


Figure 51-3 In these Hedin equations, the fully reducible vertex (green triangle of the previous figures) has been replaced by a vertex (orange triangle) that is irreducible with respect to cutting a single interaction line. The terms that are reducible with respect to cutting a single interaction line have all been gathered in a single effective interaction W represented by the red dotted line. W obeys the integral equation appearing on the second line. The loop with orange vertex is the polarization Π. The orange vertex Γ is irreducible with respect to cutting a single interaction line. It obeys the integral equation appearing on the third line. As before, the blue box is $\delta\Sigma/\delta\mathcal{G}$ where the self-energy that is differentiated appears on the first line.

whose solution is

$$\Theta = \left(1 - \mathcal{G}\mathcal{G}I - \mathcal{G}\mathcal{G}V\right)^{-1}. \tag{51.2}$$

This may also be written in the form

$$\begin{aligned}
\Theta &= \left[\left(1 - \mathcal{G}\mathcal{G}I\right)\left(1 - \left(1 - \mathcal{G}\mathcal{G}I\right)^{-1}\mathcal{G}\mathcal{G}V\right)\right]^{-1} && (51.3)\\
&= \left(1 - \left(1 - \mathcal{G}\mathcal{G}I\right)^{-1}\mathcal{G}\mathcal{G}V\right)^{-1}\left(1 - \mathcal{G}\mathcal{G}I\right)^{-1} && (51.4)\\
&= \left(1 - \Gamma\mathcal{G}\mathcal{G}V\right)^{-1}\Gamma && (51.5)
\end{aligned}$$

where we defined $\Gamma = \left(1 - \mathcal{G}\mathcal{G}I\right)^{-1}$. Returning to the second line of Fig.(51-2) and recalling that $\mathcal{G}\left(1,\overline{4}\right)$ attaches to the index $\overline{4}$ of $\Theta\left(\overline{2}^{+},\overline{2};\overline{4},3\right)$ and that $V\left(1-\overline{2}\right)$ attaches to the index 1 of $\mathcal{G}$ and $\overline{2}^{+},\overline{2}$ of $\Theta\left(\overline{2}^{+},\overline{2};\overline{4},3\right)$, we have an equation for the self-energy that looks like

$$\Sigma = -\mathcal{G}\left(1,\overline{4}\right)V\left(1-\overline{2}\right)\Theta\left(\overline{2}^{+},\overline{2};\overline{4},3\right) = -\mathcal{G}V\left(1-\Gamma\mathcal{G}\mathcal{G}V\right)^{-1}\Gamma. \tag{51.6}$$

The first product $\mathcal{G}V$ are the two terms we were just talking about. The rest of the terms obey the rules for matrix multiplication.

Algebraically, the above is equivalent to Dyson's equation plus the following set of four equations:

a) The self-energy: written in terms of $\mathcal{G}$, an effective interaction W and a vertex Γ

$$\Sigma\left(1,3\right) = -\mathcal{G}\left(1,\overline{4}\right)W\left(1,\overline{2}\right)\Gamma\left(\overline{2}^{+},\overline{2};\overline{4},3\right) \tag{51.7}$$

where we defined the effective interaction

$$W = V\left(1-\Gamma\mathcal{G}\mathcal{G}V\right)^{-1} \tag{51.8}$$

whose explicit form with indices appears below.

b) The effective interaction:

$$W\left(1,2\right) = V\left(1,2\right) + V\left(1,\overline{3}\right)\Pi\left(\overline{3},\overline{4}\right)W\left(\overline{4},2\right). \tag{51.9}$$

This is an integral equation equivalent to $V\left(1-\Gamma\mathcal{G}\mathcal{G}V\right)^{-1}$ if we define a polarization $\Pi = \Gamma\mathcal{G}\mathcal{G}$ that is a generalization of the Lindhard function (with a different sign) that includes vertex corrections. Indeed, in that case,

$$\begin{aligned}
W &= V\left(1-\Gamma\mathcal{G}\mathcal{G}V\right)^{-1} = V\left(1-\Pi V\right)^{-1} && (51.10)\\
&= V + V\Pi V + V\Pi V\Pi V + \cdots \\
&= V + V\Pi W. && (51.11)
\end{aligned}$$

Being more explicit with the indices, we can write the expression for Π.

c) The polarization:

$$\Pi\left(3,4\right) = \Gamma\left(3^{+},3;\overline{5},\overline{6}\right)\mathcal{G}\left(4,\overline{5}\right)\mathcal{G}\left(\overline{6},4\right). \tag{51.12}$$

We used the rule that an incoming Green's function attaches to the next to last index while an outgoing one attaches to the last. Note that when we restore spin indices and use the fact that $\mathcal{G}$ is diagonal in spin index, the polarization will be the only term that will lead to a factor of 2 coming from the spin sum. The expression involves the vertex Γ that we already defined. We need to be more explicit with indices.

d) The vertex: is a function Γ that came from $\Gamma = (1 - \mathcal{G}\mathcal{G}I)^{-1}$ that is equivalent to the integral equation

$$\Gamma\left(3^{+},3;\overline{5},\overline{6}\right) = \delta\left(3^{+}-\overline{5}\right)\delta\left(3-\overline{6}\right)+\Gamma\left(3^{+},3;\overline{7},\overline{8}\right)\mathcal{G}\left(\overline{9},\overline{7}\right)\mathcal{G}\left(\overline{8},\overline{10}\right)\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)}{\delta\mathcal{G}\left(\overline{9},\overline{10}\right)}. \tag{51.13}$$

The *GW* approximation that we used for the electron gas is equivalent to making the approximation $\Gamma\left(\overline{2}^{+},\overline{2};\overline{4},3\right) = \delta\left(\overline{4}-\overline{2}^{+}\right)\delta\left(3-\overline{2}\right)$. The above four equations plus Dyson's equation are what is called Hedin's equations.

To be more specific, this set of equations is illustrated in Fig.(51-3) that, for convenience and contact with the matrix equations, you should read from left to right instead of from bottom to top.

Remark 305 *Relation to the longitudinal dielectric constant: It is important physically to notice that W is the Coulomb interaction screened by the exact dielectric constant. This can be seen when you rewrite the exact result Eq.(90.29) for the dielectric constant in terms of the polarization operator that generalizes beyond RPA the non-interacting Lindhard function:*

$$\frac{1}{\epsilon^{L}(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1-\frac{e^2}{q^2\varepsilon_0}\chi^{R}_{nn}(\mathbf{q},\omega)\right) \tag{51.14}$$

$$= \frac{1}{\varepsilon_0}\left(1-V_{\mathbf{q}}\chi^{R}_{nn}(\mathbf{q},\omega)\right) \tag{51.15}$$

$$= \frac{1}{\varepsilon_0}\left(1+\frac{V_{\mathbf{q}}\Pi(\mathbf{q},\omega)}{1-V_{\mathbf{q}}\Pi(\mathbf{q},\omega)}\right) \tag{51.16}$$

$$= \frac{1}{\varepsilon_0}\left(\frac{1}{1-V_{\mathbf{q}}\Pi(\mathbf{q},\omega)}\right). \tag{51.17}$$

Comparison with the expression for W Eq.(51.10) in terms of the polarization shows that $W = V\frac{\varepsilon_0}{\varepsilon}$.

Remark 306 *Significance of the polarization: More specifically, $\Pi(\mathbf{q},\omega)$ is the sum of all diagrams that are one-interaction irreducible, i.e. that cannot be cut in two parts by cutting a single interaction line $V_{\mathbf{q}}$. Hence,*

$$\chi^{R}_{nn}(\mathbf{q},\omega) = -\frac{\Pi(\mathbf{q},\omega)}{1-V_{\mathbf{q}}\Pi(\mathbf{q},\omega)} \tag{51.18}$$

is an exact result.

52. EXERCICES FOR PART V

52.0.1 Théorie des perturbations au deuxième ordre pour la self-énergie

a) En utilisant les règles de Feynman dans l'espace des quantités de mouvement, écrivez les expressions correspondant aux deux diagrammes apparaissant à droite de la figure 38-10 des notes de cours. Ces diagrammes représentent la self-énergie irréductible au deuxième ordre en théorie des perturbations. Effectuez la somme sur les fréquences de Matsubara mais ne faites pas les intégrales.

b) Montrez, avant même de faire la somme sur les fréquences de Matsubara, que lorsque $V_{\mathbf{q}}$ est indépendant de **q,** le diagramme du milieu est égal à moins deux fois le dernier (troisième sur la figure). Le résultat net est qu'on pourrait considérer seulement le diagramme du milieu en supposant qu'un électron n'interagit qu'avec les autres électrons de spin opposé. Montrez, en remontant à l'Hamiltonien, que ce dernier résultat est général dans le cas où $V_{\mathbf{q}}$ est indépendant de **q**,(modèle de Hubbard).

c) Écrivez une expression pour la partie imaginaire de la self-énergie obtenue en (a), encore une fois sans faire les intégrales.

52.0.2 Théorie des perturbations au deuxième ordre pour la self-énergie à la Schwinger

a) Utilisez la méthode des dérivées fonctionnelles pour trouver tous les diagrammes au deuxième ordre en interaction $V_{\mathbf{q}}$ pour la self-énergie irréductible. N'oubliez pas que les fonctions de Green dans la méthode décrite en classe sont des fonctions de Green habillées, c'est-à-dire qu'elles contiennent la self-énergie et doivent donc aussi être développées en puissances de l'interaction.

b) Montrez, avant même de faire la somme sur les fréquences de Matsubara, que lorsque $V_{\mathbf{q}}$ est indépendant de **q,** le diagramme du milieu de la figure 38-10 est égal à moins deux fois le dernier (troisième sur la figure). Le résultat net est qu'on pourrait considérer seulement le diagramme du milieu en supposant qu'un électron n'interagit qu'avec les autres électrons de spin opposé. Montrez, en remontant à l'Hamiltonien, que ce dernier résultat est général dans le cas où $V_{\mathbf{q}}$ est indépendant de **q**,(modèle de Hubbard).

52.0.3 Déterminant, théorème de Wick et fonctions à plusieurs points dans le cas sans interaction

L'équation générale (36.22)

$$\frac{\delta \mathcal{G}\left(1,2\right)_{\phi}}{\delta \phi\left(3,4\right)}=\left\langle T_{\tau}\psi\left(1\right)\psi^{\dagger}\left(2\right)\psi^{\dagger}\left(3\right)\psi\left(4\right)\right\rangle_{\phi}+\mathcal{G}\left(1,2\right)_{\phi}\mathcal{G}\left(4,3\right)_{\phi}. \tag{52.1}$$

et l'équation valable dans le cas sans interaction

$$\frac{\delta \mathcal{G}\left(1,2\right)_{\phi}}{\delta \phi\left(3,4\right)}=\mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi} \tag{52.2}$$

qu'on peut facilement obtenir de l'Éq. (36.28) lorsque la self s'annule, nous apprend que dans le cas sans interaction

$$\left\langle T_\tau \psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle_\phi = \mathcal{G}(1,3)_\phi\,\mathcal{G}(4,2)_\phi - \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi \tag{52.3}$$

ou encore,

$$\left\langle T_\tau \psi(1)\,\psi(2)\,\psi^\dagger(2')\,\psi^\dagger(1')\right\rangle_\phi = \mathcal{G}(1,1')_\phi\,\mathcal{G}(2,2')_\phi - \mathcal{G}(1,2')_\phi\,\mathcal{G}(2,1')_\phi\,. \tag{52.4}$$

La formule précédente s'écrit aussi

$$\left\langle T_\tau \psi(1)\,\psi(2)\,\psi^\dagger(2')\,\psi^\dagger(1')\right\rangle_\phi = \det\begin{bmatrix} \mathcal{G}(1,1')_\phi & \mathcal{G}(1,2')_\phi \\ \mathcal{G}(2,1')_\phi & \mathcal{G}(2,2')_\phi \end{bmatrix}. \tag{52.5}$$

a) Vérifiez que le déterminant a bien les mêmes propriétés que le produit chronologique à gauche, c'est-à-dire qu'il change de signe lorsqu'on intervertit les indices (1 et 2) ou ($1'$ et $2'$).

Remark 307 *Fonction de corrélation à n points et déterminant: Cette réécriture comme un déterminant est possible aussi pour les fonctions de corrélation d'ordre supérieur. Par exemple, pour la fonction de corrélation à 6 points dans le problème suivant le résultat s'exprime comme un déterminant d'une matrice* 3×3 *de fonctions de Green. C'est la forme générale qui préserve les propriétés d'antisymmétrie du produit chronologique et qui est valable pour n'importe quelle fonction à n points dans le cas sans interactions.*

b) Vérifiez que le résultat (52.4) exprimant la fonction de corrélation à 4 points comme un produit de fonctions de corrélation à deux points dans le cas sans interaction, peut s'obtenir des règles suivantes: i) Appariez chaque $\psi(i)$ avec un $\psi^\dagger(j)$ de toute les façons possibles. ii) Chaque appariement (chaque contraction dans le jargon) donne un $-\mathcal{G}(i,j)_\phi$. iii) Le signe du produit des $-\mathcal{G}(i,j)_\phi$ est déterminé par le signe de la permutation nécessaire déplacer les $\psi(i)$ et les $\psi^\dagger(j)$ pour les mettre côte à côte dans l'ordre où ils apparaissent dans $\mathcal{G}(i,j)_\phi$, c'est-a-dire avec l'opérateur de destruction à gauche de l'opérateur de création. Ceci s'appelle le théorème de Wick et est valable pour une fonction de corrélation contenant un nombre quelconque de ψ et de $\psi^\dagger$, en autaut qu'il y a le même nombre de ψ que de $\psi^\dagger$.

52.0.4 Determinant, Wick's theorem and many-point correlation functions in the non-interacting case

The general result (36.22)

$$\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \left\langle T_\tau \psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi\,. \tag{52.6}$$

and the following equation, valid when there are no interactions (or equaivalently when the self-energy vanishes, as can be deduced from (36.28))

$$\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \mathcal{G}(1,3)_\phi\,\mathcal{G}(4,2)_\phi \tag{52.7}$$

teaches us that in the non-interacting case, the following is valid

$$\left\langle T_\tau \psi(1)\,\psi^\dagger(2)\,\psi^\dagger(3)\,\psi(4)\right\rangle_\phi = \mathcal{G}(1,3)_\phi\,\mathcal{G}(4,2)_\phi - \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi\,. \quad (52.8)$$

Changing labels, this is the same as

$$\left\langle T_\tau \psi(1)\,\psi(2)\,\psi^\dagger(2')\,\psi^\dagger(1')\right\rangle_\phi = \mathcal{G}(1,1')_\phi\,\mathcal{G}(2,2')_\phi - \mathcal{G}(1,2')_\phi\,\mathcal{G}(2,1')_\phi\,. \quad (52.9)$$

The preceeding formula can also be written as follows

$$\left\langle T_\tau \psi(1)\,\psi(2)\,\psi^\dagger(2')\,\psi^\dagger(1')\right\rangle_\phi = \det\begin{bmatrix} \mathcal{G}(1,1')_\phi & \mathcal{G}(1,2')_\phi \\ \mathcal{G}(2,1')_\phi & \mathcal{G}(2,2')_\phi \end{bmatrix}. \quad (52.10)$$

a) Verify that the determinant has the same properties as the time-ordered product to the left of the equation, namely it changes sign when indices (1 and 2) or ($1'$ and $2'$) are exchanged.

Remark 308 *Determinant and n-point correlation function: This rewriting as a determinant is possible also from higher-order correlation functions. For example, for the 6-point correlation function in the following problem, the result can be written as the determinant of a 3×3 matrix of Green's functions. That is the general form that preserves the antisymmetric properties of the time-ordering operator and that is valid for any n-point correlation function in the non-interacting case.*

b) Verify that the result (52.4) that represents the 4-point correlation function as a product of 2-point correlation functions in the non-interacting case can be obtained from the following rules: i) Pair every $\psi(i)$ with a $\psi^\dagger(j)$ in all possible ways. ii) Each pairing (or contraction in the jargon) gives a factor $-\mathcal{G}(i,j)_\phi$. iii) The sign of the proeuct of $-\mathcal{G}(i,j)_\phi$ is determined by the sign of the permutation that is necessary to displace the $\psi(i)$ and the $\psi^\dagger(j)$ to put them side by side in the order in which they appear in $\mathcal{G}(i,j)_\phi$, i.e. with the destruction operator to the left of the creation operator. This is called Wick's theorem and it is valid for a correlation function containing an arbitrary number of ψ and $\psi^\dagger$, as long as there are as many ψ as $\psi^\dagger$.

52.0.5 Cas particulier du théorème de Wick avec la méthode de Schwinger

Pour le cas sans interaction, calculez

$$\frac{\delta\mathcal{G}(1,2)}{\delta\phi(3,4)\,\delta\phi(5,6)} \quad (52.11)$$

et montrez que la fonction de corrélation à six points

$$-\left\langle T_\tau\left[\psi^\dagger(3)\,\psi(4)\,\psi^\dagger(5)\,\psi(6)\,\psi(1)\,\psi^\dagger(2)\right]\right\rangle_\phi \quad (52.12)$$

s'écrit comme une somme de six termes, chacun étant un produit de trois fonctions de Green. Montrez ensuite que le signe de chaque terme peut se déduire des permutations. Ceci est un cas particulier du théorème de Wick qui dit que dans le cas sans interaction les fonction de corrélation d'ordre plus élevé peuvent s'obtenir de toutes les "contractions" posssibles, une contraction correspondant à un appariement d'un $\psi^\dagger$ avec un ψ pour en faire une fonction de Green.

52.0.6 Fonction de Lindhard et susceptibilité magnétique:

On applique un champ magnétique extérieur $h(\mathbf{x},t)$ produisant sur un système de fermions de spin 1/2 la perturbation

$$H^{ext} = -\mu_0 \int d^3\mathbf{x} \sum_{\sigma=\pm 1} \sigma \psi_\sigma^\dagger(\mathbf{x}) \psi_\sigma(\mathbf{x}) h(\mathbf{x},t) \tag{52.13}$$

où μ_0 est le moment magnétique.

a) Utilisez la théorie de la réponse linéaire pour exprimer le coefficient de proportionalité entre le moment magnétique induit

$$M(\mathbf{k},\omega) = \mu_0 \left\langle \int d^3\mathbf{x} \int dt \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}+i\omega t} \sum_{\sigma=\pm 1} \sigma \psi_\sigma^\dagger(\mathbf{x},t) \psi_\sigma(\mathbf{x},t) \right\rangle_{hors \quad équilibre} \tag{52.14}$$

et le champ magnétique extérieur comme une fonction de réponse. Ce coefficient de proportionalité est la susceptibilité magnétique

$$\chi^R(\mathbf{k},\omega) = M(\mathbf{k},\omega)/h(\mathbf{k},\omega) \tag{52.15}$$

b) Supposez qu'il n'y a pas d'interactions dans le système et montrez, en utilisant le théorème de Wick dans le formalisme de Matsubara, que la susceptibilité magnétique est alors proportionnelle à la fonction de Lindhard.

c) Montrez que

$$\lim_{\mathbf{k}\to\mathbf{0}} \chi^R(\mathbf{k},\omega=0) = \begin{cases} \frac{3\mu_0^2 n}{2E_F} & T=0 \quad \text{(Susceptibilité de Pauli)} \\ \frac{\mu_0^2 n}{T} & T\to\infty \quad \text{(Loi de Curie)} \end{cases} \tag{52.16}$$

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Part VI

Fermions on a lattice: Hubbard and Mott

The jellium is clearly a gross caricature of real solids. It does a good job nevertheless for simple metals, like sodium or aluminum. But it is important to have more realistic models that take into account the presence of a lattice of ions. The best methods today to find the electronic charge distribution are based on Density Functional Theory (DFT), that we explain very schematically in the first Chapter of this Part. These methods give a band structure that, strictly speaking, should not be interpreted as single-particle excitations. Nevertheless, for elements in the top rows of the periodic table, the band structure found from DFT works well. If we include the long-range Coulomb interaction with the GW approximation described above, then results for band gaps for example can be quite good.

For narrow-band materials however, such as transition metal oxides that include d electrons, this is not enough. We will explore the rich Physics contained in a simple model, the Hubbard model, that was proposed to understand narrow band materials. That model adds to the band structure an on-site interaction term U that is supposed to represent the screened Coulomb interaction. We will see that in such a short-range interaction model, spin excitations that had basically disappeared from the electron-gas problem, will now play a prominent role. Even when the interaction is not too strong, we will see why the perturbative methods that we have described in the previous Part are of limited validity. When the interaction is not too strong, we can treat the problem non-perturbatively using the Two-Particle-Self-Consistent approach and others.

The Hubbard model will also allow us to understand why certain materials that are predicted to be good metals by band structure theory are in fact insulators. Insulating behavior can be induced by the interaction U when it is larger than the bandwidth. Such interaction-induced insulators are known as Mott insulators. And the transition between the metallic and the insulating phase that occurs as a function of U is called the Mott transition. The best known method to treat materials that are close to a Mott transition is Dynamical Mean-Field Theory and its cluster generalizations, that we will explain. High-temperature superconductors and layered organic conductors are examples of systems that display Mott insulating phases.

In the next Part we will use the Hubbard model to introduce broken symmetry states with ferromagnetism as an example. In this Part, we restrict ourselves to the "normal" paramagnetic state.

Definition 34 *Note that it is usual for physicist to call "correlations" all effects that go beyond DFT. Chemists often refer to correlations when Hartree-Fock theory is not sufficient.*

53. DENSITY FUNCTIONAL THEORY

The presence of a static lattice of ions creates bands, as we know from one-electron theory. How do we generalize this to the many-body case with electron-electron interactions. In particular, how do we go beyond Hartree-Fock theory?

Modern versions of band structure calculations, now more frequently refered to as electronic structure calculations, are based on Density Functional Theory (DFT). This is a ground state or thermal equilibrium method that is also used for molecules. We begin by describing the general method, then its implementation for band-structure calculations and then finite temperature generalizations.

53.1 The ground state energy is a functional of the local density

The approach is based on a simple theorem of Hohenberg and Kohn [1].

Theorem 35 *When there is a unique ground state, its ground state energy is a unique functional of the single-electron density.*

We present the version of Levy [2, 3] and Lieb [134]. In both cases, we use the variational principle for the ground state: the ground state wave function is that which minimizes the energy

$$E[\Psi] = \langle\Psi| H |\Psi\rangle .$$

with the constraint that with the constraint that $\langle\Psi|\Psi\rangle = 1$. So I need to prove the variational principle first. Here is the proof. The theorem has to wait a little bit.

Proof: We can expand $|\Psi\rangle$ on a complete basis of energy eigenstates

$$|\Psi\rangle = \sum_i a_i |i\rangle . \tag{53.1}$$

Then the average energy is given by

$$\begin{aligned} \langle\Psi| H |\Psi\rangle &= \sum_{i,j} a_j^* a_i \langle j| H |i\rangle & (53.2)\\ &= \sum_i a_i^* a_i E_i & (53.3) \end{aligned}$$

where the last line follows because by hypothesis the Hamiltonian is diagonal in that basis. With E_0 the lowest energy state, the inequality follows

$$\sum_i a_i^* a_i E_i \geq \left(\sum_i a_i^* a_i \right) E_0. \tag{53.4}$$

The prefactor on the right-hand side simplifies with the norm of the wave function in the denominator, which proves the theorem.

To continue, let

$$H = \widehat{T}_{kin} + \hat{V}_c + \hat{V}_l \tag{53.5}$$

where $\widehat{T}_{kin}$ is the kinetic energy, $\hat{V}_c$ the Coulomb interaction between electrons and $\hat{V}_l$ the interaction between the electrons and the positive lattice of ions. We are working in the limit where the kinetic energy of the ions is neglected, so there are no phonons. With $n_l(\mathbf{r}')$ the charge density of the lattice we can write

$$\begin{aligned}
\langle\Psi|\hat{V}_l|\Psi\rangle &= \langle\Psi|\int d^3\mathbf{r}\int d^3\mathbf{r}'\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}')|\Psi\rangle & (53.6)\\
&= \int d^3\mathbf{r}\langle\Psi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Psi\rangle\int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') & (53.7)\\
&= \int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r}) & (53.8)
\end{aligned}$$

where in the last line I have defined the lattice potential

$$V_l(\mathbf{r}) \equiv \int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') \tag{53.9}$$

and the one-body electronic density

$$n(\mathbf{r}) \equiv \int d^3\mathbf{r}\langle\Psi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Psi\rangle. \tag{53.10}$$

Hohenberg and Kohn first proved that in the ground state, $V_l(\mathbf{r})$ leads to a unique density $n(\mathbf{r})$.That shows that the ground state energy is a unique functional of $n(\mathbf{r})$ since $V_l(\mathbf{r})$ determines the Hamiltonian (kinetic energy and electron-electron interactions are always the same). That theorem, that assumes that the ground state is unique, is proven by contradition as follows. Assume that the potentials $V_l(\mathbf{r})$ and $V_l'(\mathbf{r})$ lead to the same density $n(\mathbf{r})$. The many-particle wave functions $|\Psi\rangle$ and $|\Psi'\rangle$ must be different since they correspond to different Schrödinger equations. The variational property then tells us that

$$\begin{aligned}
E' &= \langle\Psi'|H'|\Psi'\rangle < \langle\Psi|H'|\Psi\rangle = \langle\Psi|H - V_\ell + V_\ell'|\Psi\rangle. & (53.11)\\
E' &< E + \int d\mathbf{r}n(\mathbf{r})[V_l'(\mathbf{r}) - V_l(\mathbf{r})]. & (53.12)
\end{aligned}$$

Redoing this calculation with primed and non-primed system exchanging roles, we find that

$$E < E' + \int d\mathbf{r}n(\mathbf{r})[V_l(\mathbf{r}) - V_l'(\mathbf{r})]. \tag{53.13}$$

Adding the two equations, we have that

$$E + E' < E + E' \tag{53.14}$$

which cannot be true since the ground state is unique by hypothesis, so E is not equal to E'. This proves that the hypothesis that $V_l(\mathbf{r})$ and $V_l'(\mathbf{r})$ can both lead to the same density $n(\mathbf{r})$ cannot be correct (unless $V_l(\mathbf{r})$ and $V_l'(\mathbf{r})$ differ by a constant, in which case the corresponding wave functions are identical.). Hence, given $V_l(\mathbf{r})$, there is no other potential $V_l'(\mathbf{r})$ that can lead to the same density $n(\mathbf{r})$. This is equivalent to saying, and that is the important step, that the ground state energy is a unique functional of the density.

A more illuminating approach in my opinion, is that of Levy and Lieb [2, 3] [134]. If we take the set of all normalized wave functions, the variational principle can be formulated as

$$E = \min_{\Psi} \langle \Psi | \widehat{T}_{kin} + \hat{V}_c + \hat{V}_l | \Psi \rangle .$$

We now perform the minimization in two steps. First with respect to all wave functions that have the same one-particle density, then with respect to the one-particle density

$$\begin{aligned} E &= \min_{n} \min_{\Psi \to n} \langle \Psi | \widehat{T}_{kin} + \hat{V}_c + \hat{V}_l | \Psi \rangle \\ E &= \min_{n} \left[\left(\min_{\Psi \to n} \langle \Psi | \widehat{T}_{kin} + \hat{V}_c | \Psi \rangle \right) + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] \qquad (53.15) \\ &= \min_{n} \left[F[n] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] . \qquad (53.16) \end{aligned}$$

where we have defined

$$\boxed{F[n] = \min_{\Psi \to n} \langle \Psi | \widehat{T}_{kin} + \hat{V}_c | \Psi \rangle .} \qquad (53.17)$$

That functional of $n(\mathbf{r})$ contains kinetic energy and Coulomb interaction between electrons. It is independent of the lattice potential and is thus a universal property of the inhomogeneous electron gas. We say inhomogeneous because we have to find this function for densities that depend on position.

We can then write

$$\boxed{E[V_l] = \min_{n(\mathbf{r})} \left[F[n] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right]} . \qquad (53.18)$$

From that point of view, the Hohenberg-Kohn ground state energy E is a functional of the external potential and is the Legendre transform of the Levy-Lieb functional F with

$$\frac{\delta E[V_l]}{\delta V_l(\mathbf{r})} = n(\mathbf{r}) \qquad (53.19)$$

which can in principle be inverted to write $V_l(\mathbf{r})$ as a function of $n(\mathbf{r})$ and then write $E[V_l]$ as a functional of $n(\mathbf{r})$, namely $E[V_l[n(\mathbf{r})]]$. The inverse Legendre transform leads to

$$\frac{\delta F[n]}{\delta n(\mathbf{r})} = -V_l(\mathbf{r}) . \qquad (53.20)$$

What have we achieved? We have shown that a) the ground state energy depends only on $n(\mathbf{r})$ instead of the whole wave function. b) The functional $F[n]$ is universal in the sense that it depends only on $n(\mathbf{r})$ and nothing else. If we can find the exact $F[n]$ for all possible $n(\mathbf{r})$, it can be applied to all situations. When the density does not vary too violently, we can just find out the functional $F[n]$ by solving the inhomogeneous electron gas by whatever method we can, Monte Carlo for example.

53.2 The Kohn-Sham approach

How can we transform the general ideas of the previous section into a calculational tool? The Hartree contribution to the potential energy depends only on density.

It is less clear how to write the kinetic energy and the rest of the contributions to the Coulomb interaction (exchange for example) in a way that depends only on density. In the Thomas-Fermi approach, we wrote the kinetic energy as a function of the local Fermi wave vector, and hence as a function of the density. Nevertheless, that is not very precise when the density changes on short length scales. Kohn and Sham [116] proposed to expand the density in terms of orthogonal one-body orbitals for N particles in a paramagnetic state:

$$n(\mathbf{r}) = \sum_{i=1,\sigma}^{N/2} \left|\phi_{i,\sigma}^{KS}(\mathbf{r})\right|^2. \tag{53.21}$$

If the wave function was simply obtained by filling these orthogonal orbitals $\phi_{KS}(\mathbf{r})$, whatever they are, up to the Fermi level, the corresponding kinetic energy would be easy to compute

$$T_{KS} = \langle \Psi_{KS}| \widehat{T}_{kin} |\Psi_{KS}\rangle = \sum_{i=1,\sigma} \int d^3\mathbf{r} \phi_{i,\sigma}^{KS}(\mathbf{r}) \left(\frac{-\nabla^2}{2m}\right) \phi_{i,\sigma}^{KS}(\mathbf{r}). \tag{53.22}$$

The Kohn-Sham method then proposes to write for the universal functional

$$F[n] = \langle \Psi_{KS}| \widehat{T}_{kin} |\Psi_{KS}\rangle + \frac{1}{2}\int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|} + E_{xc}[n].$$

The above equation defines the exchange correlation functional $E_{xc}[n]$. Going back to the definition of $F[n]$, we see that

$$\begin{aligned} E_{xc}[n] &= \min_{\Psi\to n} \langle \Psi| \widehat{T}_{kin} + \hat{V}_c |\Psi\rangle - \min_{\Psi_{KS}\to n} \langle \Psi_{KS}| \widehat{T}_{kin} |\Psi_{KS}\rangle \\ &\quad -\frac{1}{2}\int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|}. \end{aligned} \tag{53.23}$$

Note that the Kohn-Sham expression for the kinetic energy is not exact.

Years of experience have yielded good approximations for the universal functional $E_{xc}[n]$. The simplest approximation, the Local Density Approximation (LDA) reads, for real orbitals,

$$\begin{aligned} E_{xc}^{LDA}[n] &= -\frac{1}{2}\min_{\Psi_{KS}\to n} \sum_{\sigma,\sigma'} \sum_{i,j}^{N/2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \delta_{\sigma,\sigma'} \frac{e^2 \phi_{i,\sigma}^{KS}(\mathbf{r}) \phi_{j,\sigma}^{KS}(\mathbf{r}) \phi_{i,\sigma'}^{KS}(\mathbf{r}') \phi_{j,\sigma'}^{KS}(\mathbf{r}')}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|} \\ &\quad + \int d^3\mathbf{r} C^X n^{4/3}(\mathbf{r}). \end{aligned}$$

The first term is the Kohn-Sham exchange energy computed from $\langle \Psi| \hat{V}_c |\Psi\rangle$ with the Kohn-Sham wave function. Instead of minimizing with respect to the Kohn-Sham orbitals restricted to a given density and then with respect to the density, one minimizes with respect to the Kohn-Sham orbitals, obtaining equations that have the structure of the integro-differential Hartree-Fock equation. What has been achieved is that we have an auxiliary non-interacting electron problem, obeying Fermi-statistics obviously, that should give a good approximation to the ground-state energy and ground-state density.

Hartree-Fock equations that are valid for any variational state formed by a Slater determinant are discussed in Appendix C.

It is important to realize that the Kohn-Sham orbitals serve to compute the ground-state single-particle density. The eigenstates are Bloch states with a band index. The corresponding eigenenergies cannot be interpreted as exact single-particle excitations. They may however serve as a starting point for further calculations using many-body theory, as I explain in the next Chapter on the Hubbard model.

53.3 *Finite temperature

Mermin [5] has used the Feynmann variational principle to show that in the presence of an external potential, the grand potential is a functional of the density and that there is a universal part to it.

We have already shown, with ϱ the density matrix, that

$$\Omega[\varrho] < \Omega[\varrho'] + \langle H - H' \rangle_{\varrho'} . \tag{53.24}$$

We assume that the difference between ϱ and ϱ' is only the lattice potential but that suffices to state that there is really an inequality and that the two sides cannot be equal. Writing explicitly the difference between the two Hamiltonians,

$$\Omega[\varrho] < \Omega[\varrho'] + \int d^3\mathbf{r} n'(\mathbf{r}) (V_l(\mathbf{r}) - V_l'(\mathbf{r})) . \tag{53.25}$$

We could also use the inequality by interchanging the role of ϱ and ϱ' so that the following inequality is also valid

$$\Omega[\varrho'] < \Omega[\varrho] + \int d^3\mathbf{r} n(\mathbf{r}) (V_l'(\mathbf{r}) - V_l(\mathbf{r})) . \tag{53.26}$$

If the densities are identical for the two different lattice potentials, then $n'(\mathbf{r}) = n(\mathbf{r})$ and adding the two inequalities together we find the absurd result

$$\Omega[\varrho] + \Omega[\varrho'] < \Omega[\varrho'] + \Omega[\varrho] . \tag{53.27}$$

Hence, if the two lattice potentials are different, the densities have to differ. In other words the local density is uniquely determined by the external lattice potential.

If we know the external lattice potential, we can write down the density matrix ϱ in the usual way. Since there is a one-to-one correspondance between $V_l(\mathbf{r})$ and $n(\mathbf{r})$, the density matrix ϱ is a functional of $n(\mathbf{r})$ and

$$\Omega[n] = \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) + \mathcal{F}[n] \tag{53.28}$$

where

$$\mathcal{F}[n] = \left\langle \widehat{T}_{kin} + \hat{V}_c \right\rangle_n - TS[n] \tag{53.29}$$

with S the entropy $-\mathrm{Tr}[\varrho \ln \varrho]$ determined from the density matrix that is uniquely determined by the density.

One thus obtains a minimization problem with respect to the density $n(\mathbf{r})$ that is very similar to what we had at zero temperature.

Remark 309 *The original Hohenberg-Kohn theorem is along the lines of the arguments in this section. We could also formulate the Mermin result in a manner similar to that of Levy for the ground state. The density matrix would replace the wave function.*

53.4 Improving DFT with better functionals

DFT is based on the existence of a universal functional of the density. However, this functional is unknown, so a major part of the work in that field has been

to improve the quality of the functional. A well known example is the Perdew, Burke, Ernzerhof functional [190]. Another well known author in that field that has helped make DFT a truly first principles approach is Marvin L. Cohen [221]. Note that going beyond the LDA approximation leads to more general functionals of $n(\mathbf{r})$ that can depend for example on derivatives of the density, for example the Laplacian of the density or the square of the gradient (to make sure we that $F[n]$ is a scalar) etc.

Another direction for improvement by Car and Parrinello [50] has been to combine molecular dynamics with DFT to go beyond the pair-potential approximation, thereby making possible the simulation of both covalently bonded and metallic systems and allowing the application of density-functional theory to much larger systems than previously feasible.

I note without proof for now that there is an exact expression for the exchange correlation energy $E_{xc}[n]$. Given the density $n(\mathbf{r})$ we can write this exchange-correlation energy as follows [120],

$$E_{xc}(\mathbf{r}) = \frac{\delta \Phi^{xc}_{DFT}[n]}{\delta n(\mathbf{r})} \tag{53.30}$$

where

$$\Phi^{xc}_{DFT}[n] = T \sum_{iq_n} \int d^3\mathbf{r} \int d^3\mathbf{r}' \int_0^1 d\lambda \frac{\chi^{\lambda}_{\rho\rho}(\mathbf{r}, \mathbf{r}'; iq_n)}{4\pi\varepsilon_0 |\mathbf{r} - \mathbf{r}'|} \tag{53.31}$$

where the charge density is $\rho(\mathbf{r}) = \sqrt{\lambda} e\, n(\mathbf{r})$ and the corresponding susceptibility $\chi^{\lambda}_{\rho\rho}(\mathbf{r}, \mathbf{r}'; iq_n)$ is calculated for a Coulomb potential where the electric charge is λe^2. One uses this expression to find more accurate exchange-correlation functionals [**?**].

53.5 DFT and many-body perturbation theory

DFT has been designed to find ground states. The eigenenergies of the Kohn Sham orbitals are just the result of a parametrization of the density. There is nothing in the theory that garantees that they represent single-particle excited states. To find excited states and even improve ground state energies, it was proposed to use the many-body perturbation method developed for the electron gas [199][100]. You can read about electronic structure and interactions for example in this book [152]. The idea is to expand the field operators $\psi_\sigma(\mathbf{r})$ using the Kohn-Sham orbitals. In that basis, the effect of interactions is minimized, but it is still there. One can then use any many-body method to find excited states and other interesting properties. The first method to use is the RPA to find the dielectric constant. The corresponding self-energy with the screened interaction is refered to in this context as the GW approximation. These calculations [20] can be seen as an approximation for the exact equations of Hedin [91, 92] who also performed the first full calculation for the electron gas. Hedin's equations have been derived above in Chap. 51.

One had to wait till the mid 80's to see applications to real materials [99]. As shown in Fig. (53-1), spectacular agreement with experiment for band gaps has been achieved in the latest version of the approach [239]. In that approach, a quasiparticle approximation is taken for the Green's function, which is determined self-consistently. This helps remove the influence of the choice of basis for the Kohn-Sham orbitals.

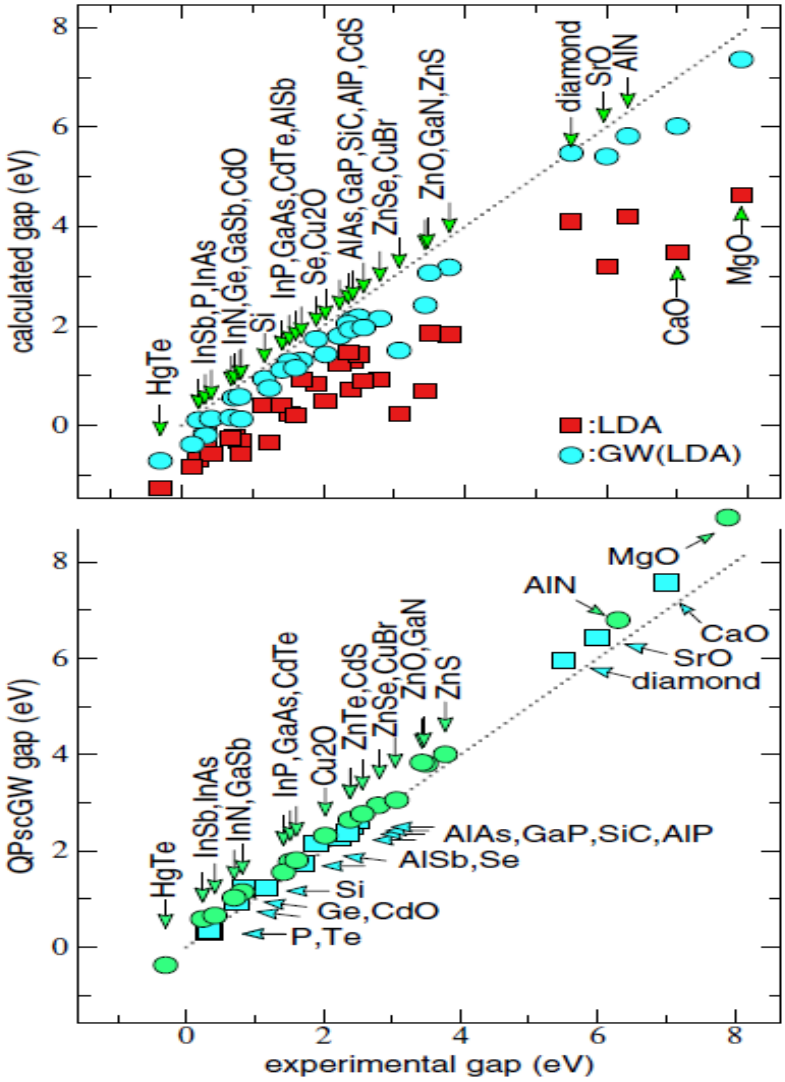


Figure 53-1 Exprimental band gaps for semi-conductors and insulators compared with theory. The calculations for the top figures labeled LDA are just the gaps in the Kohn-Sham eigenenergies, while the other ones are obtained from GW. The essentially exact agreement in the bottom figure is for quasiparticle self-consistent GW. The figure is taken from M. van Schilfgaarde et al. PRL **96**, 226402 (2006).

Yet, this approach fails for late transition metals oxides, which are insulators, but predicted to be metals by DFT based methods. A partial remedy for this was to include an orbital-dependent potential U, that acts only on the d or f orbitals [15, 136], the so-called LDA+U method. In order of increasing localization of the orbitals, meaning larger interactions, we find: $5d, 4d$, $3d, 4f$, and $5f$. Within a given row of the periodic table, moving from left to right also increases localization. But what is U? That takes me to the next topic.

53.6 Model Hamiltonians

In parallel efforts to understand properties of materials, the study of simple Hamiltonians revealed very rich physics. One of the first difficult problems that was tackled was that of the Kondo Hamiltonian. That Hamiltonian was suggested by Nobel Prize winner PW Anderson in his study of a model, now known as the Anderson impurity model, that introduced a double occupancy cost U for electrons on an impurity with localized orbital [10]. In the Kondo problem, an isolated impurity with a local moment is hybridized antiferromagnetically with a conduction-electron sea. At high temperature, this local moment is free. At low temperature, there is a crossover to a state where the localized moment essentially disappears by forming a highly entangled singlet state with the conduction sea. A full solution of that problem had to wait for the renormalization group of Nobel Prize winner Ken Wilson [253]. The solution to this problem explained in particular the resistivity minimum found in dilute alloys.

Another important model was proposed independently in 1964 by Hubbard, Kanamori and Gutwiller. Known today as the Hubbard model, this model has two non-commuting terms. A term that represents electrons moving on a lattice with one orbital per site. That term is diagonal in a plane-wave basis. The other term represents the energy cost U associated with double occupancy and is diagonal in the site basis. This model was proposed to understand emergent phases of matter such as ferromagnetism. But in the end, it revealed itself as a way to explain antiferromagnetism and the metal-insulator transition, or Mott transition. The latter problem was by far the most difficult one. The interaction-induced metal insulator transition was proposed by Peierls and Mott around 1937 as an explanation for the discrepancy between the band picture of solids and observation in materials sur as NiO.

Early explanations of the Mott transition at half-filling, all based on the Hubbard model, included a) Hubbard who proposed that the original density of states is split in two by U so that when U is small enough, a metal is recovered [98] b) Brinkmann and Rice who suggested that the effective mass of electrons diverges at the transition [44], a result recovered by the modern slave-boson approach of Kotliar and Ruckenstein [122] c) Slater who associated the transition to an emergent long-range antiferromagnetic order [220]. The latter explanation is invalid for what are called today Mott insulators in a paramagnetic state.

54. THE HUBBARD MODEL

Let me step back. Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. The Kohn-Sham orbitals give highly accurate electronic density and energy for the ground state. If the problem has been solved for a translationally invariant lattice, the one-particle states will be Bloch states indexed by crystal momentum $\mathbf{k}$ and band index n. Nevertheless, these one-particle states cannot be used to build single-particle states that diagonalize the many-body Hamiltonian. More specifically, if we expand the creation-annihilation operators in that basis using the general formulas for one-particle and two-particle parts of the Hamiltonian, it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

After providing a "derivation" of the model, we will solve limiting cases that will illustrate one limit where states are extended, and one limit where they are localized, giving a preview of the Mott transition.

Finding an effective Hamiltonian for a few bands near the Fermi level starting from the full electronic structure is a delicate matter that necessitates a much more detailed treatment than the one exposed here. The procedure to find the effective Hamiltonian is called "downfolding". This means that one wants to obtain an effective Hamiltonian that focuses on a few bands near the Fermi level. This is in a sense our "model space". These methods, that I will not explain, include cRPA [21] where the dielectric constant is computed by using in the bubbles all particle hole-pairs that include at least one of the bands that we do not wish to consider in our model space. The resulting dielectric constant does not screen the Coulomb interaction in the sense of Thomas-Fermi as discussed above. The Coulomb interaction is smaller but still long range. It is only if the model space is metallic that the Coulomb interaction will become truly short-range. For examples of derivations of model Hamiltonians, you can also look at Refs. [171] and [172].

The approach that follows to "derive" the Hubbard model is just heuristic.

54.1 Assumptions behind the Hubbard model

A qualitative derivation of the model is as follows. Start from the general Hamiltonian Eq.(36.1). The field operators can be expanded in single-particle eigenstates. For the case of interest to us, these would be Bloch states $\phi_{n\mathbf{k}}(\mathbf{r}) \equiv \langle \mathbf{r} | n\mathbf{k} \rangle$ with band index n and crystal momentum $\mathbf{k}$, so that

$$\psi(\mathbf{r}) = \sum_{n\mathbf{k}} \phi_{n\mathbf{k}}(\mathbf{r}) c_{n\mathbf{k}}. \tag{54.1}$$

Since screening suggests that in the end we need to consider short range interactions that are better described in a localized basis, we can use the Wannier basis

$w_n(\mathbf{r}-\mathbf{R}_i)$. In that case, the expansion takes the form,

$$\psi(\mathbf{r}) = \sum_{n\mathbf{R}_i} w_n(\mathbf{r}-\mathbf{R}_i)\, c_{n\mathbf{R}_i}. \tag{54.2}$$

The kinetic energy operator with the potential from the lattice, for example, can be lumped together. They then look as follows

$$\sum_\sigma \int d^3\mathbf{r}\psi^\dagger_\sigma(\mathbf{r})\left[\left(-\frac{\nabla^2}{2m}\right)+V_\ell(\mathbf{r})\right]\psi_\sigma(\mathbf{r}) \tag{54.3}$$

$$= \sum_\sigma \sum_{n\mathbf{R}_i m\mathbf{R}_j} c^\dagger_{\sigma,n\mathbf{R}_i}\langle n\mathbf{R}_i|\,\widehat{T}_{kin}+\widehat{V}_\ell\,|m\mathbf{R}_j\rangle\, c^\dagger_{\sigma,m\mathbf{R}_j} \tag{54.4}$$

where

$$\langle n\mathbf{R}_i|\,\widehat{T}_{kin}+\widehat{V}_\ell\,|m\mathbf{R}_j\rangle \tag{54.5}$$

$$\equiv \int d^3\mathbf{r} w^*_n(\mathbf{r}-\mathbf{R}_i)\left[\left(-\frac{\nabla^2}{2m}\right)+V_\ell(\mathbf{r})\right] w_m(\mathbf{r}-\mathbf{R}_j). \tag{54.6}$$

Remark 310 *There is an arbitrariness in the definition of the Wannier functions. Normally, we take for a single band m*

$$w_m(\mathbf{r}-\mathbf{R}_j) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}\phi_{m\mathbf{k}}(\mathbf{r}). \tag{54.7}$$

However, there is an arbitrariness. We can instead perform a unitary transformation

$$W_\ell(\mathbf{r}-\mathbf{R}_j) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}\sum_m U_{\ell m}\phi_{m\mathbf{k}}(\mathbf{r}) \tag{54.8}$$

that gives a different set of equally valid orthonormal Wannier orbitals. This has led the group of Vanderbilt to define "maximally localized orbitals" [154][223]. These are not necessarily the best to obtain effectif models but they are quite popular.

In cases where a single band crosses the Fermi level and is far in energy from other bands, we can appeal to perturbation-theory ideas and assume that we can focus on that single band that crosses the Fermi level. I then drop the band index and use the short-hand notation $\langle n\mathbf{R}_i|\,\widehat{T}_{kin}\,|n\mathbf{R}_j\rangle \equiv \langle i|\,\widehat{T}_{kin}\,|j\rangle$. The Hamiltonian in the presence of the Coulomb interaction then takes the form

$$H = \sum_\sigma\sum_{i,j} c^\dagger_{i\sigma}\langle i|\,\widehat{T}_{kin}+\hat{V}_l\,|j\rangle\, c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\langle i|\langle j|\,\hat{V}_c\,|k\rangle\,|l\rangle\, c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{l\sigma'}c_{k\sigma} \tag{54.9}$$

where the first term contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. Remember that $\langle i|$ and $|k\rangle$ belong to the same one-particle Hilbert space as do $\langle j|$ and $|l\rangle$. Here, $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) are creation and annihilation operators for electrons of spin σ in the Wannier orbital centered around site i. A single many-particle state formed by filling orbitals, leading to a Slater determinant as wave function, cannot diagonalize this Hamiltonian because of the interaction part that empties orbitals and fills other ones. The true eigenstates are linear combinations of Slater determinants.

The one-body part by itself is essentially the DFT band structure. In 1964, Hubbard, Kanamori and Gutzwiller did the most drastic of approximations, hoping to have a model simple enough to solve. They assumed that $\langle i|\langle j|\,\hat{V}_c\,|k\rangle\,|l\rangle$ would be much larger than all other interaction matrix elements when all lattice

sites are equal. Defining $t_{ij} \equiv \langle i| \widehat{T} |j\rangle$ and $U \equiv \langle i| \langle i| \hat{V}_c |i\rangle |i\rangle$, and using $c_{i\sigma}c_{i\sigma} = 0$ they were left with

$$H = \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{i} U c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} \tag{54.10}$$

$$= \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \tag{54.11}$$

$$= \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow}. \tag{54.12}$$

In this expression, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the density of spin σ electrons, $t_{ij} = t^{*}_{ji}$ is the hopping amplitude, and U is the screened Coulomb repulsion that acts only on electrons on the same site. Most of the time, one considers hopping only to nearest neighbors. In general, we write $-t, -t', -t''$ respectively for the first-, second- and third-nearest neighbor hopping amplitudes. To go from the first to the second line we used the Pauli exclusion principle $c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma} = 0$.

Remark 311 *This last statement is important. To obtain the Hubbard model where up electrons interact only with down, we had to assume that the Pauli exclusion principle is satisfied exactly. So approximation methods that do not satisfy this constraint are suspicious.*

The model can be solved exactly only in one dimension using the Bethe ansatz, and in infinite dimension. The latter solution is the basis for Dynamical Mean Field Theory (DMFT) that we will discuss below. Despite the fact that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable [101]. A laser interference pattern can be used to create an optical lattice potential using the AC Stark effect. One can control tunneling between potential minima as well as the interation of atoms between them and basically build a physical system that will be described by the Hubbard Hamiltonian. This kind of experimental setup in a sense is an analog computer. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of cold atoms, one can find conditions where the Hubbard model description is very accurate. By the way, in optical lattices, interesting physics occurs mostly in the nano Kelvin range. Discussing how such low temperatures are achieved would distract us to much.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a Mott insulator. The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe high-temperature superconductivity, depending on lattice and range of interaction parameters.

54.2 Where spin fluctuations become important

In deriving the Hubbard model we have used the Pauli exclusion principle. Electrons do not interact with electrons of the same spin since this means they would

be in the same state. In other words, we have taken into account the fact that exchange has gotten rid of that type of interactions. This is discussed further from the point of view of diagrams in Sec. (56.4). The consequence of this is that spin now starts to play an important role, contrary to the case of the electron gas. In fact, almost all manifestations of magnetism in solids originates from exchange, not from direct magnetic-dipole magnetic-dipole interactions. An easy way to see this is to rewrite the Hubbard interaction in terms of density-density interaction $(n_{i\downarrow}+n_{i\uparrow})^2$ and spin-spin interaction $S_i^z S_i^z$ as follows:

$$Un_{i\downarrow}n_{i\uparrow} = \frac{U}{4}\left(n_{i\downarrow}+n_{i\uparrow}\right)^2 - \frac{U}{4}\left(n_{i\downarrow}-n_{i\uparrow}\right)^2 \tag{54.13}$$

$$= \frac{U}{4}n_i n_i - \frac{U}{4}S_i^z S_i^z. \tag{54.14}$$

To gain a feeling of the Physics contained in the Hubbard model, let us first discuss two limiting cases where it can be solved exactly.

54.3 The non-interacting limit $U = 0$

As a simple example that comes back often in the context of high-temperature superconductivity, consider a square lattice in two dimensions with nearest-neighbor hopping only. Then, when $U = 0$, we have

$$H_0 = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} \tag{54.15}$$

where t_{ij} is a Hermitian matrix. When there is no magnetic field the one-body states can all be taken real and t_{ij} is symmetric. To take advantage of translational invariance we use our Fourier transforms

$$c_{i\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma} \tag{54.16}$$

$$c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma}^\dagger \tag{54.17}$$

with $\mathbf{r}_i$ the position of site i, and

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = N\delta_{\mathbf{k},0}. \tag{54.18}$$

Here N is the number of atoms and we take the lattice spacing a to be unity. Defining $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}$ and noting that the hopping matrix depends only on the distance to the neighbors $\boldsymbol{\delta}$, we find

$$H_0 = \frac{1}{N}\sum_{\mathbf{r}_i,\boldsymbol{\delta},\sigma}\sum_{\mathbf{k}'} t_{\boldsymbol{\delta}} e^{-i\mathbf{k}'\cdot\mathbf{r}_i} c_{\mathbf{k}'\sigma}^\dagger \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_i+\boldsymbol{\delta})} c_{\mathbf{k}\sigma}$$

$$= \sum_{\mathbf{k},\boldsymbol{\sigma}} \overbrace{\sum_{\boldsymbol{\delta}} t_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}}^{\varepsilon_{\mathbf{k}}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \tag{54.19}$$

$$H = \sum_{\mathbf{k},\boldsymbol{\sigma}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \tag{54.20}$$

In the case of nearest-neighbor hopping only, on a two-dimensional square lattice for example where $t_{ij} = -t$ for nearest-neighbor hopping, we have the dispersion relation

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y),$$

where I have assumed that the lattice spacing, or distance δ between nearest-neighbors, is equal to unity. Clearly, if the Fermi wave vector is sufficiently small, we can define $t^{-1} = 2m_b$ and approximate the dispersion relation by its quadratic expansion, as in the free electron limit

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) \sim C + \frac{k_x^2 + k_y^2}{2m_b}. \tag{54.21}$$

54.4 The strongly interacting, atomic, limit $t = 0$

If there are no hoppings and only disconnected atomic sites,

$$K = U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \tag{54.22}$$

there are two energy levels, correspondig to empty, singly (zero energy) and doubly occupied site (energy U). It is apparently much simpler than the previous problem. But not quite. A simple thing to compute is the partition function. Since each site is independent, $Z = Z_1^N$ where Z_1 is the partition function for one site. We find, since there are four possible states on a site, empty, spin up, spin down and doubly occupied,

$$Z_1 = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta(U-2\mu)}. \tag{54.23}$$

Already at this level we see that there are "correlations". Z_1can be factored into $\left(1 + e^{\beta\mu}\right)^2$ only if there are no interactions.

Things become more subtle when we consider the "dynamics", as embodied for example in the Green function

$$\mathcal{G}_\sigma(\tau) = -\left\langle T_\tau \left[c_\sigma(\tau)\, c_\sigma^\dagger \right] \right\rangle. \tag{54.24}$$

We can consider only one site at a time since the Hamiltonian is diagonal in site indices. Imagine using Lehman representation. It is clear that when the time evolution operator acts on the intermediate state, we will need to know if in this intermediate state the system is singly or doubly occupied. We cannot trace only on up electrons without worrying about down electrons. The Lehman representation gives a staightforward way of obtaining the Green function.

We can also proceed with the equation of motion approach, a procedure we will adopt to introduce the concept of hierarchy of equations (the analog of the BBGKY hierarchy in classical systems). All that we need is

$$\frac{\partial c_\sigma}{\partial \tau} = [K, c_\sigma] = [U n_\sigma n_{-\sigma} - \mu n_\sigma, c_\sigma] = -U c_\sigma n_{-\sigma} + \mu c_\sigma. \tag{54.25}$$

From this, the equation of motion for the Green function is

$$\begin{aligned} \frac{\partial \mathcal{G}_\sigma(\tau)}{\partial \tau} &= -\delta(\tau) - \left\langle T_\tau \left[[K, c_\sigma(\tau)]\, c_\sigma^\dagger \right] \right\rangle & (54.26) \\ &= -\delta(\tau) + \mu \mathcal{G}_\sigma(\tau) + U \left\langle T_\tau \left[c_\sigma(\tau)\, n_{-\sigma}(\tau)\, c_\sigma^\dagger \right] \right\rangle & (54.27) \end{aligned}$$

The structure of the equation of motion is a very general result. One-body Green functions are coupling to higher order correlation functions. Let us write down the equation of motion for that higher order correlation function that we define as follows

$$\mathcal{G}_{2,\sigma}(\tau) = -\left\langle T_\tau \left[c_\sigma(\tau)\, n_{-\sigma}(\tau)\, c_\sigma^\dagger \right] \right\rangle . \tag{54.28}$$

Following the usual approach, and recalling that here $\partial n_{-\sigma}(\tau)/\partial\tau = [K, n_{-\sigma}(\tau)] = 0$ because the Hamiltonian preserves the number of particles, we find with the help of Eq.(54.25) and of the equal-time anticommutator $\left\{c_\sigma n_{-\sigma}, c_\sigma^\dagger\right\} = n_{-\sigma}$ arising from the derivative of the θ function in the time-ordered product,

$$\frac{\partial \mathcal{G}_{2,\sigma}(\tau)}{\partial\tau} = -\delta(\tau)\langle n_{-\sigma}\rangle + \mu\mathcal{G}_{2,\sigma}(\tau) - U\mathcal{G}_{2,\sigma}(\tau) . \tag{54.29}$$

Instead of generating a higher order correlation function in the term coming from $[K, c_\sigma(\tau)]$, as is usually the case, the system of equations has closed since $n_{-\sigma}n_{-\sigma} = n_{-\sigma}$. This is a very special case. Equations (54.27) and (54.29) form a closed set of equations that is easy to solve in Matsubara frequencies where they become

$$(i\omega_n + \mu)\,\mathcal{G}_\sigma(i\omega_n) = 1 + U\mathcal{G}_{2,\sigma}(i\omega_n) \tag{54.30}$$

$$(i\omega_n + \mu)\,\mathcal{G}_{2,\sigma}(i\omega_n) = \langle n_{-\sigma}\rangle + U\mathcal{G}_{2,\sigma}(i\omega_n) . \tag{54.31}$$

Substituting the second equation in the first

$$(i\omega_n + \mu)\,\mathcal{G}_\sigma(i\omega_n) = 1 + \frac{U\langle n_{-\sigma}\rangle}{(i\omega_n + \mu - U)} . \tag{54.32}$$

Since

$$\frac{U\langle n_{-\sigma}\rangle}{(i\omega_n+\mu)(i\omega_n+\mu-U)} = \frac{U\langle n_{-\sigma}\rangle}{U}\left[\frac{1}{(i\omega_n+\mu-U)} - \frac{1}{(i\omega_n+\mu)}\right] \tag{54.33}$$

we are left with

$$\mathcal{G}_\sigma(i\omega_n) = \frac{1-\langle n_{-\sigma}\rangle}{i\omega_n+\mu} + \frac{\langle n_{-\sigma}\rangle}{i\omega_n+\mu-U} \tag{54.34}$$

$$\mathcal{G}^R_\sigma(\omega) = \frac{1-\langle n_{-\sigma}\rangle}{\omega+i\eta+\mu} + \frac{\langle n_{-\sigma}\rangle}{\omega+i\eta+\mu-U} .$$

The imaginary part gives us the single-particle spectral weight. Instead of a single delta function located at a $\mathbf{k}$ dependent position, we have two delta functions that are completely independent of $\mathbf{k}$, as we must expect for a localized state. The two levels correspond respectively to the electron afinity and ionization potential of the atom. Physically speaking, if the fraction of sites occupied by down electrons is $\langle n_{-\sigma}\rangle$, then a spin up electron will have an energy $-\mu + U$ a fraction $\langle n_{-\sigma}\rangle$ of the time, and an energy $-\mu$ for a fraction $1 - \langle n_{-\sigma}\rangle$ of the time. And that is independent of the momentum. That is very different from a quasiparticle. There is no pole at $\omega = 0$ unless $\mu = 0$.

The non-interacting limit is not a good starting point for this problem clearly. One expects perturbation theory to breakdown. This is simple to see for example at half filling when $\langle n_{-\sigma}\rangle = 1/2$ and $\mu = U/2$. Then,

$$\mathcal{G}^R_\sigma(\omega) = \frac{1}{2}\left(\frac{1}{\omega+i\eta+U/2} + \frac{1}{\omega+i\eta-U/2}\right) = \frac{(\omega+i\eta)}{(\omega+i\eta)^2 - \left(\frac{U^2}{4}\right)} \tag{54.35}$$

$$= \frac{1}{(\omega+i\eta) - \frac{U^2}{4(\omega+i\eta)}} \tag{54.36}$$

so that clearly, the retarded self-energy $\Sigma^R(\omega) = \frac{U^2}{4(\omega+i\eta)}$ is singular at low frequency, not good news for perturbation theory. It gets rid of the pole that is at $\omega = 0$ when there is no interaction.

If t is not zero but $U/t \gg 1$, then we have a Mott insulator. In a Mott insulator, the two peaks that we just found in the single-particle spectral weight are somewhat broadened, but there is a gap at zero frequency. We will leave this concept aside for the moment and discuss the weak coupling case.

55. *THE PEIERLS SUBSTITUTION ALLOWS ONE TO COUPLE GENERAL TIGHT-BINDING MODELS TO THE ELECTROMAGNETIC FIELD

Suppose we have tight-binding bands of atomic or Wannier orbitals. That problem arises for example when we focus on a few correlated bands near the Fermi level. It is in general necessary to go a localized basis where short-range interactions, Hubbard or Hund's for example, are easiest to write. In this Chapter, I try to answer the question "How do I write the interaction with the electromagnetic field when we take into account only a finite number of bands?"

In the presence of the electromagnetic field, we still have the usual intra-atomic transitions, say electric-dipole transitions. But there are extra contributions coming from hopping between atoms. We know, for example, that the vector potential for a uniform electric field couples to the uniform current operator. There is a contribution to that current that is just the gradient of the dispersion relation $\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{\mathbf{k}}$. The gauge-invariant current also has an additional term. In linear reponse, this later contribution gave the diamagnetic term, that depended inversely on the mass. So, intuitively, we expect that the velocity and inverse mass tensor must come in. To derive everything in the most general way with a finite basis in a tight-binding model, our best guide is gauge invariance. In fact, without gauge invariance as a guide, we may be inclined to think that if there are several bands labeled by n then the current operator is $\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{\mathbf{k}n}$. This is incorrect for general response functions, as I will show. So, here we go.

We already know from Sec. (11.1) that under a gauge transformation, one-particle wave functions in first quantization tranform as follow

$$\psi'(\mathbf{r},t) = e^{ie\Lambda(\mathbf{r},t)/\hbar}\psi(\mathbf{r},t) \tag{55.1}$$

or in Dirac's notation,

$$\langle \mathbf{r}|\ \psi'(t)\rangle = e^{ie\Lambda(\mathbf{r},t)/\hbar}\langle \mathbf{r}|\ \psi(t)\rangle\,. \tag{55.2}$$

Suppose that $\psi(\mathbf{r},t)$ is expanded in a finite set of Wannier orbitals (or some other local orbitals) as in Eq. (54.2)

$$\psi(\mathbf{r},t) = \sum_{n\mathbf{R}_i+\mathbf{r}_\mu} w_n\left(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu\right) c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{55.3}$$

where n is a band index in the simplest cas, or more generally an orbital index (Recall the ambiguity in the definition of the Wannier functions discussed in Sec. (54.1)). Here I have generalized Eq. (54.2) by allowing several atoms that are located at position $\mathbf{r}_\mu$ with respect to the unit cell that is itself located at $\mathbf{R}_i$. Since $w_n\left(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu\right)$ are just basis functions that we take as given, under a

gauge transformation the destruction operator must transform in such a way that the wave-function transforms properly

$$c'_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) = e^{ie\Lambda(\mathbf{R}_i+\mathbf{r}_\mu,t)/\hbar} c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t)\,. \tag{55.4}$$

and analogously for the creation operators. Something has happened here! Instead of $\Lambda(\mathbf{r},t)/\hbar$, I have written $\Lambda(\mathbf{R}_i+\mathbf{r}_\mu,t)/\hbar$. While we can continue to take into account intra-atomic transitions since we have localized orbitals, the finite basis means that for hopping between different atoms, we do not have arbitrary spatial resolution since our basis is finite. So we have no choice but to consider only electromagnetic fields that vary on a scale that is larger than the inter-atomic distance. In all the usual condensed-matter experiments, this is the case. With the most powerful lasers today, [256] one can apply fields of the order of $10^2\,\mathrm{V}/\mathrm{\AA}$ that vary over the wavelength of light, namely distances of the order of 10^4 atoms, and even with micromagnets, the magnetic field varies by one Tesla on the scale of one micron, or 10^{-6} meters, or 10^4 atoms [192].

Given the effect of a gauge transformation on orbitals, we see that interaction terms that depend only on density or spin are automatically gauge independent, whereas the kinetic energy in a Wannier basis will be gauge invariant if any given term in the presence of a vector potential takes the form

$$e^{i\frac{e}{\hbar}\int_{\mathbf{R}_i+\mathbf{r}_\mu}^{\mathbf{R}_j+\mathbf{r}_\nu}\mathbf{A}(\mathbf{r},t)\cdot d\mathbf{r}} c^\dagger_{m\mathbf{R}_j+\mathbf{r}_\nu}(t)\, c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{55.5}$$

which is invariant under a gauge transformation $\mathbf{A}\to\mathbf{A}+\boldsymbol{\nabla}\Lambda$, as we can see from the way the operators transform in Eq. 55.4. The above assumes that the integral is taken along the straight line connecting $\mathbf{R}_i+\mathbf{r}_\mu$ and $\mathbf{R}_j+\mathbf{r}_\nu$ and that $\mathbf{A}(\mathbf{r},t)$ does not vary much over the path of integration, or that it can be replaced by its value in the mid point. In other words, the phase in the above exponential is

$$\frac{e}{\hbar}\int_{\mathbf{R}_i+\mathbf{r}_\mu}^{\mathbf{R}_j+\mathbf{r}_\nu}\mathbf{A}(\mathbf{r},t)\cdot d\mathbf{r} = \mathbf{A}\left(\frac{\mathbf{R}_j+\mathbf{r}_\nu+\mathbf{R}_i+\mathbf{r}_\mu}{2}\right)\cdot(\mathbf{R}_j+\mathbf{r}_\nu-\mathbf{R}_i-\mathbf{r}_\mu) \tag{55.6}$$

The effect of the magnetic induction will come from the part of the vector potential that cannot be represented by a gradient. The flux of this field thus depends on the path chosen to go from one site to the other. The above choice is physically correct because if we write the equations of motion for the Green's function in a gauge invariant manner, factoring out the trivial gauge dependence of the Green's function, discussed in Sec. 32.3, the resulting equations of motion depend on the magnetic flux in the manner expected from path integral considerations. Namely, recall that the Green's function describing propagation from one site to another site goes through all possible intermediate sites. On any given path, these three sites define a surface and the magnetic flux through this surface appears in the equation of motion for the gauge invariant Green's function when the above definition is used. [176] [114]

The current operator on the lattice is obtained from

$$\mathbf{j} = -\frac{\delta H}{\delta \mathbf{A}} \tag{55.7}$$

as we saw in Eq. (11.26).

Remark 312 *When the magnetic flux* $\oint \mathbf{A}(\mathbf{r},t)\cdot d\mathbf{r}$ *through a unit cell is equal to* nh/e*, where* n *is an integer, it is as if the magnetic field was absent. There is thus a periodicity associated with the magnetic field that may or may not be commensurate with the lattice. This induces a spectrum of Landau levels in two*

dimensions that gives a complicated but beautiful fractal picture, often referred to as a Hofstadter butterfly. [94] The magnetic fields necessary to observe this effect are unattainable in solid state systems. It is however possible to engineer the Peierls substitution in optical lattices of cold atoms [105] [?] This has lead to the suggestion and to the observation of this spectrum of Landau Levels in cold atom experiments. [5] [161] [6]

Remark 313 *Be careful with the semiclassical definition of the band current: Suppose we want to compute the current-current correlation function to obtain the conductivity. We need the current operator. A common assumptions for DC calculations is to consider the contribution of each electronic band b separately and to take $\frac{e}{\hbar}\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{\mathbf{k}b}$ as the current vertex in each band. This is the semi-classical approximation. Note however that the current given by Eq. (55.7) above will in general include interband transitions. To see this, first choose to represent the electric field with a time-dependent vector potential that is independent of position. In that case, thanslational invariance is preserved. Going to a Fourier basis then, for each value of $\mathbf{k}$, the kinetic energy operator takes the form of an $M\times M$ matrix where M is the number of orbitals in the unit cell. The Hamiltonian in that form is said to be in the orbital basis. The band basis is obtained by diagonalizing the $M\times M$ matrix for each value of $\mathbf{k}$. In the orbital basis, the Fourier transform gives*

$$c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t)=\left(\frac{1}{N}\right)\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{r}_\mu)}c_{n\mathbf{k}}(t) \tag{55.8}$$

which means that the effect of the vector potential for the electric field can be included by doing the substitution

$$\mathbf{k}\rightarrow\mathbf{k}-\frac{e}{\hbar}\mathbf{A}(t) \tag{55.9}$$

Writing the Hamiltonian in the orbital basis then, the expression for the current Eq.(55.7) in that basis can evaluated from

$$\mathbf{j}_{mn}(\mathbf{k})=-\frac{\delta H_{mn}(\mathbf{k})}{\delta\mathbf{A}}=\frac{e}{\hbar}\frac{\partial H_{mn}(\mathbf{k})}{\partial\mathbf{k}}\equiv\frac{e}{\hbar}\nabla_{\mathbf{k}}H_{mn}(\mathbf{k}). \tag{55.10}$$

Since H_{mn} is not diagonal in the orbital basis, the current in that basis is not diagonal either. Nevertheless, if interband transitions can be neglected in the DC limit, we can recover the expected semi-classical result. Indeed, let $U_{mb}(\mathbf{k})$ be the unitary transformation that goes from the orbital to the band basis, namely $H_{mn}(\mathbf{k})U_{nb}(\mathbf{k})=\varepsilon_{\mathbf{k}b}U_{mb}(\mathbf{k})$ and assume that there are no interband transitions. Then

$$\begin{aligned}
U^{\dagger}_{bm}(\mathbf{k})\,\mathbf{j}_{mn}(\mathbf{k})\,U_{nb}(\mathbf{k}) &= \frac{e}{\hbar}U^{\dagger}_{bm}(\mathbf{k})\left(\nabla_{\mathbf{k}}H_{mn}(\mathbf{k})\right)U_{nb}(\mathbf{k}) && (55.11)\\
&= \frac{e}{\hbar}\nabla_{\mathbf{k}}\left(U^{\dagger}_{bm}(\mathbf{k})\,H_{mn}(\mathbf{k})\,U_{nb}(\mathbf{k})\right) && (55.12)\\
&\quad -\frac{e}{\hbar}\nabla_{\mathbf{k}}U^{\dagger}_{bm}(\mathbf{k})\left(H_{mn}(\mathbf{k})\,U_{nb}(\mathbf{k})\right) && (55.13)\\
&\quad -\frac{e}{\hbar}\left(U^{\dagger}_{bm}(\mathbf{k})\,H_{mn}(\mathbf{k})\right)\nabla_{\mathbf{k}}U_{nb}(\mathbf{k}) && (55.14)\\
&= \frac{e}{\hbar}\nabla_{\mathbf{k}}\left(U^{\dagger}_{bm}(\mathbf{k})\,\varepsilon_{\mathbf{k}b}U_{mb}(\mathbf{k})\right)-\frac{e}{\hbar}\left(\nabla_{\mathbf{k}}U^{\dagger}_{bm}(\mathbf{k})\right)\varepsilon_{\mathbf{k}b}U_{mb}(\mathbf{k}) && (55.15)\\
&\quad -\frac{e}{\hbar}U^{\dagger}_{bn}(\mathbf{k})\,\varepsilon_{\mathbf{k}b}\left(\nabla_{\mathbf{k}}U^{\dagger}_{nb}(\mathbf{k})\right) && (55.16)\\
&= \frac{e}{\hbar}\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}b} && (55.17)
\end{aligned}$$

where the last step is justified by the fact that we have unitary matrices so that $U^{\dagger}_{bm}(\mathbf{k})\,U_{mb}(\mathbf{k})=1$ and $\nabla_{\mathbf{k}}\left(U^{\dagger}_{bm}(\mathbf{k})\,U_{mb}(\mathbf{k})\right)=\nabla_{\mathbf{k}}(1)=0$ for all bands b. The

above steps are just another derivation of the Hellmann-Feynman theorem. [74] The above arguments do not work any more for second derivatives encountered for the diamagnetic current or in expressions for the Hall current. The multiband case for the Hall current must be considered carefully and it is the expression for the current in the orbital basis that must be used. [177]

Remark 314 *In electronic structure calculations, it is customary to omit the factor $e^{i\mathbf{k}\cdot\mathbf{r}_\mu}$ in the expression for the Fourier transforms Eq. (55.8). This is natural sine translational invariance is from one unit cell to the next. However, this means that when the current is calculated from $-\nabla_{\mathbf{k}} H(\mathbf{k})$, some intra unit-cell currents are neglected. This can be corrected by modifying the expression for the current [232]. The easiest way however is to include the Bloch phase even within a unit cell, as I have done above. [177] You can find the expression for the current that includes gradients of the periodic part of the Bloch function in this reference [179].*

Remark 315 *Recall our discussion on the arbitrariness in the definition of Wannier orbitals in Sec. 54.1. [153] This does not influence the Peierls substitution.*

Remark 316 *The scalar potential should be included with the time derivative as usual.*

Remark 317 *For a mathematical derivation of the Peierls substitution and corrections, see for example Ref. [183].*

56. THE HUBBARD MODEL IN THE FOOTSTEPS OF THE ELECTRON GAS

In this Chapter, we follow the same steps as the electron gas and derive RPA equations for the response functions. While spin fluctuations did not play a prominent role in the electron gas, they will be dominant in the Hubbard model and we will see why. RPA for the Hubbard model however has a major deficiency: It does not satisfy the Pauli exclusion principle, as we will see. This had no major consequence for the eletron gas, but in the case of the Hubbard model this is crucial. We will see how to cure this problem and others using the Two-Particle Self-Consistent Approach in the next Chapter.

56.1 Single-particle properties

Following functional methods of the Schwinger school[23, 25, 151], we begin, as we have done earlier, with the generating function with source fields ϕ_σ and field destruction operators ψ in the grand canonical ensemble

$$\ln Z\left[\phi\right]=\ln \mathrm{Tr}\quad[e^{-\beta\left(\widehat{H}-\mu\widehat{N}\right)}\mathrm{T}_\tau\left(e^{-\psi_{\overline{\sigma}}^{\dagger}\left(\overline{1}\right)\phi_{\overline{\sigma}}\left(\overline{1},\overline{2}\right)\psi_{\overline{\sigma}}\left(\overline{2}\right)}\right)] \tag{56.1}$$

We adopt the convention that 1 stands for the position and imaginary time indices $(\mathbf{r}_1,\tau_1)$. The over-bar means summation over every lattice site and integration over imaginary-time from 0 to β, and $\overline{\sigma}$ summation over spins. T_τ is the time-ordering operator. Before, the spin index was included in the labels.

The propagator in the presence of the source field is obtained from functional differentiation

$$\mathcal{G}_\sigma\left(1,2\right)_\phi=-\left\langle T_\tau\psi_\sigma\left(1\right)\psi_\sigma^{\dagger}\left(2\right)\right\rangle_\phi=-\frac{\delta\ln Z\left[\phi\right]}{\delta\phi_\sigma\left(2,1\right)}. \tag{56.2}$$

Physically, relevant correlation functions are obtained for $\phi=0$ but it is extremely convenient to keep finite ϕ in intermediate steps of the calculation.

Using the equation of motion for the field ψ and the definition of the self-energy, one obtains the Dyson equation in the presence of the source field [110]

$$\left(\mathcal{G}_0^{-1}-\phi\right)\mathcal{G}=1+\Sigma\mathcal{G}\quad;\quad\mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\phi-\Sigma \tag{56.3}$$

where, from the commutator of the interacting part of the Hubbard Hamiltonian H, one obtains

$$\begin{aligned}\Sigma_\sigma\left(1,\overline{1}\right)_\phi\mathcal{G}_\sigma\left(\overline{1},2\right)_\phi &= -U\left\langle T_\tau\psi_{-\sigma}^{\dagger}\left(1^+\right)\psi_{-\sigma}\left(1\right)\psi_\sigma\left(1\right)\psi_\sigma^{\dagger}\left(2\right)\right\rangle_\phi &(56.4)\\ &= -U\left[\frac{\delta\mathcal{G}_\sigma\left(1,2\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)}-\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi\mathcal{G}_\sigma\left(1,2\right)_\phi\right] &(56.5)\end{aligned}$$

The imaginary time in 1^+ is infinitesimally larger than in 1. This formula can be deduced from our previous one with the Coulomb interaction by specializing to a local interaction only between opposite spins. That removes one integral and one spin sum.

As in the electron gas, we need to know response functions, more specifically $\delta\mathcal{G}_\sigma(1,2)_\phi/\delta\phi_{-\sigma}(1^+,1)$.

56.2 Response functions

Response (four-point) functions for spin and charge excitations can be obtained from functional derivatives ($\delta\mathcal{G}/\delta\phi$) of the source-dependent propagator. We will see that a linear combination of these response functions is related to $\delta\mathcal{G}_\sigma(1,2)_\phi/\delta\phi_{-\sigma}(1^+,1)$ above. Following the standard approach and using matrix notation to abbreviate the summations and integrations we have,

$$\mathcal{G}\mathcal{G}^{-1} = 1 \tag{56.6}$$

$$\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1} + \mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi} = 0. \tag{56.7}$$

Using the Dyson equation (56.3) $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma$ this may be rewritten

$$\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} = \mathcal{G}\circ\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}, \tag{56.8}$$

where the symbol $\circ$ reminds us that the neighboring labels of the propagators have to be the same as those of the ϕ in the functional derivative. If perturbation theory converges, we may write the self-energy as a functional of the propagator. From the chain rule, one then obtains an integral equation for the response function in the particle-hole channel that is the analog of the Bethe-Salpeter equation in the particle-particle channel

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\circ\mathcal{G} + \mathcal{G}\left[\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right]\mathcal{G}. \tag{56.9}$$

The labels of the propagators in the last term are attached to the self energy, as in Eq.(56.8) [1].

In the Coulomb-gas case, we have solved this equation in the RPA approximation, where only charge fluctuations are involved. Here let us drop any special assumption, other than spin-rotation invariance, concerning the form of the irreducible vertices. We will see that in general, both spin and charge fluctuations influence the self-energy, contrary to the Coulomb gas where only charge fluctuations were involved.

Remark 318 *In the RPA approximation for the Coulomb gas, the spin fluctuations are given by a single bubble. The diagrams that are reducible with respect to the Coulomb interaction all vanish. See the exercises.*

To obtain spin and charge fluctuations from the above formula, we restore spin indices explicitly and represent coordinates with numbers (in our previous

[1] To remind ourselves of this, we may also adopt an additional "vertical matrix notation" convention and write Eq.(7) as $\frac{\delta G}{\delta\phi} = G\circ G + G\left[\begin{smallmatrix}\frac{\delta\Sigma}{\delta G}\\ \frac{\delta G}{\delta\phi}\end{smallmatrix}\right]G$.

convention, numbers included spin labels, but not here). When the external field is diagonal in spin indices we need only one spin label on $\mathcal{G}$ and ϕ. The response function that can be used then to build both spin and charge fluctuations is

$$\begin{aligned} -\frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} &= \left\langle T_\tau \psi_\sigma^\dagger\left(1^+\right)\psi_\sigma\left(1\right)\psi_{\sigma'}^\dagger\left(2^+\right)\psi_{\sigma'}\left(2\right)\right\rangle_\phi - \mathcal{G}_\sigma\left(1,1^+\right)_\phi \mathcal{G}_{\sigma'}\left(2,2^+\right)_\phi \\ &= \left\langle T_\tau n_\sigma\left(1\right) n_{\sigma'}\left(2\right)\right\rangle_\phi - \left\langle n_\sigma\left(1\right)\right\rangle_\phi \left\langle n_{\sigma'}\left(2\right)\right\rangle_\phi . \end{aligned} \tag{56.10}$$

The charge and spin given by

$$n_i \equiv n_{i\uparrow} + n_{i\downarrow} \tag{56.11}$$

$$S_i^z \equiv n_{i\uparrow}\left(\tau\right) - n_{i\downarrow}\left(\tau\right). \tag{56.12}$$

Hence, the charge fluctuations are obtained from

$$\chi_{ch}\left(1,2\right) = -\sum_{\sigma,\sigma'} \frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} \tag{56.13}$$

and the spin fluctuations from

$$\chi_{sp}\left(1,2\right) = -\sum_{\sigma,\sigma'} \sigma \frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} \sigma'. \tag{56.14}$$

We thus need the spin dependence in the integral equation for the susceptibilities to compute $\chi_{ch}\left(1,2\right)$ and $\chi_{sp}\left(1,2\right)$. It reads:

$$\frac{\delta \mathcal{G}_\sigma}{\delta\phi_{\sigma'}} = \mathcal{G}\cdot\mathcal{G}\delta_{\sigma,\sigma'} + \mathcal{G}_\sigma\left[\frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\overline{\sigma}}}\frac{\delta\mathcal{G}_{\overline{\sigma}}}{\delta\phi_{\sigma'}}\right]\mathcal{G}_\sigma. \tag{56.15}$$

Let us focus on the integral equation for the charge fluctuations which is obtained by doing the sums over spins: There is a sum over $\overline{\sigma}$. The spin indices on the Green's function are unnecessary when there is rotational invariance, hence we dropped them. From the above Eq.(56.15) we can compute χ_{ch} by performing the sum over spins. If we use that, by rotational invariance, $\mathcal{G}_\sigma$ is independent of spin direction σ while the quantities

$$\sum_\sigma \frac{\delta \mathcal{G}_\sigma}{\delta\phi_{\sigma'}} \; ; \; \sum_\sigma \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\sigma'}} \tag{56.16}$$

are independent of σ' and

$$\sum_{\sigma'} \frac{\delta \mathcal{G}_\sigma}{\delta\phi_{\sigma'}} \tag{56.17}$$

is independent of σ, the result can be written as follows

$$\chi_{ch} = -\sum_{\sigma,\sigma'} \frac{\delta \mathcal{G}_\sigma}{\delta\phi_{\sigma'}} = -2\mathcal{G}\cdot\mathcal{G} - \mathcal{G}\left[\sum_\sigma \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\sigma'''}} \sum_{\sigma''}\sum_{\sigma'} \frac{\delta\mathcal{G}_{\sigma''}}{\delta\phi_{\sigma'}}\right]\mathcal{G} \tag{56.18}$$

where we introduced a label σ''' in Eq.(56.18) that does not influence the result. The irreducible charge vertex is given by[2] $U_{ch} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} + \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}$. In other words, Eq.(56.18) may be written as

$$\boxed{\chi_{ch} = -2\mathcal{G}\cdot\mathcal{G} + \mathcal{G}\left[\left(\frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow} + \frac{\delta\Sigma_\downarrow}{\delta\mathcal{G}_\uparrow}\right)\chi_{ch}\right]\mathcal{G}} \tag{56.19}$$

[2] Using spin rotational invariance (SU(2) symmetry) we have that several relations, such as $\frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} = \frac{\delta\Sigma_\downarrow}{\delta\mathcal{G}_\uparrow}$. This is used without further comments.

Similarly, to find the integral equation for the spin response function, we notice that

$$\sum_{\sigma} \sigma \frac{\delta \Sigma_{\sigma}}{\delta \mathcal{G}_{\sigma'}} \sigma' = \left(\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\sigma'}} - \frac{\delta \Sigma_{\downarrow}}{\delta \mathcal{G}_{\sigma'}} \right) \sigma' \tag{56.20}$$

$$= \left(\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} - \frac{\delta \Sigma_{\downarrow}}{\delta \mathcal{G}_{\uparrow}} \right) \tag{56.21}$$

We have taken σ' up $(+1)$ and then down (-1) and used rotational invariance $\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} = \frac{\delta \Sigma_{\downarrow}}{\delta \mathcal{G}_{\downarrow}}$ and $\frac{\delta \Sigma_{\downarrow}}{\delta \mathcal{G}_{\uparrow}} = \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}}$ to see that the result is independent of σ'. This means that the general spin resolved response function Eq.(56.15) yieds for the spin susceptibility, given $(\sigma'')^2 = 1$

$$\begin{aligned} \chi_{sp} &= -\sum_{\sigma,\sigma'} \sigma \frac{\delta \mathcal{G}_{\sigma}}{\delta \phi_{\sigma'}} \sigma' = -2\mathcal{G}\hat{\cdot}\mathcal{G} \\ &\quad -\mathcal{G} \left[\sum_{\sigma''} \sum_{\sigma'} \left(\sum_{\sigma} \sigma \frac{\delta \Sigma_{\sigma}}{\delta \mathcal{G}_{\sigma''}} \sigma'' \right) \sigma'' \frac{\delta \mathcal{G}_{\sigma''}}{\delta \phi_{\sigma'}} \sigma' \right] \mathcal{G}. \\ &= -2\mathcal{G}\hat{\cdot}\mathcal{G} + \mathcal{G} \left[\left(\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} \right) \sum_{\sigma''} \sum_{\sigma'} \sigma'' \frac{\delta \mathcal{G}_{\sigma''}}{\delta \phi_{\sigma'}} \sigma' \right] \mathcal{G} \end{aligned} \tag{56.22}$$

so that finally,

$$\boxed{\chi_{sp} = -2\mathcal{G}\hat{\cdot}\mathcal{G} - \mathcal{G} \left[\left(\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} \right) \chi_{sp} \right] \mathcal{G}} \tag{56.23}$$

In summary, we define irreducible vertices appropriate for spin and charge responses as follows,

$$\begin{aligned} \boxed{U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}}} \\ \boxed{U_{ch} = \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} + \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}}} \end{aligned} \tag{56.24}$$

56.3 Hartree-Fock and RPA

As an example of calculation of response functions, consider the Hartree-Fock approximation which corresponds to factoring the four-point function in the definition of the self-energy Eq.(56.4) as if there were no interactions, in which case it is easy to see that $\frac{\delta \mathcal{G}_{\sigma}(1,2)_{\phi}}{\delta \phi_{-\sigma}(1^+,1)} = 0$. To be more specific, starting from

$$\Sigma_{\sigma}(1,\overline{1})_{\phi} \mathcal{G}_{\sigma}(\overline{1},2)_{\phi} = -U \left\langle T_{\tau} \psi^{\dagger}_{-\sigma}(1^+) \psi_{-\sigma}(1) \psi_{\sigma}(1) \psi^{\dagger}_{\sigma}(2) \right\rangle_{\phi} \tag{56.25}$$

$$= -U \left[\frac{\delta \mathcal{G}_{\sigma}(1,2)_{\phi}}{\delta \phi_{-\sigma}(1^+,1)} - \mathcal{G}_{-\sigma}(1,1^+)_{\phi} \mathcal{G}_{\sigma}(1,2)_{\phi} \right] \tag{56.26}$$

the Hartree-Fock approximation is

$$\Sigma^H_{\sigma}(1,\overline{1})_{\phi} \mathcal{G}^H_{\sigma}(\overline{1},2)_{\phi} = U \mathcal{G}^H_{-\sigma}(1,1^+)_{\phi} \mathcal{G}^H_{\sigma}(1,2)_{\phi}.$$

Multiplying the above equation by $\left(G^H_{\sigma}\right)^{-1}$, we are left with

$$\Sigma^H_{\sigma}(1,2)_{\phi} = U \mathcal{G}^H_{-\sigma}(1,1^+)_{\phi} \delta(1-2), \tag{56.27}$$

so that

$$\left.\frac{\delta\Sigma_{\uparrow}^{H}\left(1,2\right)_{\phi}}{\delta\mathcal{G}_{\downarrow}^{H}\left(3,4\right)_{\phi}}\right|_{\phi=0}=U\delta\left(1-2\right)\delta\left(3-1\right)\delta\left(4-2\right), \tag{56.28}$$

and

$$\left.\frac{\delta\Sigma_{\uparrow}^{H}\left(1,2\right)_{\phi}}{\delta\mathcal{G}_{\uparrow}^{H}\left(3,4\right)_{\phi}}\right|_{\phi=0}=0.$$

which, when substituted in the integral equation (56.9) for the response function, tells us that we have generated the random phase approximation (RPA) with, from Eq.(56.24), $U_{sp}=U_{ch}=U$. Indeed, when the irreducible vertex comes from the Hartree term, the same structure as the one found before for the electron gas results. The charge susceptibility that follows from the result of the previous section Eq.(56.19) for χ_{ch} and the definition U_{ch} for the corresponding irreducible vertex Eq.(56.24) is

$$\chi_{ch}\left(1,2\right)=\chi^{(0)}\left(1,2\right)-\frac{1}{2}\chi^{(0)}\left(1,\overline{3}\right)U_{ch}\chi_{ch}\left(\overline{3},2\right) \tag{56.29}$$

with $\chi^{(0)}\left(1,2\right)=-2\mathcal{G}\left(1,2\right)\mathcal{G}\left(2,1\right)$. The Fourier transform is

$$\chi_{ch}\left(q\right)=\chi^{(0)}\left(q\right)-\frac{U_{ch}}{2}\chi^{(0)}\left(q\right)\chi_{ch}\left(q\right). \tag{56.30}$$

Since at this point the self-energy is a constant, we take for $\mathcal{G}$ the non-interacting Green's function. In Fourier-Matsubara space, $\chi_0(q)$ then is the Lindhard function that, in analytically continued retarded form is, for a discrete lattice of N sites,

$$\chi^{0R}(\mathbf{q},\omega)=-\frac{2}{N}\sum_{\mathbf{k}}\frac{f\left(\zeta_{\mathbf{k}}\right)-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)}{\omega+i\eta+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}. \tag{56.31}$$

Similarly, for the spin susceptibility, using the integral equation Eq.(56.23) and the definition U_{sp} for the corresponding irreducible vertex Eq.(56.24), we obtain

$$\chi_{sp}\left(q\right)=\chi^{(0)}\left(q\right)+\frac{U_{sp}}{2}\chi^{(0)}\left(q\right)\chi_{sp}\left(q\right). \tag{56.32}$$

The equations for the spin and charge fluctuations can easily be solved and yield, respectively

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} \tag{56.33}$$

$$\chi_{ch}(q) = \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)} \tag{56.34}$$

It is known on general grounds [23] that RPA satisfies conservation laws. We will describe the general methods that lead to approximations that are consistent with conservation laws in a later chapter. But it is easy to check that for a special case. Since spin and charge are conserved, then the equalities $\chi_{sp}^{R}(\mathbf{q}=\mathbf{0},\omega)=0$ and $\chi_{ch}^{R}(\mathbf{q}=\mathbf{0},\omega)=0$ for $\omega\neq0$ follow from the corresponding equality for the non-interacting Lindhard function $\chi^{0R}(\mathbf{q}=\mathbf{0},\omega)=0$.

Remark 319 *If we had used dressed Green's function to compute the Lindhard susceptibility, the conservation law $\chi_{sp,ch}\left(\mathbf{q}=\mathbf{0},i\omega_n\right)=0$ for $i\omega_n\neq0$ would have been violated, as shown in Eq.(50.6) and in Appendix A of Ref.[255]. In general, irreducible vertices and self-energy (and corresponding Green's functions) must be taken at the same level of approximation.*

56.4 RPA and violation of the Pauli exclusion principle

RPA has a drawback that is particularly important for the Hubbard model. It violates the Pauli exclusion principle that is assumed to be satisfied exactly in its definition where up spins interact only with down spins. To see this requires a bit more thinking. We derive a sum rule that rests on the use of the Pauli exclusion principle and check that it is violated by RPA to second order in U.

First note that if we sum the spin and charge susceptibilities over all wave vectors $\mathbf{q}$ and all Matsubara frequencies iq_n, we obtain local, equal-time correlation functions, namely

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_{sp}(\mathbf{q},iq_n) = \left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 2\langle n_\uparrow n_\downarrow\rangle \tag{56.35}$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_{ch}(\mathbf{q},iq_n) = \left\langle (n_\uparrow + n_\downarrow)^2 \right\rangle - \langle n_\uparrow + n_\downarrow\rangle^2 = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle + 2\langle n_\uparrow n_\downarrow\rangle - n^2 \tag{56.36}$$

where on the right-hand side, we used the Pauli exclusion principle $n_\sigma^2 = \left(c_\sigma^\dagger c_\sigma\right)\left(c_\sigma^\dagger c_\sigma\right) = c_\sigma^\dagger c_\sigma - c_\sigma^\dagger c_\sigma^\dagger c_\sigma c_\sigma = c_\sigma^\dagger c_\sigma = n_\sigma$ that follows from $c_\sigma^\dagger c_\sigma^\dagger = c_\sigma c_\sigma = 0$. This is the simplest version of the Pauli exclusion principle. Full antisymmetry is another matter [32, 106]. We call the first of the above displayed equations the local spin sum-rule and the second one the local charge sum-rule. For RPA, adding the two sum rules yields

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\left(\chi_{sp}(\mathbf{q},iq_n) + \chi_{ch}(\mathbf{q},iq_n)\right) = \tag{56.37}$$

$$\frac{T}{N}\sum_{q}\left(\frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} + \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)}\right) = 2n - n^2. \tag{56.38}$$

Since the non-interacting susceptibility $\chi_0(q)$ satisfies the sum rule, we see by expanding the denominators that in the interacting case it is violated already to second order in U because $\chi_0(q)$ being real and positive, (See Eq.(58.12)), the quantity $\sum_q \chi_0(q)^3$ cannot vanish.

56.5 Why RPA violates the Pauli exclusion principle from the point of view of diagrams

Let us return to the original Coulomb interaction that does not depend on spins. You can go back to Fig.(37-7) for a refresher. Take only the first order diagram with a single Coulomb interaction and two momentum integrals. Take the same spin direction for the incoming particle-hole pair, say on top, and for the outgoing particle-hole pair, say on the bottom. In the case where we have no momentum dependence on the interaction line, the two diagrams have identical values and opposite sign, so they cancel each other. When the spins are different for

the incoming and for the outgoing particle-hole pair, only the reducible diagram contributes. We have arranged the Hubbard model so that this happens automatically, namely we have used the Pauli exclusion principle so that electrons of a given spin interact only with electrons of the opposite spin. But that works only for diagrams to that order. This corresponds to the fact that RPA satisfies the Pauli exclusion principle to first order in U, as we just saw in the previous section.

However, there are many more diagrams. To satisfy the Pauli exclusion principle, we would need to take into account exact cancellations between all diagrams that are obtained by interchanging the end or the beginning of Green's functions lines. For example, consider the diagram where we have three bubbles and two interaction lines. Take up spins for the first and last bubble and down spin for the middle bubble. Now consider the diagram obtained by taking one Green's function line of the first bubble and making it land at the end of the interaction that begins the last bubble while the Green's function that used to land there now lands at the end of the interaction line of the first bubble. We have then a diagram that has an opposite sign to the first one since two fermions were exchanged. The values of that diagram and of the first one are identical for a contact (i.e. momentum-independent) interactions. Hence, as soon as we move beyond first order in interaction, there are exact cancellations between diagrams that are not taken into account if we sum only bubbles, even if up electrons interact only with down.

56.6 RPA, phase transitions and the Mermin-Wagner theorem

The RPA predicts that the normal state is sometimes unstable, namely that if we decrease the temperature, spin fluctuations at zero frequency start, in certain cases, to diverge. Below the temperature where that occurs, the spin susceptibility is negative, which is prohibited by thermodynamic stability. This indicates that a paramagnetic ground state is an unstable state. This happens even in two-dimensions with RPA because

$$\chi_0(q) = \int \frac{d\omega'}{\pi} \frac{\chi''_{sp}(\mathbf{q},\omega')\omega'}{\omega'^2 + q_n^2}$$

is positive so that the expression for the spin susceptibility

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U\chi_0(q)} \tag{56.39}$$

is quite likely to become negative for a U sufficiently large.

By the way, why does a negative spin susceptibility at $q_n = 0$ signal an instability? Because there is a thermodynamic inequality that says that susceptibilities of the form dA/da, where A and a are thermodynamically conjugate variables, are positive since entropy is a maximum at equilibrium. But there is another way to look at this from the thermodynamic sum rule in Sec. 10.10.1

$$\chi_{sp}(\mathbf{Q},0) = \int \frac{d\omega}{\pi} \frac{\chi''_{sp}(\mathbf{Q},\omega)}{\omega}. \tag{56.40}$$

Indeed, if the left-hand side is negative, this means that the imaginary part of the spin susceptibility for positive frequencies has to be negative.[3] This violates

[3] It is positive at negative frequencies since it must be odd.

the positivity criterion imposed by stability, Sec. 10.6, namely $\chi''_{sp}(\mathbf{Q},\omega)\omega > 0$. Hence, the system is unstable.

Such an instability in two dimensions at finite temperature is prohibited by the Mermin-Wagner theorem that says that a continuous symmetry cannot be broken in two dimensions at finite temperature. We will come back on this theorem in a later chapter, but for now the theorem may intuitively be understood as follows. If there is long-range order in the presence of a continuous symmetry, there will be a term in the free energy that will be proportional to $|\nabla\phi|^2$, where ϕ is the angle representing the deviation of the spins say, from their equilibrium position. The equipartition theorem then says that

$$\mathbf{q}^2 \left\langle \phi_{\mathbf{q}} \phi_{-\mathbf{q}} \right\rangle = \frac{T}{2}. \tag{56.41}$$

Thus, in two dimensions, the thermal fluctuations of that angle are infinite, proving the theorem by contradiction:

$$\left\langle \phi^2 \right\rangle = \int_0^\infty \frac{d^2q}{q^2} \frac{T}{2} = \infty.$$

We may think that the instability will occur for U so large that anyway RPA does not apply. This is not the case. Let us illustrate that this happens with a specific example where in fact the instability occurs for infinitesimal U.

We evaluate the Lindhard function Eq.(56.31) at zero frequency in the case where we have only nearest neighbor hopping on a cubic lattice, in other words, $\varepsilon_{\mathbf{k}} = -2t\left(\cos k_x + \cos k_y + \cos k_z\right)$. In $d = 2$ this would be replaced by $\zeta_{\mathbf{k}} = \varepsilon_{\mathbf{k}} = -2t\left(\cos k_x + \cos k_y\right)$. Then, if we take $\mu = 0$, which in this case corresponds to half-filling, and choose the wave vector corresponding to an antiferromagnetic fluctuation, namely $Q = (\pi, \pi, \pi)$ that leads to a phase $+1$ or -1 on alternating sites, we find

$$\chi^{0R}(\mathbf{Q}, 0) = -\frac{2}{N} \sum_{\mathbf{k}} \frac{2f\left(\varepsilon_{\mathbf{k}}\right) - 1}{2\varepsilon_{\mathbf{k}}} \tag{56.42}$$

because of the equality $f(-\varepsilon) = 1 - f(\varepsilon)$ and the co-called nesting property $\varepsilon_{\mathbf{k}} = -\varepsilon_{\mathbf{k}+\mathbf{Q}}$. But $2f\left(\varepsilon_{\mathbf{k}}\right) - 1 = -\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)$ which allows one to write by using the definition of the density of states $N(\varepsilon)$

$$\begin{aligned}
\chi^{0R}(\mathbf{Q}, 0) &= \frac{2}{N} \sum_{\mathbf{k}} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} && (56.43)\\
&\sim 2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} && (56.44)\\
&\sim \int d\varepsilon N(\varepsilon) \frac{\tanh\left(\beta\varepsilon/2\right)}{2\varepsilon}. && (56.45)
\end{aligned}$$

This last result takes the same form in $d = 2$. You just need to replace the density of states by the two-dimensional one. The last integral diverges when $T \to 0$ or $\beta \to \infty$. Indeed, take $N(\varepsilon)$ constant near the Fermi level, up to a cutoff energy $\pm E_F$. Near the Fermi level, $\varepsilon = 0$, when $\varepsilon > T$ we can approximate $\tanh\left(\beta\varepsilon/2\right)/2\varepsilon \sim 1/4T$. So we can extract the logarithmically divergent part of the integral as follows:

$$\begin{aligned}
\int d\varepsilon N(\varepsilon) \frac{\tanh\left(\beta\varepsilon/2\right)}{2\varepsilon} &\sim \int_T^{E_F} d\varepsilon N(0) \frac{1}{\varepsilon}\\
&\sim N(0) \ln\left(\frac{E_F}{T}\right). && (56.46)
\end{aligned}$$

For T sufficiently small, $\chi^{0R}(\mathbf{Q},0)$ diverges, which means that at a certain temperature, the denominator of the spin susceptibility Eq.(56.33) goes through zero, even with infinitesimal U. At that temperature, the spin susceptibility diverges. Below that it is negative, signaling an instability.

This instability signals a second-order phase transition that it physical. In two dimensions, $N(\varepsilon)$ has a logarithmic divergence at $\varepsilon = 0$ so the above result must be modified. We would obtain a $\ln^2(E_F/T)$ instead of $\ln(E_F/T)$. Nevertheless, the qualitative result would be the same. There is an instability even in the presence of an infinitesimal U. However, in two-dimensions, one cannot have a phase transition that breaks a continuous symmetry at finite temperature in two dimensions. That is the content of the Mermin Wagner theorem.[159, 95] Hence, RPA fails miserably on many grounds in two dimensions: It violates the Pauli exclusion principle and the Mermin-Wagner theorem. The approach in the next section fixes these two problems and more.

57. THE TWO-PARTICLE-SELF-CONSISTENT APPROACH

The two-particle-self-consistent approach (TPSC) is designed to remedy the deficiencies found above in the study of the the one-band Hubbard model. It is also possible to generalize to cases where near-neighbor interactions are included.

TPSC is valid from weak to intermediate coupling. Hence, on the negative side, it does not describe the Mott transition. Nevertheless, there is a large number of physical phenomena that it allows to study. An important one is antiferromagnetic fluctuations. It is extremely important physically that in two dimensions there is a wide range of temperatures where there are huge antiferromagnetic fluctuations in the paramagnetic state, without long-range order, as imposed by the Mermin-Wagner theorem. The standard way to treat fluctuations in many-body theory, the Random Phase Approximation (RPA) misses this and also, as we saw, the RPA also violates the Pauli exclusion principle in an important way. The composite operator method (COM), by F. Mancini, is another approach that satisfies the Mermin-Wagner theorem and the Pauli exclusion principle. [147, 148, 146] The Fluctuation Exchange Approximation (FLEX) [30, 31], and the self-consistent renormalized theory of Moriya-Lonzarich [164, 137, 166] are other approaches that satisfy the Mermin-Wagner theorem at weak coupling. Each has its strengths and weaknesses, as discussed in Refs. [255, 8]. Weak coupling renormalization group approaches become uncontrolled when the antiferromagnetic fluctuations begin to diverge [70, 210, 130, 97]. Other approaches include the effective spin-Hamiltonian approach [238].

In summary, the advantages and disadvantages of TPSC are as follows. Advantages:

- There are no adjustable parameters.
- Several exact results are satisfied: Conservation laws for spin and charge, the Mermin-Wagner theorem, the Pauli exclusion principle in the form $\left\langle n_{\uparrow}^{2}\right\rangle = \langle n_{\uparrow}\rangle$, the local moment and local-charge sum rules and the f sum-rule.
- Consistency between one and two-particle properties serves as a guide to the domain of validity of the approach. (Double occupancy obtained from sum rules on spin and charge equals that obtained from the self-energy and the Green function).
- Up to intermediate coupling, TPSC agrees within a few percent with Quantum Monte Carlo (QMC) calculations. Note that QMC calculations can serve as benchmarks since they are exact within statistical accuracy, but they are limited in the range of physical parameter accessible.
- We do not need to assume that Migdal's theorem applies to be able to obtain the self-energy.

The main successes of TPSC include

- Understanding the physics of the pseudogap induced by precursors of a long-range ordered phase in two dimensions. For this understanding, one needs

a method that satisfies the Mermin-Wagner theorem to create a broad temperature range where the antiferromagnetic correlation length is larger than the thermal de Broglie wavelength. That method must also allow one to compute the self-energy reliably. Only TPSC does both.

- Explaining the pseudogap in electron-doped cuprate superconductors over a wide range of dopings.
- Finding estimates of the transition temperature for d-wave superconductivity that were found later in agreement with quantum cluster approaches such as the Dynamical Cluster Approximation.
- Giving quantitative estimates of the range of temperature where quantum critical behavior can affect the physics.

The drawbacks of this approach, that I explain as we go along, are that

- It works well in two or more dimensions, not in one dimension [1] [174].
- It is not valid at strong coupling, except at very high temperature and large U where it recovers the atomic limit [58].
- It is not valid deep in the renormalized classical regime [245].
- For models other than the one-band Hubbard model, one usually runs out of sum rules and it is in general not possible to find all parameters self-consistently. With nearest-neighbor repulsion, it has been possible to find a way out [60].

For detailed comparisons with QMC calculations, discussions of the physics and detailed comparisons with other approaches, you can refer to Ref.[255, 8]. You can read Ref.[236] for a review of the work related to the pseudogap and superconductivity up to 2005 including detailed comparisons with Quantum Cluster approaches in the regime of validity that overlaps with TPSC (intermediate coupling). A more recent review appeared in Ref. [235].

57.1 TPSC First step: two-particle self-consistency for $\mathcal{G}^{(1)}$, $\Sigma^{(1)}$, $\Gamma_{sp}^{(1)} = U_{sp}$ and $\Gamma_{ch}^{(1)} = U_{ch}$

Details of the more formal derivation may be also be found in Ref. [7]. In conserving approximations, the self-energy is obtained from a functional derivative $\Sigma\left[\mathcal{G}\right] = \delta\Phi\left[\mathcal{G}\right]/\delta\mathcal{G}$ of Φ the Luttinger-Ward functional, which is itself computed from a set of diagrams. We will see this approach later in the course. To liberate ourselves from diagrams and find results that are valid beyond perturbation theory, we start instead from the exact expression for the self-energy, Eq.(56.4)

$$\Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},2\right)_\phi = -U\left\langle T_\tau \psi^\dagger_{-\sigma}\left(1^+\right)\psi_{-\sigma}\left(1\right)\psi_\sigma\left(1\right)\psi^\dagger_\sigma\left(2\right)\right\rangle_\phi$$

and notice that when label 2 equals 1^+, the right-hand side of this equation is equal to double-occupancy $\langle n_\uparrow n_\downarrow\rangle$. Factoring as in Hartree-Fock amounts to assuming

[1] Modifications have been proposed in zero dimension to use as impurity solver for DMFT [78]

no correlations. Instead, we should insist that $\langle n_\uparrow n_\downarrow \rangle$ should be obtained self-consistently. After all, in the Hubbard model, there are only two local four point functions: $\langle n_\uparrow n_\downarrow \rangle$ and $\left\langle n_\uparrow^2 \right\rangle = \left\langle n_\downarrow^2 \right\rangle$. The latter is given exactly, through the Pauli exclusion principle, by $\left\langle n_\uparrow^2 \right\rangle = \left\langle n_\downarrow^2 \right\rangle = \langle n_\uparrow \rangle = \langle n_\downarrow \rangle = n/2$, when the filling n is known. In a way, $\langle n_\uparrow n_\downarrow \rangle$ in the self-energy equation (56.4), can be considered as an initial condition for the four point function when one of the points, 2, separates from all the others which are at 1. When that label 2 does not coincide with 1, it becomes more reasonable to factor *à la* Hartree-Fock. These physical ideas are implemented by postulating

$$\Sigma_\sigma^{(1)}\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma^{(1)}\left(\overline{1},2\right)_\phi = A_\phi \mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)_\phi \mathcal{G}_\sigma^{(1)}\left(1,2\right)_\phi \tag{57.1a}$$

where A_ϕ depends on external field and is chosen such that the exact result [2]

$$\Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},1^+\right)_\phi = U\left\langle n_\uparrow\left(1\right) n_\downarrow\left(1\right)\right\rangle_\phi \tag{57.2}$$

is satisfied. It is easy to see that the solution is

$$A_\phi = U\frac{\left\langle n_\uparrow\left(1\right) n_\downarrow\left(1\right)\right\rangle_\phi}{\left\langle n_\uparrow\left(1\right)\right\rangle_\phi \left\langle n_\downarrow\left(1\right)\right\rangle_\phi}. \tag{57.3}$$

Substituting A_ϕ back into our *ansatz* Eq.(58.3) we obtain our first approximation for the self-energy by right-multiplying by $\left(\mathcal{G}_\sigma^{(1)}\right)^{-1}$:

$$\Sigma_\sigma^{(1)}\left(1,2\right)_\phi = A_\phi \mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)_\phi \delta\left(1-2\right). \tag{57.4}$$

We are now ready to obtain irreducible vertices using the prescription of section 56.2, Eq.(56.24), namely through functional derivatives of Σ with respect to $\mathcal{G}$. In the calculation of U_{sp}, the functional derivative of $\langle n_\uparrow n_\downarrow \rangle / \left(\langle n_\uparrow \rangle \langle n_\downarrow \rangle\right)$ drops out, so we are left with [3],

$$\begin{aligned} \left.\frac{\delta\Sigma_\uparrow^{(1)}\left(1,2\right)_\phi}{\delta\mathcal{G}_\downarrow^{(1)}\left(3,4\right)_\phi}\right|_{\phi=0} - \left.\frac{\delta\Sigma_\uparrow^{(1)}\left(1,2\right)_\phi}{\delta\mathcal{G}_\uparrow^{(1)}\left(3,4\right)_\phi}\right|_{\phi=0} &= U_{sp}\delta\left(1-2\right)\delta\left(3-1\right)\delta\left(4-2\right) \\ U_{sp} &= A_{\phi=0} = U\frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}. \end{aligned} \tag{57.5}$$

The renormalization of this irreducible vertex may be physically understood as coming from the physics described by Kanamori and Brueckner [255] (in the latter case in the context of nuclear physics): The value of the bare interaction is renormalized down by the fact that the two-particle wave function will want to be smaller where U is larger. In the language of perturbation theory, one must sum the Born series to compute how two particles scatter off each other and not work in the first Born approximation. This completes the derivation of the *ansatz* that is central to TPSC.

The functional-derivative procedure generates an expression for the charge vertex U_{ch} which involves the functional derivative of $\langle n_\uparrow n_\downarrow \rangle / \left(\langle n_\uparrow \rangle \langle n_\downarrow \rangle\right)$ which contains six point functions that one does not really know how to evaluate. But, if we again assume that the vertex U_{ch} is a constant, it is simply determined by the requirement that charge fluctuations also satisfy the fluctuation-dissipation

[2] See footnote (14) of Ref. [8] for a discussion of the choice of limit 1^+ vs 1^-.

[3] For $n > 1$, all particle occupation numbers must be replaced by hole occupation numbers.

theorem and the Pauli exclusion principle, as in Eq.(56.36). In summary, spin and charge fluctuations are obtained from

$$\chi_{sp}(q) = \frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} \tag{57.6}$$

$$\chi_{ch}(q) = \frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}. \tag{57.7}$$

with the irreducible vertices determined from the sum rules

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle \tag{57.8}$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)} = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2. \tag{57.9}$$

along with the relations that relates U_{sp} to double occupancy, Eq.(57.5).

Remark 320 *Note that, in principle, $\Sigma^{(1)}$ also depends on double-occupancy, but since $\Sigma^{(1)}$ is a constant, it is absorbed in the definition of the chemical potential and we do not need to worry about it in this case. That is why the non-interacting irreducible susceptibility $\chi^{(1)}(q) = \chi_0(q)$ appears in the expressions for the susceptibility, even though it should be evaluated with $\mathcal{G}^{(1)}$ that contains $\Sigma^{(1)}$. A rough estimate of the renormalized chemical potential (or equivalently of $\Sigma^{(1)}$), is given in the appendix of Ref. ([8]). One can check that spin and charge conservation are satisfied by the TPSC susceptibilities.*

Remark 321 *$U_{sp}\langle n_\uparrow\rangle\langle n_\downarrow\rangle = U\langle n_\uparrow n_\downarrow\rangle$ can be understood as correcting the Hatree-Fock factorization so that the correct double occupancy be obtained. Expressing the irreducible vertex in terms of an equal-time correlation function is inspired by the approach of Singwi [219] to the electron gas. But TPSC is different since it also enforces the Pauli exclusion principle and connects to a local correlation function, namely $\langle n_\uparrow n_\downarrow\rangle$.*

57.2 TPSC Second step: an improved self-energy $\sum^{(2)}$

Collective charge and spin excitations can be obtained accurately from Green's functions that contain a simple self-energy, as we have just seen. Such modes are emergent objects that are less influenced by details of the single-particle properties than the other way around, especially at finite temperature where the lowest fermionic Matsubara frequency is not zero. The self-energy on the other hand is much more sensitive to collective modes since these are important at low frequency. The second step of TPSC is thus to find a better approximation for the self-energy. This is similar in spirit to what is done in the electron gas [141] where plasmons are found with non-interacting particles and then used to compute an improved approximation for the self-energy. This two step process is also analogous to renormalization group calculations where renormalized interactions are evaluated to one-loop order and quasiparticle renormalization appears only to two-loop order [158, 40, 258].

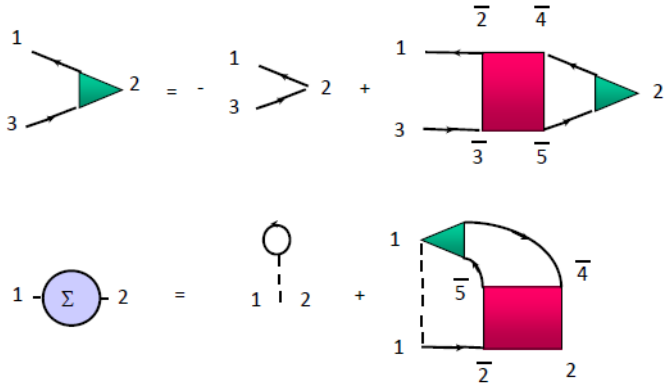


Figure 57-1 Exact expression for the three point vertex (green triangle) in the first line and for the self-energy in the second line. Irreducible vertices are the red boxes and Green's functions solid black lines. The numbers refer to spin, space and imaginary time coordinates. Symbols with an over-bard are summed/integrated over. The self-energy is the blue circle and the bare interaction U the dashed line.

The procedure will be the same as for the electron gas. But before we move to the algebra, we can understand physically the result by looking at Fig. 57-1 that shows the exact diagrammatic expressions for the three-point vertex (green triangle) and self-energy (blue circle) in terms of Green's functions (solid black lines) and irreducible vertices (red boxes). The bare interaction U is the dashed line. One should keep in mind that we are not using perturbation theory despite the fact that we draw diagrams. Even within an exact approach, the quantities defined in the figure have well defined meanings. The numbers on the figure refer to spin, space and imaginary time coordinates. When there is an over-bar, there is a sum over spin and spatial indices and an integral over imaginary time.

In TPSC, the irreducible vertices in the first line of Fig. 57-1 are local, i.e. completely momentum and frequency independent. They are given by U_{sp} and U_{ch}. If we set point 3 to be the same as point 1, then we can obtain directly the TPSC spin and charge susceptibilities from that first line. In the second line of the figure, the exact expression for the self-energy is displayed[4]. The first term on the right-hand side is the Hartree-Fock contribution. In the second term, one recognizes the bare interaction U at one vertex that excites a collective mode represented by the green triangle and the two Green's functions. The other vertex is dressed, as expected. In the electron gas, the collective mode would be the plasmon. If we replace the irreducible vertex using U_{sp} and U_{ch} found for the collective modes, we find that here, both types of modes, spin and charge, contribute to the self-energy [247].

Moving now to the algebra, let us repeat our procedure for the electron gas to show how to obtain an improved approximation for the self-energy that takes advantage of the fact that we have found accurate approximations for the low-frequency spin and charge fluctuations. We begin from the general definition of the self-energy Eq.(56.4) obtained from Dyson's equation. The right-hand side of that equation can be obtained either from a functional derivative with respect to an external field that is diagonal in spin, as in our generating function Eq.(56.1), or by a functional derivative of $\left\langle \psi_{-\sigma}(1)\,\psi^{\dagger}_{\sigma}(2)\right\rangle_{\phi_t}$ with respect to a transverse

[4] In the Hubbard model the Fock term cancels with the same-spin Hartree term

external field ϕ_t, namely an external field that is not diagonal in spin indices.

Working first in the longitudinal channel, the right-hand side of the general definition of the self-energy Eq.(56.4) may be written as

$$\Sigma_\sigma\left(1,\overline{1}\right)\mathcal{G}_\sigma\left(\overline{1},2\right)=-U\left[\left.\frac{\delta\mathcal{G}_\sigma\left(1,2\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)}\right|_{\phi=0}-\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi\mathcal{G}_\sigma\left(1,2\right)_\phi\right]. \quad (57.10)$$

The last term is the Hartree-Fock contribution. It gives the exact result for the self-energy in the limit $\omega\to\infty$.[255] The $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ term is thus a contribution to lower frequencies and it comes from the spin and charge fluctuations. Right-multiplying the last equation by $\mathcal{G}^{-1}$ and replacing the lower energy part $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ by its general expression in terms of irreducible vertices, Eq.(56.9) (recalling that for $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ the first term vanishes) we find

$$\begin{aligned}\Sigma_\sigma^{(2)}\left(1,2\right) &= U\mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)\delta\left(1-2\right) \quad (57.11)\\ &\quad -U\mathcal{G}_\sigma^{(1)}\left(1,\overline{3}\right)\left[\left.\frac{\delta\Sigma_\sigma^{(1)}\left(\overline{3},2\right)_\phi}{\delta\mathcal{G}_{\overline{\sigma}}^{(1)}\left(\overline{4},\overline{5}\right)_\phi}\right|_{\phi=0}\left.\frac{\delta\mathcal{G}_{\overline{\sigma}}^{(1)}\left(\overline{4},\overline{5}\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)_\phi}\right|_{\phi=0}\right].\end{aligned}$$

Every quantity appearing on the right-hand side of that equation has to be taken from the TPSC results. This means in particular that the irreducible vertices $\delta\Sigma_\sigma^{(1)}/\delta\mathcal{G}_{\sigma'}^{(1)}$ are at the same level of approximation as the Green functions $\mathcal{G}_\sigma^{(1)}$ and self-energies $\Sigma_\sigma^{(1)}$. In other approaches one often sees renormalized Green functions $\mathcal{G}^{(2)}$ appearing on the right-hand side along with unrenormalized vertices, $\delta\Sigma_\sigma/\delta\mathcal{G}_{\sigma'}\to U$. We will see later in the context of electron-phonon interactions that this is equivalent to assuming, without justification, that the so-called Migdal's theorem applies to spin and charge fluctuations.

In terms of U_{sp} and U_{ch} in Fourier space, the above formula[247] reads,

$$\Sigma_\sigma^{(2)}(k)_{long}=Un_{-\sigma}+\frac{U}{4}\frac{T}{N}\sum_q\left[U_{sp}\chi_{sp}^{(1)}(q)+U_{ch}\chi_{ch}^{(1)}(q)\right]\mathcal{G}_\sigma^{(1)}(k+q). \quad (57.12)$$

This can be seen simply by noting in Eq.(57.11) that

$$\begin{aligned}\frac{\delta\Sigma_\sigma^{(1)}}{\delta\mathcal{G}_\sigma^{(1)}}\frac{\delta\mathcal{G}_\sigma^{(1)}}{\delta\phi_{-\sigma}} &= \frac{1}{2}\left(U_{ch}-U_{sp}\right)\frac{1}{4}\left(\chi_{ch}-\chi_{sp}\right) \quad (57.13)\\ \frac{\delta\Sigma_\sigma^{(1)}}{\delta\mathcal{G}_{-\sigma}^{(1)}}\frac{\delta\mathcal{G}_{-\sigma}^{(1)}}{\delta\phi_{-\sigma}} &= \frac{1}{2}\left(U_{ch}+U_{sp}\right)\frac{1}{4}\left(\chi_{ch}+\chi_{sp}\right). \quad (57.14)\end{aligned}$$

The approach to obtain a self-energy formula that takes into account both longitudinal and transverse fluctuations is detailed in Ref.([8]). Crossing symmetry, rotational symmetry and sum rules and comparisons with QMC dictate the final formula for the improved self-energy $\Sigma^{(2)}$ as we now sketch.

There is an ambiguity in obtaining the self-energy formula [168]. Within the assumption that only U_{sp} and U_{ch} enter as irreducible particle-hole vertices, the self-energy expression in the transverse spin fluctuation channel is different. What do we mean by that? Consider the exact formula for the self-energy represented symbolically by the diagram of Fig. 57-2. This is the so-called Schwinger-Dyson equation. It can be understood from the fact that $\Sigma\mathcal{G}$ is a four-point function, which means two Green's functions in, and two out that scatter in the middle. One of the Green's functions has disappeared because to obtain Σ, we need to multiply by $\mathcal{G}^{-1}$. In the figure, the textured box is the fully reducible vertex

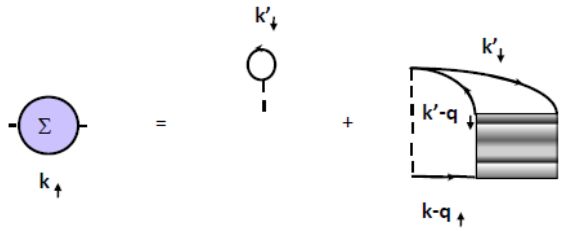


Figure 57-2 Exact self-energy in terms of the Hartree-Fock contribution and of the fully reducible vertex Γ represented by a textured box.

$\Gamma\left(q, k-k', k+k'-q\right)$ that depends in general on three momentum-frequency indices. $\Gamma\left(q, k-k', k+k'-q\right)$ comes from the four-point function in the definition of the self-energy $\left.\frac{\delta \mathcal{G}_\sigma\left(1,\overline{2}\right)_\phi}{\delta \phi_{-\sigma}\left(1^+,1\right)}\right|_{\phi=0} \mathcal{G}_\sigma^{-1}\left(\overline{2},3\right)_\phi$ with two incoming Green's function and one outgoing one explicitly written down. The other outgoing Green's function is removed by $\mathcal{G}_\sigma^{-1}\left(\overline{2},3\right)_\phi$. The longitudinal version of the self-energy corresponds to expanding the fully reducible vertex $\Gamma\left(q, k-k', k+k'-q\right)$ in terms of diagrams that are irreducible in the longitudinal (parallel spins) channel illustrated in Fig. 57-1. This takes good care of the singularity of Γ when its first argument q is near (π, π). The transverse version [168, 8] does the same for the dependence on the second argument $k-k'$, which corresponds to the other (antiparallel spins) particle-hole channel. But the fully reducible vertex obeys crossing symmetry. In other words, interchanging two fermions just leads to a minus sign. One then expects that averaging the two possibilities gives a better approximation for Γ since it preserves crossing symmetry in the two particle-hole channels [168]. By considering both particle-hole channels only, we neglect the dependence of Γ on $k+k'-q$ because the particle-particle channel is not singular. The final formula that we obtain is [168]

$$\Sigma_\sigma^{(2)}(k) = U n_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right]\mathcal{G}_\sigma^{(1)}(k+q). \qquad (57.15)$$

The superscript (2) reminds us that we are at the second level of approximation. $\mathcal{G}_\sigma^{(1)}$ is the same Green's function as that used to compute the susceptibilities $\chi^{(1)}(q)$. Since the self-energy is constant at that first level of approximation, this means that $\mathcal{G}_\sigma^{(1)}$ is the non-interacting Green's function with the chemical potential that gives the correct filling. That chemical potential $\mu^{(1)}$ is slightly different from the one that we must use in $\left(\mathcal{G}^{(2)}\right)^{-1} = iq_n + \mu^{(2)} - \varepsilon_{\mathbf{k}} - \Sigma^{(2)}$ to obtain the same density [126]. Estimates of $\mu^{(1)}$ may be found in Ref. [8, 126]. Further justifications for the above formula are given below in Sect. (57.3).

Remark 322 *Note that a spin fluctuation has $S = 1$, to that is why, physically, there is a factor of 3 in front of the spin fluctuations.*

57.3 TPSC, internal accuracy checks

How can we make sure that TPSC is accurate? We will show sample comparisons with benchmark Quantum Monte Carlo calculations, but we can check the accuracy in other ways. For example, we have already mentioned that the f-sum rule Eq.(58.5) is exactly satisfied at the first level of approximation (i.e. with $n_{\mathbf{k}}^{(1)}$ on the right-hand side). Suppose that on the right-hand side of that equation, one uses $n_{\mathbf{k}}$ obtained from $\mathcal{G}^{(2)}$ instead of the Fermi function. One should find that the result does not change by more than a few percent. This is what happens when agreement with QMC is good.

When we are in the Fermi liquid regime, another way to verify the accuracy of the approach is to verify if the Fermi surface obtained from $\mathcal{G}^{(2)}$ satisfies Luttinger's theorem very closely. Luttinger's theorem says that even an interacting system, when there is a jump in $n_{\mathbf{k}}$ at the Fermi surface at $T = 0$ (as we have seen in the electron gas) then the particle density is determined by the number of $\mathbf{k}$ points inside the Fermi surface, as in the non-interacting case.

Finally, there is a consistency relation between one- and two-particle quantities (Σ and $\langle n_\uparrow n_\downarrow \rangle$). The relation

$$\Sigma_\sigma\left(1,\bar{1}\right)\mathcal{G}_\sigma\left(\bar{1},1^+\right) \equiv \frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{G}\right) = \frac{T}{N}\sum_{\mathbf{k}}\sum_{n}\Sigma(\mathbf{k},iq_n)\mathcal{G}(\mathbf{k},iq_n)e^{-iq_n0^-} = U\left\langle n_\uparrow n_\downarrow\right\rangle \tag{57.16}$$

should be satisfied exactly for the Hubbard model. In standard many-body books [142], it is encountered in the calculation of the free energy through a coupling-constant integration. We have seen this in the previous Chapter 43. In TPSC, it is not difficult to show [5] that the following equation

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right) = U\left\langle n_\uparrow n_\downarrow\right\rangle \tag{57.17}$$

is satisfied exactly with the self-consistent $U\langle n_\uparrow n_\downarrow\rangle$ obtained with the susceptibilities[6]. An internal accuracy check consists in verifying by how much $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(2)}\right)$ differs from $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right)$. Again, in regimes where we have agreement with Quantum Monte Carlo calculations, the difference is only a few percent.

The above relation between Σ and $\langle n_\uparrow n_\downarrow\rangle$ gives us another way to justify our expression for $\Sigma^{(2)}$. Suppose one starts from Fig. 57-1 to obtain a self-energy expression that contains only the longitudinal spin fluctuations and the charge fluctuations, as was done in the first papers on TPSC [245]. One finds that each of these separately contributes an amount $U\langle n_\uparrow n_\downarrow\rangle/2$ to the consistency relation Eq.(57.17). Similarly, if we work only in the transverse spin channel [168, 8] we find that each of the two transverse spin components also contributes $U\langle n_\uparrow n_\downarrow\rangle/2$ to $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right)$. Hence, averaging the two expressions also preserves rotational invariance. In addition, one verifies numerically that the exact sum rule (Ref. [255] Appendix A)

$$-\int\frac{d\omega'}{\pi}\Sigma''^R_\sigma(\mathbf{k},\omega') = U^2 n_{-\sigma}\left(1-n_{-\sigma}\right) \tag{57.18}$$

determining the high-frequency behavior is satisfied to a higher degree of accuracy with the symmetrized self-energy expression Eq. (57.15).

Eq. (57.15) for $\Sigma^{(2)}$ is different from so-called Berk-Schrieffer type expressions [29] that do not satisfy [7] the consistency condition between one- and two-particle

[5] Appendix B or Ref. [255]

[6] FLEX does not satisfy this consistency requirement. See Appendix E of [255]. In fact double-occupancy obtained from ΣG can even become negative [16].

[7] [255] Appendix E)

properties, $\frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{G}\right) = U\left\langle n_\uparrow n_\downarrow\right\rangle$.

Remark 323 *Schemes, such as the fluctuation exchange approximation (FLEX), that we will discuss later, use on the right-hand side $G^{(2)}$, are thermodynamically consistent (Sect. 74.1) and might look better. However, as we just saw, in Fig. 58-2, FLEX misses some important physics. The reason [255] is that the vertex entering the self-energy in FLEX is not at the same level of approximation as the Green's functions. Indeed, since the latter contain self-energies that are strongly momentum and frequency dependent, the irreducible vertices that can be derived from these self-energies should also be frequency and momentum dependent, but they are not. In fact they are the bare vertices. It is as if the quasi-particles had a lifetime while at the same time interacting with each other with the bare interaction. Using dressed Green's functions in the susceptibilities with momentum and frequency independent vertices leads to problems as well. For example, the conservation law $\chi_{sp,ch}\left(\mathbf{q}=\mathbf{0},iq_n\right)=0$ is violated in that case, as shown in Appendix A of Ref.[255]. Further criticism of conserving approaches appears in Appendix E of Ref.[255] and in Ref.[8].*

58. TPSC, BENCHMARKING AND PHYSICAL ASPECTS

In this chapter, we present a physically motivated approach to TPSC and benchmark the theory by comparing with Quantum Monte Carlo simulations. We also discuss physical consequences of the approach, in particular the appearance of a pseudogap that is the precursor of long-range order that occurs only at zero temperature. We show that this physics seems to be realized in electron-doped cuprates.

58.1 Physically motivated approach, spin and charge fluctuations

As basic physical requirements, we would like our approach to satisfy a) conservation laws, b) the Pauli exclusion principle and c) the Mermin Wagner theorem. The standard RPA approach satisfies the first requirement but not the other two as we saw in Sec. 56.4.

How can we go about curing this violation of the Pauli exclusion principle while not damaging the fact that RPA satisfies conservation laws? The simplest way is to proceed in the spirit of Fermi liquid theory and assume that the effective interaction (irreducible vertex in the jargon) is renormalized. This renormalization has to be different for spin and charge so that

$$\chi_{sp}(q) = \frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} \tag{58.1}$$

$$\chi_{ch}(q) = \frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}. \tag{58.2}$$

In practice $\chi^{(1)}(q)$ is the same[1] as the Lindhard function $\chi_0(q)$ for $U = 0$ but, strictly speaking, there is a constant self-energy term that is absorbed in the definition of μ [8]. We are almost done with the collective modes. Substituting the above expressions for $\chi_{sp}(q)$ and $\chi_{ch}(q)$ in the two sum-rules, local-spin and local-charge appearing in Eqs.(56.35,56.36), we could determine both U_{sp} and U_{ch} if we knew $\langle n_\uparrow n_\downarrow \rangle$. The following *ansatz*

$$U_{sp} \langle n_\uparrow \rangle \langle n_\downarrow \rangle = U \langle n_\uparrow n_\downarrow \rangle \tag{58.3}$$

gives us the missing equation. Now notice that U_{sp}, or equivalently $\langle n_\uparrow n_\downarrow \rangle$ depending on which of these variables you want to treat as independent, is determined self-consistently. That explains the name of the approach, "Two-Particle-Self-Consistent". Since the the sum-rules are satisfied exactly, when we add them up the resulting equation, and hence the Pauli exclusion principle, will also be satisfied exactly. In other words, in Eq.(56.38) that follows from the Pauli exclusion

[1] The meaning of the superscripts differs from that in Ref. [255]. Superscripts (2) (1) here correspond respectively to (1) (0) in Ref. [255]

principle, we now have U_{sp} and U_{ch} on the left-hand side that arrange each other in such a way that there is no violation of the principle. In standard many-body theory, two-particle self-consistency is achieved in a much more complicated by solving parquet equations. [106, 32]

The ansatz Eq.(58.3) is inspired from the work of Singwi [219, 102] and was also found independently by M. R. Hedeyati and G. Vignale [90]. The whole procedure was justified in the previous Chapter. For now, let us just add a few physical considerations.

Since U_{sp} and U_{ch} are renormalized with respect to the bare value, one might have expected that one should use the dressed Green's functions in the calculation of $\chi_0(q)$. It is explained in appendix A of Ref.[255] that this would lead to a violation of the results $\chi^R_{sp}(\mathbf{q}=\mathbf{0},\omega)=0$ and $\chi^R_{ch}(\mathbf{q}=\mathbf{0},\omega)=0$. In the present approach, the f-sum rule

$$\int \frac{d\omega}{\pi}\omega\chi''_{ch,sp}(\mathbf{q},\omega) = \lim_{\eta\to 0} T\sum_{iq_n}\left(e^{-iq_n\eta}-e^{iq_n\eta}\right) iq_n\chi_{ch,sp}(\mathbf{q},iq_n) \quad (58.4)$$

$$= \frac{1}{N}\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}}-2\epsilon_{\mathbf{k}}\right)n_{\mathbf{k}\sigma} \quad (58.5)$$

is satisfied with $n_{\mathbf{k}\sigma}=n^{(1)}_{\mathbf{k}\sigma}$, the same as the Fermi function for the non-interacting case since it is computed from $\mathcal{G}^{(1)}$. [2] The right-hand side of the first line above is just the equal-time commutator calculated in imaginary time. The denominators containing U_{sp} or U_{ch} above, will lead to contributions to the sum that are of order $1/(iq_n)^2$ or higher, so that the convergence factor are not needed which means that they do not contribute. So, then only the contribution $\chi^{(1)}$ from the numerator contributes, which explains the result, which is essentially the non-interacting one where Luttinger's theorem is obviously satisfied.

Remark 324 *$U_{sp}\langle n_\uparrow\rangle\langle n_\downarrow\rangle = U\langle n_\uparrow n_\downarrow\rangle$ can be understood as correcting the Hatree-Fock factorization so that the correct double occupancy be obtained. Expressing the irreducible vertex in terms of an equal-time correlation function is inspired by the approach of Singwi [219] to the electron gas. But TPSC is different since it also enforces the Pauli exclusion principle and connects to a local correlation function, namely $\langle n_\uparrow n_\downarrow\rangle$.*

58.2 Mermin-Wagner, Kanamori-Brueckner

The functional form of the results that we found for spin and charge fluctuations have the RPA form but the renormalized interactions U_{sp} and U_{ch} must be computed from

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle \quad (58.6)$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)} = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2. \quad (58.7)$$

[2] For the conductivity with vertex corrections [27], the f-sum rule with $n_{\mathbf{k}\sigma}$ obtained from $G^{(2)}$ is satisfied.

With the *ansatz* Eq.(58.3), the above system of equations is closed and the Pauli exclusion principle is enforced. The first of the above equations is solved self-consistently with the U_{sp} ansatz. This gives the double occupancy $\langle n_\uparrow n_\downarrow \rangle$ that is then used to obtain U_{ch} from the next equation. The fastest way to numerically compute $\chi^{(1)}(q)$ is to use fast Fourier transforms [27].

These TPSC expressions for spin and charge fluctuations were obtained by enforcing the conservations laws and the Pauli exclusion principle. In particular, TPSC satisfies the f-sum rule Eq.(58.5). But we obtain for free a lot more of the physical results, namely Kanamori-Brueckner renormalization and the Mermin-Wagner theorem.

Let us begin with Kanamori-Brueckner renormalization of U. Many years ago, Kanamori in the context of the Hubbard model [112], and Brueckner in the context of nuclear physics, introduced the notion that the bare U corresponds to computing the scattering of particles in the first Born approximation. In reality, we should use the full scattering cross section and the effective U should be smaller. From Kanamori's point of view, the two-body wave function can minimize the effect of U by becoming smaller to reduce the value of the probability that two electrons are on the same site. The maximum energy that this can cost is the bandwidth since that is the energy difference between a one-body wave function with no nodes and one with the maximum allowed number. Let us see how this physics comes out of our results. Far from phase transitions, we can expand the denominator of the local moment sum-rule equation to obtain

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi^{(1)}(q)\left(1+\frac{1}{2}U_{sp}\chi^{(1)}(q)\right) = n - 2\frac{U_{sp}}{U}\langle n_\uparrow\rangle\langle n_\downarrow\rangle\,. \tag{58.8}$$

Since $\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_0(q) = n - 2\langle n_\uparrow\rangle\langle n_\downarrow\rangle$, we are can solve for U_{sp} and obtain [3].

$$U_{sp} = \frac{U}{1+\Lambda U} \tag{58.9}$$

$$\Lambda \equiv \frac{1}{n^2}\frac{T}{N}\sum_{iq_n}\sum_{\mathbf{q}}\left(\chi^{(1)}\right)^2(\mathbf{q},iq_n)\,. \tag{58.10}$$

We see that at large U, U_{sp} saturates to $1/\Lambda$, which in practice we find to be of the order of the bandwidth. For those that are familiar with diagrams, note that the Kanamori-Brueckner physics amounts to replacing each of the interactions U in the ladder or bubble sum for diagrams in the particle-hole channel by infinite ladder sums in the particle-particle channel [52]. This is not quite what we obtain here since $\left(\chi^{(1)}\right)^2$ is in the particle-hole channel, but in the end, numerically, the results are close and the Physics seems to be the same. One cannot make strict comparisons between TPSC and diagrams since TPSC is non-perturbative.

While Kanamori-Brueckner renormalization, or screening, is a quantum effect that occurs even far from phase transitions, when we are close we need to worry about the Mermin-Wagner theorem. To satisfy this theorem, approximate theories must prevent $\langle n_\uparrow n_\downarrow\rangle$ from taking unphysical values. This quantity is positive and bounded by its value for $U=\infty$ and its value for non-interacting systems, namely $0 \le \langle n_\uparrow n_\downarrow\rangle \le n^2/4$. Hence, the right-hand side of the local-moment sum-rule Eq.(58.6) is contained in the interval $\left[n, n-\frac{1}{2}n^2\right]$. To see how the Mermin-Wagner theorem is satisfied, write the self-consistency condition Eq.(58.6) in the form

$$\frac{T}{N}\sum_{q}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\chi^{(1)}(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle. \tag{58.11}$$

[3] There is a misprint of a factor of 2 in Ref. [255]. It is corrected in Ref.[58].

Consider increasing $\langle n_\uparrow n_\downarrow \rangle$ on the left-hand side of this equation. The denominator becomes smaller, hence the integral larger. To become larger, $\langle n_\uparrow n_\downarrow \rangle$ has to decrease on the right-hand side. There is thus negative feedback in this equation that will make the self-consistent solution finite. This, however, does not prevent the expected phase transition in three dimensions [59]. To see this, we need to look in more details at the phase space for the integral in the sum rule.

As we know from the spectral representation for χ,

$$\chi_{ch,sp}\left(\mathbf{q}, iq_n\right) = \int \frac{d\omega'}{\pi} \frac{\chi''_{ch,sp}\left(\mathbf{q},\omega'\right)}{\omega' - iq_n} = \int \frac{d\omega'}{\pi} \frac{\omega' \chi''_{ch,sp}\left(\mathbf{q},\omega'\right)}{\left(\omega'\right)^2 + \left(\omega_n\right)^2}. \tag{58.12}$$

the zero Matsubara frequency contribution is always the largest. There, we find the so-called Ornstein-Zernicke form for the susceptibility.

Ornstein-Zernicke form Let us focus on the zero Matsubara frequency contribution and expand the denominator near the point where $1-\frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0) = 0$. The wave vector $\mathbf{Q}$ is that where $\chi^{(1)}$ is maximum. We find [59],

$$\begin{aligned} \chi_{sp}\left(\mathbf{q}+\mathbf{Q}, \omega + i\eta\right) &\simeq \frac{\chi^{(1)}(\mathbf{Q},0)}{1 - \frac{1}{2}U_{sp}\chi^{(1)} - \frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}}{\partial\mathbf{Q}^2}q^2 - \frac{1}{2}U_{sp}\frac{\partial\chi^{(1)}}{\partial\omega}\omega} \\ &\sim \frac{\xi^2}{1+\xi^2 q^2 - i\omega/\omega_{sp}}, \end{aligned} \tag{58.13}$$

where all quantities in the denominator are evaluated at $(\mathbf{Q}, 0)$. On dimensional grounds,

$$-\frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}(\mathbf{Q},0)}{\partial\mathbf{Q}^2} \Big/ \left(1 - \frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0)\right)$$

scales (noted $\sim$) as the square of a length, ξ, the correlation length. That length is determined self-consistently. Since, $\omega_{sp} \sim \xi^{-2}$, all finite Matsubara frequency contributions are negligible if $2\pi T/\omega_{sp} \sim 2\pi T\xi^2 \gg 1$. That condition in the form $\omega_{sp} \ll T$ justifies the name of the regime we are interested in, namely the renormalized classical regime. The classical regime of a harmonic oscillator occurs when $\omega \ll T$. The regime here is "renormalized" classical because at temperatures above the degeneracy temperature, the system is a free classical gas. As temperature decreases below the Fermi energy, it becomes quantum mechanical, then close to the phase transition, it becomes classical again.

Substituting the Ornstein-Zernicke form for the susceptibility in the self-consistency relation Eq.(58.6), we obtain

$$T\int \frac{d^d\mathbf{q}}{(2\pi)^d} \frac{1}{q^2 + \xi^{-2}} = \widetilde{C} \tag{58.14}$$

where $\widetilde{C}$ contains non-zero Matsubara frequency contributions as well as $n - 2\langle n_\uparrow n_\downarrow \rangle$. Since $\widetilde{C}$ is finite, this means that in two dimensions ($d = 2$), it is impossible to have $\xi^{-2} = 0$ on the left-hand side otherwise the integral would diverge logarithmically. This is clearly a dimension-dependent statement that proves the Mermin-Wagner theorem. In two-dimensions, we see that the integral gives a logarithm that leads to

$$\xi \sim \exp\left(C'/T\right).$$

where in general, C' can be temperature dependent [59]. When C' is not temperature dependent, the above result is similar to what is found at strong coupling in the non-linear sigma model. The above dimensional analysis is a bit expeditive. A more careful analysis [165, 202] yields prefactors in the temperature dependence of the correlation length.

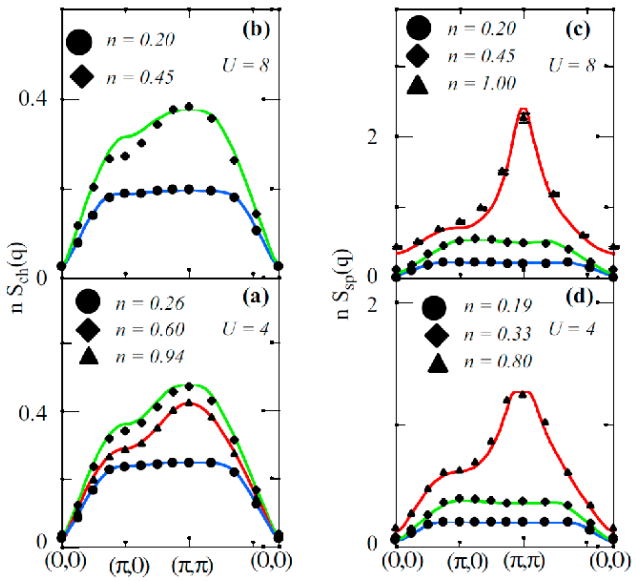


Figure 58-1 Wave vector $(\mathbf{q})$ dependence of the spin and charge structure factors for different sets of parameters. Solid lines are from TPSC and symbols are QMC data. Monte Carlo data for $n = 1$ and $U = 8t$ are for 6×6 clusters and $T = 0.5t$; all other data are for 8×8 clusters and $T = 0.2t$. Error bars are shown only when significant. From Ref. [245].

58.3 Benchmarking

Quantum Monte Carlo calculations, that we explain in a later Chapter of this book, can be considered exact within statistical sampling. Hence they can be used as benchmarks for any approximation scheme. In this section, we present a few benchmarks on spin and charge fluctuations, and then on self-energy. More comparisons may be found in Refs. [236] and [245, 255, 247, 129] and others quoted in these papers.

58.3.1 Spin and charge fluctuations

The set of TPSC equations for spin and charge fluctuations Eqs.(58.6,58.7,58.3) is rather intuitive and simple. The agreement of calculations with benchmark QMC calculations is rather spectacular, as shown in Fig.(58-1). There, one can see the results of QMC calculations of the structure factors, i.e. the Fourier transform of the equal-time charge and spin correlation functions, compared with the corresponding TPSC results.

This figure allows one to watch the Pauli exclusion principle in action. At $U = 4t$, Fig.(58-1a) shows that the charge structure factor does not have a monotonic dependence on density. This is because, as we approach half-filling, the spin fluctuations are becoming so large that the charge fluctuations have to decrease so that the sum still satisfies the Pauli exclusion principle, as expressed by Eq.(56.38). This kind of agreement is found even at couplings of the order of the bandwidth and when second-neighbor hopping t' is present [242, 243].

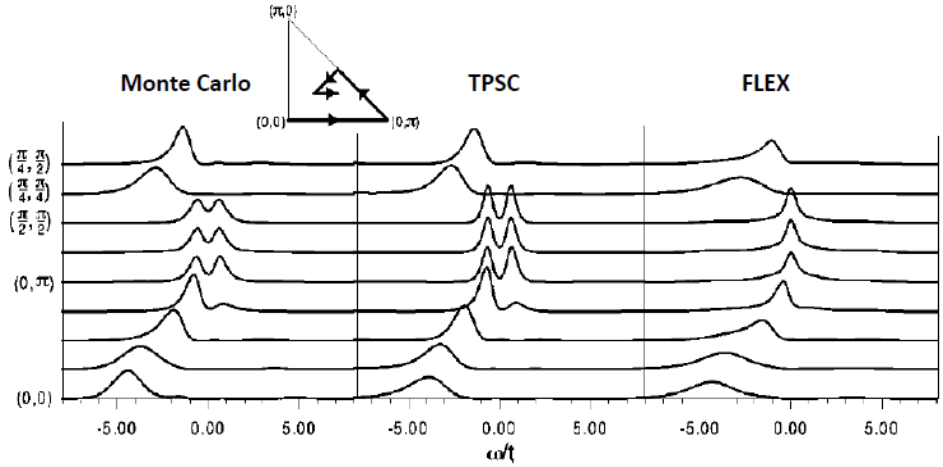
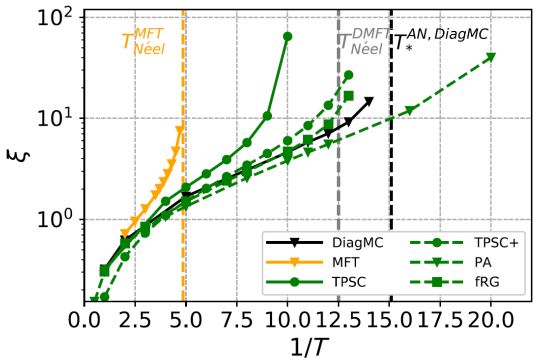


Figure 58-2 Single-particle spectral weight $A(\mathbf{k},\omega)$ for $U = 4$, $\beta = 5$, $n = 1$, and all independent wave vectors $\mathbf{k}$ of an 8×8 lattice. Results obtained from maximum entropy inversion of Quantum Monte Carlo data on the left panel, from TPSC in the middle panel and form the FLEX approximation on the right panel. (Relative error in all cases is about 0.3%). Figure from Ref.[168]

Remark 325 *Even though the entry in the renormalized classical regime is well described by TPSC [128], equation (58.3) for U_{sp} fails deep in that regime because $\Sigma^{(1)}$ becomes too different from the true self-energy. At $n = 1$, $t' = 0$, deep in the renormalized classical regime, U_{sp} becomes arbitrarily small, which is clearly unphysical. However, by assuming that $\langle n_\uparrow n_\downarrow \rangle$ is temperature independent below T_X, a property that can be verified from QMC calculations, one obtains a qualitatively correct description of the renormalized-classical regime. One can even drop the ansatz and take $\langle n_\uparrow n_\downarrow \rangle$ from QMC on the right-hand side of the local moment sum-rule Eq.(58.6) to obtain U_{sp}.*

58.3.2 Self-energy

We check that the formula for the self-energy Eq.(57.15) is accurate by comparing in Fig. 58-2 the spectral weight (imaginary part of the Green's function) obtained from Eq.(57.15) with that obtained from Quantum Monte Carlo calculations. The latter are exact within statistical accuracy and can be considered as benchmarks. The meaning of the curves are detailed in the caption. The comparison is for half-filling in a regime where the simulations can be done at very low temperature and where a non-trivial phenomenon, the pseudogap, appears. This all important phenomenon is discussed further below in subsection 59.1 and in the first case study, Sect. 59.2. In the third panel, we show the results of another popular Many-Body Approach, the FLuctuation Exchange Approximation (FLEX) [30]. It misses [63] the physics of the pseudogap in the single-particle spectral weight because it uses fully dressed Green's functions and assumes that Migdal's theorem applies, i.e. that the vertex does not need to be renormalized consequently Ref.[255, 163]. The same problem exists in the corresponding version of the GW approximation. [92]



Remark 326 *The dressing of one vertex in the second line of Fig. 57-1 means that we do not assume a Migdal theorem. Migdal's theorem arises in the case of electron-phonon interactions [142]. There, the small ratio m/M, where m is the electronic mass and M the ionic mass, allows one to show that the vertex corrections are negligible. This is extremely useful to formulate the Eliashberg theory of superconductivity.*

Remark 327 *In Refs. [255, 168] we used the notation $\Sigma^{(1)}$ instead of $\Sigma^{(2)}$. The notation of the present paper is the same as that of Ref. [8]*

58.3.3 TPSC+, Beyond TPSC

TPSC has been compared to a number of other state of the art methods in [208]. Fig. (58.3.3) for the Hubbard model at half-filling at $U = 2t$ shows the correlation length as a function of temperature. The DiagMC result can be considered exact. This is one of the cases where TPSC is at its worse. It is expected that it does not work in the renormalized classical regime. An improvement of TPSC, namely TPSC+ gives better results.

59. *ANTIFERROMAGNETISM CLOSE TO HALF-FILLING AND PSEUDOGAP IN TWO DIMENSIONS

We return to the normal state and look at the dominant instability in the half-filled case $n = 1$. In that case, the Fermi surface of the Hubbard model with nearest-neighbor hopping exhibits the phenomenon of nesting. For example, the Fermi surface in the two-dimensional case is a diamond, as illustrated in Fig. (?). All the points of the flat surfaces are connected by the same wave vector $\mathbf{Q} = (\pi, \pi)$ which leads to a very large susceptibility. Whereas at low filling the maximum susceptibility is at $q = 0$, in the present case it is a local maximum that is smaller than the maximum at $\mathbf{Q}$, as we will see.

Let us compute the spin susceptibility at that nesting wave vector. Nesting in the present case means that

$$\zeta_{\mathbf{p}+\mathbf{Q}} = -2t \left(\cos \left(k_x + \pi \right) + \cos \left(k_y + \pi \right) \right) = -\zeta_{\mathbf{p}}. \tag{59.1}$$

Using this result we find that the zero-frequency susceptibility at that wave vector $\mathbf{Q}$ is

$$\chi_0^R \left(\mathbf{Q}, 0 \right) = -\frac{2}{N} \sum_{\mathbf{p}} \frac{f\left(\zeta_{\mathbf{p}}\right) - f\left(\zeta_{\mathbf{p}+\mathbf{Q}}\right)}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{Q}}} = -\frac{2}{N} \sum_{\mathbf{p}} \frac{f\left(\zeta_{\mathbf{p}}\right) - f\left(-\zeta_{\mathbf{p}}\right)}{2\zeta_{\mathbf{p}}} \tag{59.2}$$

$$= \frac{1}{N} \sum_{\mathbf{p}} \frac{1 - 2f\left(\zeta_{\mathbf{p}}\right)}{\zeta_{\mathbf{p}}} = \int d\varepsilon N\left(\varepsilon\right) \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon}. \tag{59.3}$$

Assume that the density of states is a constant. For $\varepsilon \gg T$, we are integrating $1/\varepsilon$. However, for $\varepsilon < T$ the singularity in the denominator of the integrand is cutoff. In other words, we obtain a contribution that diverges at low temperature like $\ln\left(W/T\right)$ where W is the bandwidth. This means that at sufficiently low temperature, the criterion $1 - \frac{U}{2}\chi_0^R\left(\mathbf{Q}, 0\right) = 0$ will always be satisfied whatever the value of U and there will be a transition to a state characterized by the wave vector $\mathbf{Q}$. This is the antiferromagnetic state where spins alternate in direction from one site to the other. In two dimensions for example, the chemical potential at $n = 1$ sits right at a logarithmic van Hove singularity in $N\left(\varepsilon\right)$ so that in fact $\chi_0^R\left(\mathbf{Q}, 0\right)$ scales like $\ln^2\left(W/T\right)$, which is larger than the single power of ln that one would obtain at $q = 0$.

When there is no nesting, like when the next-nearest neighbor hopping t' contributes, the susceptibility does not diverge at low temperature. In that case, the transition will occur only if U is large enough.

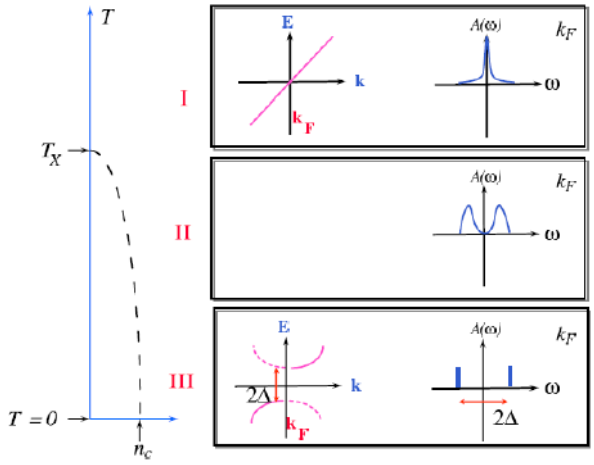


Figure 59-1 Cartoon explanation of the pseudogap due to precursors of long-range order. When the antiferromagnetic correlation length ξ becomes larger than the thermal de Broglie wavelength, there appears precursors of the $T = 0$ Bogoliubov quasi-particles for the long-range ordered antiferromagnet. This can occur only in the renormalized classical regime, below the dashed line on the left of the figure.

59.1 Pseudogap in the renormalized classical regime

When we compared TPSC with Quantum Monte Carlo simulations and with FLEX in Fig. 58-2 above, perhaps you noticed that at the Fermi surface, the frequency dependent spectral weight has two peaks instead of one. In addition, at zero frequency, it has a minimum instead of a maximum. That is called a pseudogap. A cartoon explanation [236] of this pseudogap is given in Fig. 59-1. At high temperature we start from a Fermi liquid, as illustrated in panel I. Now, suppose the ground state has long-range antiferromagnetic order as in panel III, in other words at a filling between half-filling and n_c. In the mean-field approximation we have a gap and the Bogoliubov transformation from fermion creation-annihilation operators to quasi-particles has weight at both positive and negative energies. In two dimensions, because of the Mermin-Wagner theorem, as soon as we raise the temperature above zero, long-range order disappears, but the antiferromagnetic correlation length ξ remains large so we obtain the pseudogap illustrated in panel II. As we will explain analytically below, the pseudogap survives as long as ξ is much larger than the thermal de Broglie wave length $\xi_{th} \equiv v_F/(\pi T)$ in our usual units. At the crossover temperature T_X, the relative size of ξ and ξ_{th} changes and we recover the Fermi liquid.

We now proceed to sketch analytically where these results come from starting from finite T. Details and more complete formulae may be found in Refs. [245, 247, 255, 246][1]. We begin from the TPSC expression (57.15) for the self-energy. Normally one has to do the sum over bosonic Matsubara frequencies first, but the zero Matsubara frequency contribution has the correct asymptotic behavior in fermionic frequencies iq_n so that, as in Sect.58.2, one can once more isolate on the right-hand side the contribution from the zero Matsubara frequency. In the

[1] Note also the following study from zero temperature [38]

renormalized classical regime then, we have [2]

$$\Sigma(\mathbf{k}_F, ik_n) \propto T \int q^{d-1} dq \frac{1}{q^2 + \xi^{-2}} \frac{1}{ik_n - \varepsilon_{\mathbf{k}_F+\mathbf{Q}+\mathbf{q}}} \tag{59.4}$$

where $\mathbf{Q}$ is the wave vector of the instability. This integral can be done analytically in two dimensions [255, 244]. But it is more useful to analyze limiting cases [247]. Expanding around the points known as hot spots where $\varepsilon_{\mathbf{k}_F+\mathbf{Q}} = 0$, we find after analytical continuation that the imaginary part of the retarded self-energy at zero frequency takes the form

$$\Sigma''^R(\mathbf{k}_F, 0) \propto -\pi T \int d^{d-1} q_\perp dq_{||} \frac{1}{q_\perp^2 + q_{||}^2 + \xi^{-2}} \delta(v'_F q_{||}) \tag{59.5}$$

$$\propto \frac{\pi T}{v'_F} \xi^{3-d}. \tag{59.6}$$

In the last line, we just used dimensional analysis to do the integral.

The importance of dimension comes out clearly [247]. In $d = 4$, $\Sigma''^R(\mathbf{k}_F, 0)$ vanishes as temperature decreases, $d = 3$ is the marginal dimension and in $d = 2$ we have that $\Sigma''^R(\mathbf{k}_F, 0) \propto \xi/\xi_{th}$ that diverges at zero temperature. In a Fermi liquid the quantity $\Sigma''^R(\mathbf{k}_F, 0)$ vanishes at zero temperature, hence in three or four dimensions one recovers the Fermi liquid (or close to one in $d = 3$). But in two dimensions, a diverging $\Sigma''^R(\mathbf{k}_F, 0)$ corresponds to a vanishingly small $A(\mathbf{k}_F, \omega = 0)$ as we can see from

$$A(\mathbf{k}, \omega) = \frac{-2\Sigma''^R(\mathbf{k}_F, \omega)}{(\omega - \varepsilon_{\mathbf{k}} - \Sigma'^R(\mathbf{k}_F, \omega))^2 + \Sigma''^R(\mathbf{k}_F, \omega)^2}. \tag{59.7}$$

Fig. 31 of Ref.[236] illustrates graphically the relationship between the location of the pseudogap and large scattering rates at the Fermi surface. At stronger U the scattering rate is large over a broader region, leading to a depletion of $A(\mathbf{k},\omega)$ over a broader range of $\mathbf{k}$ values.

Remark 328 *Note that the condition $\xi/\xi_{th} \gg 1$, necessary to obtain a large scattering rate, is in general harder to satisfy than the condition that corresponds to being in the renormalized classical regime. Indeed, $\xi/\xi_{th} \gg 1$ corresponds $T/v_F \gg \xi^{-1}$ while the condition $\omega_{sp} \ll T$ for the renormalized classical regime corresponds to $T \gg \xi^{-2}$, with appropriate scale factors, because ω_{sp} scales as ξ^{-2} as we saw in Eq. (58.13) and below.*

To understand the splitting into two peaks seen in Figs. 58-2 and 59-1 consider the singular renormalized contribution coming from the spin fluctuations in Eq. (59.4) at frequencies $\omega \gg v_F \xi^{-1}$. Taking into account that contributions to the integral come mostly from a region $q \leq \xi^{-1}$, one finds

$$\Sigma'^R(\mathbf{k}_F, \omega) = \left(T \int q^{d-1} dq \frac{1}{q^2 + \xi^{-2}} \right) \frac{1}{ik_n - \varepsilon_{\mathbf{k}_F+\mathbf{Q}}}$$

$$\equiv \frac{\Delta^2}{\omega - \varepsilon_{\mathbf{k}_F+\mathbf{Q}}} \tag{59.8}$$

which, when substituted in the expression for the spectral weight (59.7) leads to large contributions when

$$\omega - \varepsilon_{\mathbf{k}} - \frac{\Delta^2}{\omega - \varepsilon_{\mathbf{k}_F+\mathbf{Q}}} = 0 \tag{59.9}$$

[2] This formula is similar to one that appeared in Ref.[131]

or, equivalently,

$$\omega = \frac{(\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}_F+\mathbf{Q}}) \pm \sqrt{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}_F+\mathbf{Q}})^2 + 4\Delta^2}}{2}, \tag{59.10}$$

which, at $\omega = 0$, corresponds to the position of the hot spots[3]. At finite frequencies, this turns into the dispersion relation for the antiferromagnet [209].

It is important to understand that analogous arguments hold for any fluctuation that becomes soft because of the Mermin-Wagner theorem,[255, 60] including superconducting ones [255, 7, 126]. The wave vector $\mathbf{Q}$ would be different in each case.

To understand better when Fermi liquid theory is valid and when it is replaced by the pseudogap instead, it is useful to perform the calculations that lead to $\Sigma''^R(\mathbf{k}_F, 0) \propto \xi/\xi_{th}$ in the real frequency formalism. The details may be found in Appendix D of Ref. [255].

59.2 Pseudogap in electron-doped cuprates

High-temperature superconductors are made of layers of CuO_2 planes. The rest of the structure is commonly considered as providing either electron or hole doping of these planes depending on chemistry. At half-filling, or zero-doping, the ground state is an antiferromagnet. As one dopes the planes, one reaches a doping, so-called optimal doping, where the superconducting transition temperature T_c is maximum. Let us start from optimal hole or electron doping and decrease doping towards half-filling. That is the underdoped regime. In that regime, one observes a curious phenomenon, the pseudogap. What this means is that as temperature decreases, physical quantities behave as if the density of states near the Fermi level was decreasing. Finding an explanation for this phenomenon has been one of the major challenges of the field [229, 175].

To make progress, we need a microscopic model for high-temperature superconductors. Band structure calculations [9, 186] reveal that a single band crosses the Fermi level. Hence, it is a common assumption that these materials can be modeled by the one-band Hubbard model. Whether this is an oversimplification is still a subject of controversy [189, 135, 191, 218, 140, 87]. Indeed, spectroscopic studies [51, 189] show that hole doping occurs on the oxygen atoms. The resulting hole behaves as a copper excitation because of Zhang-Rice [259] singlet formation. In addition, the phase diagram [215, 143, 3, 2, 89, 113] and many properties of the hole-doped cuprates can be described by the one-band Hubbard model. Typically, the band parameters that are used are: nearest-neighbor hopping $t = 350$ to 400 meV and next-nearest-neighbor hopping $t' = -0.15$ to $-0.3t$ depending on the compound [9, 186]. Third-nearest-neighbor hopping $t'' = -0.5t'$ is sometimes added to fit finer details of the band structure [186]. The hoppings beyond nearest-neighbor mean that particle-hole symmetry is lost even at the band structure level.

In electron-doped cuprates, the doping occurs on the copper, hence there is little doubt that the single-band Hubbard model is even a better starting point in this case. Band parameters [155] are similar to those of hole-doped cuprates. It is sometimes claimed that there is a pseudogap only in the hole-doped cuprates. The origin of the pseudogap is indeed probably different in the hole-doped cuprates.

[3] For comparisons with paramagnon theory see [205].

But even though the standard signature of a pseudogap is absent in nuclear magnetic resonance [261] (NMR) there is definitely a pseudogap in the electron-doped case as well [17], as can be seen in optical conductivity [180] and in Angle Resolved Photoemission Spectroscopy (ARPES) [18]. As we show in the rest of this section, in electron-doped cuprates strong evidence for the origin of the pseudogap is provided by detailed comparisons of TPSC with ARPES as well as by verification with neutron scattering [167] that the TPSC condition for a pseudogap, namely $\xi > \xi_{th}$, is satisfied. The latter length makes sense from weak to intermediate coupling when quasi-particles exist above the pseudogap temperature. In strong coupling, i.e. for values of U larger than that necessary for the Mott transition, there is evidence that there is another mechanism for the formation of a pseudogap. This is discussed at length in Refs. [216, 88] [4]. The recent discovery [222] that at sufficiently large U there is a first order transition in the paramagnetic state between two kinds of metals, one of which is highly anomalous, gives a sharper meaning to what is meant by strong-coupling pseudogap.

Let us come back to modeling of electron-doped cuprates. Evidence that these are less strongly coupled than their hole-doped counterparts comes from the fact that a) The value of the optical gap at half-filling, ~ 1.5 eV, is smaller than for hole doping, ~ 2.0 eV [231]. b) In a simple Thomas-Fermi picture, the screened interaction scales like $\partial\mu/\partial n$. Quantum cluster calculations [216] show that $\partial\mu/\partial n$ is smaller on the electron-doped side, hence U should be smaller. c) Mechanisms based on the exchange of antiferromagnetic calculations with U/t at weak to intermediate coupling [31, 129] predict that the superconducting T_c increases with U/t. Hence T_c should decrease with increasing pressure in the simplest model where pressure increases hopping t while leaving U essentially unchanged. The opposite behavior, expected at strong coupling where $J = 4t^2/U$ is relevant [113, 119], is observed in the hole-doped cuprates. d) Finally and most importantly, there is detailed agreement between TPSC calculations [127, 88, 236] and measurements such as ARPES [18, 156], optical conductivity [180] and neutron [167] scattering.

To illustrate the last point, consider Fig. 59-2 that compares TPSC calculations with experimental results for ARPES. Apart from a tail in the experimental results, the agreement is striking. [5]. In particular, if there was no interaction, the Fermi surface would be a line (red) on the momentum distribution curve (MDC). Instead, it seems to disappear at symmetrical points displaced from $(\pi/2, \pi/2)$. These points, so-called hot spots, are linked by the wave vector (π, π) to other points on the Fermi surface. This is where the antiferromagnetic gap would open first if there was long-range order. The pull back of the weight from $\omega = 0$ at the hot spots is close to the experimental value: 100 meV for the 15% doping shown, and 300 meV for 10% doping (not shown). More detailed ARPES spectra and comparisons with experiment are shown in Ref. [236]. The value of the temperature T^* at which the pseudogap appears [127] is also close to that observed in optical spectroscopy [180]. In addition, the size of the pseudogap is about ten times T^* in the calculation as well as in the experiments. For optical spectroscopy, vertex corrections (see Sect. **??**) have to be added to be more quantitative. Experimentally, the value of T^* is about twice the antiferromagnetic transition temperature up to $x = 0.13$. That can be obtained [127] by taking $t_z = 0.03t$ for hopping in the third direction. Recall that in strictly two dimensions, there is no long-range order. Antiferromagnetism appears on a much larger range of dopings for electron-doped than for hole-doped cuprates.

These TPSC calculations have predicted the value of the pseudogap temperature at $x = 0.13$ before it was observed experimentally [156] by a group unaware

[4] See also conclusion of Ref.[236].

[5] Such tails tend to disappear in more recent laser ARPES measurements on hole-doped compounds [118].

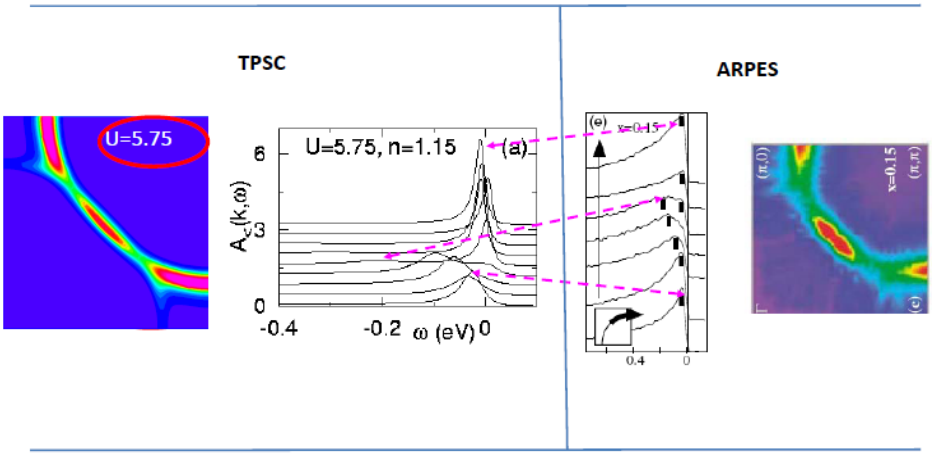
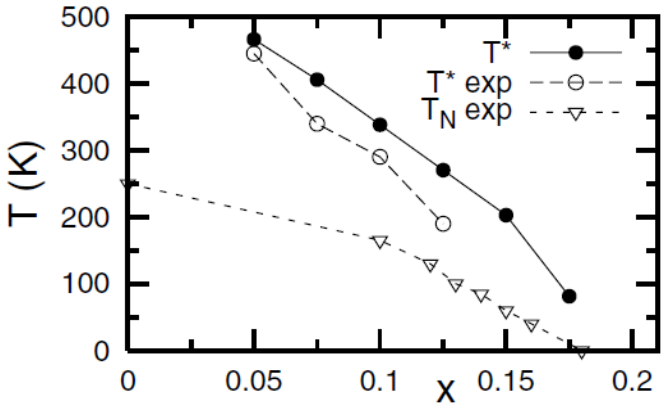


Figure 59-2 On the left, results of TPSC calculations [127, 236] at optimal doping, $x = 0.15$, corresponding to filling 1.15, for $t = 350$ meV, $t' = -0.175t$, $t_J = 0.05t$, $U = 5.75t$, $T = 1/20$. The left-most panel is the magnitude of the spectral weight times a Fermi function, $A(\mathbf{k},\omega) f(\omega)$ at $\omega = 0$, so-called momentum-distribution curve (MDC). Red (dark black) indicates larger value and purple (light grey) smaller value. The next panel is $A(\mathbf{k},\omega) f(\omega)$ for a set of fixed $\mathbf{k}$ values along the Fermi surface. These are so-called energy-dispersion curves (EDC). The two panels to the right are the corresponding experimental results [18] for $Nd_{2-x}Ce_xCuO_4$. Dotted arrows show the correspondence between TPSC and experiment.

of the theoretical prediction in Fig.59.2. In addition, the prediction that ξ should scale like ξ_{th} at the pseudogap temperature has been verified in neutron scattering experiments [167] in the range $x = 0.04$ to $x = 0.15$. The range of temperatures and doping explored in that work is shown in Fig. 59.2. Note that the antiferromagnetic phase boundary, that occurs here because of coupling in the third dimension, is at a location different from earlier estimates that appear in Fig. 59.2. However, the location of the pseudogp temperature has not changed. At the doping that corresponds to optimal doping, T^* becomes of the order of 100 K, more than four times lower than at $x = 0.04$. The antiferromagnetic correlation length ξ beyond optimal doping begins to decrease and violate the scaling of ξ with ξ_{th}. In that doping range, T^* and the superconducting transition temperature are close. Hence it is likely that there is interference between the two phenomena [42], an effect that has not yet been taken into account in TPSC.

An important prediction that one should verify is that inelastic neutron scattering will find over-damped spin fluctuations in the pseudogap regime and that the characteristic spin fluctuation energy will be smaller than k_BT whenever a pseudogap is present. Equality should occur above T^*.

Finally, note that the agreement found in Fig. 59-2 between ARPES and TPSC is for $U \sim 6t$. At smaller values of U the antiferromagnetic correlations are not strong enough to produce a pseudogap in that temperature range. For larger U, the weight near $(\pi/2, \pi/2)$ disappears, in disagreement with experiments. The same value of U is found for the same reasons in strong coupling calculations with Cluster Perturbation Theory (CPT) [216] and with slave boson methods [257]. Recent first principle calculations [250] find essentially the same value of U. In that approach, the value of U is fixed, whereas in TPSC it was necessary to increase U by about 10% moving towards half-filling to get the best agreement with experiment. In any case, it is quite satisfying that weak and strong coupling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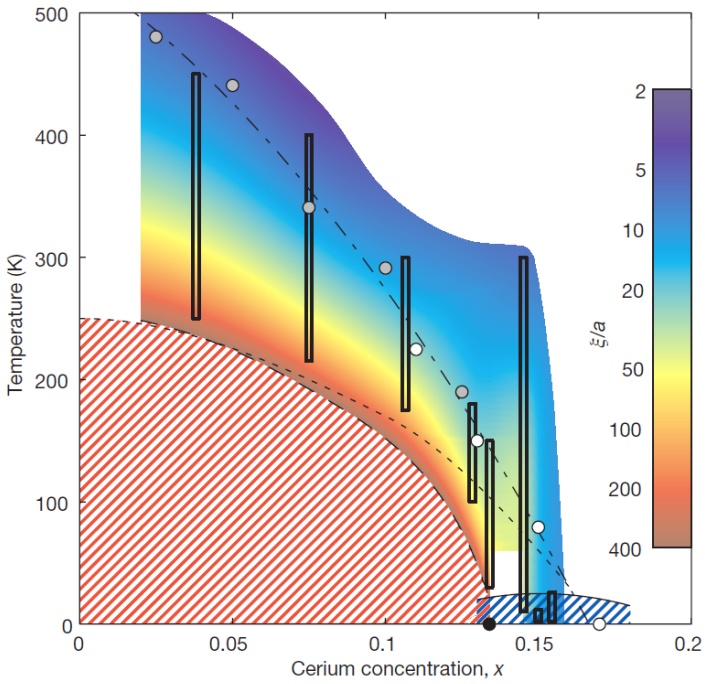
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methods agree on the value of U for electron-doped cuprates. This value of U is very near the critical value for the Mott transition at half-filling [185]. Hence, antiferromagnetic fluctuations at finite doping can be very well described by Slater-like physics (nesting) in electron-doped cuprates.

For recent calculations including the effect of the third dimension on the pseudogap see [211]. Finally, note that the analog of the above mechanism for the pseudogap has also been seen in two-dimensional charge-density wave dichalcogenides [39].

60. DYNAMICAL MEAN-FIELD THEORY AND MOTT TRANSITION-I

In this Chapter, we will see a physically motivated derivation of dynamical mean-field theory and discuss the results found by this method on the Mott transition. A more rigorous approach to the derivation will appear later in this book. There are many review articles. We quote from Ref.[103] amongs others.

The band picture of electrons explained very well the occurence of metals, with bands that are unfilled, and insulators, with filled bands. De Boer and Verwey (1937) reported that many transition-metal oxides with a partially filled d-electron band were exceptions. They were often poor conductors and indeed often insulators. NiO became the prototypical example. following their report, Peierls (1937) pointed out the importance of the electron-electron correlation: According to Mott (1937), Peierls noted

> "it is quite possible that the electrostatic interaction between the electrons prevents them from moving at all. At low temperatures the majority of the electrons are in their proper places in the ions. The minority which have happened to cross the potential barrier find therefore all the other atoms occupied, and in order to get through the lattice have to spend a long time in ions already occupied by other electrons. This needs a considerable addition of energy and so is extremely improbable at low temperatures."

Peierls is explaining that at half-filling, every unit cell is occupied by one carrier in the presence of strong Coulomb repulsion. And the electrons cannot move because of the large Coulomb repulsion it would cost. Later, Slater found another way to obtain an insulator at half-filling even when Coulomb interactions are weak. This is when long-range antiferromagnetic order leads to a doubling of the unit cell. We have already seen in the previous Chapter that perfect nesting could lead to a diverging antiferromagnetic susceptibility, and hence to a phase transition with arbitrarily weak interaction. In that case, the Brillouin zone becomes half the size so the band split in two and the lower band is now full. The Mott insulator and the antiferromagnetic insulator are conceptually very different. One has long-range order while the other does not.

In the 1970's vanadium oxide became an example of a material showing a Mott transition. The phase diagram appears in Fig. 60. The substitution of vanadium by another metal with d electrons is modeled here as pressure. The accuracy of this hypothesis is confirmed by real pressure experiments that appear on the same plot (see the top and bottom horizontal axis). Pressure increases the overlap between orbitals, hence the kinetic energy and tends to delocalize electrons. We see on this phase diagram a finite temperature first order transition between a metal and an insulator without long-range order. This material has a three-dimensional lattice structure.

Layered organic conductors are quasi two-dimensional materials with a half-filled band. These are soft materials, so one can apply pressure and have a sizeable effect on the electronic structure. One observes a first-order metal-insulator transition at high-temperature that ends at a critical point. For both materials there

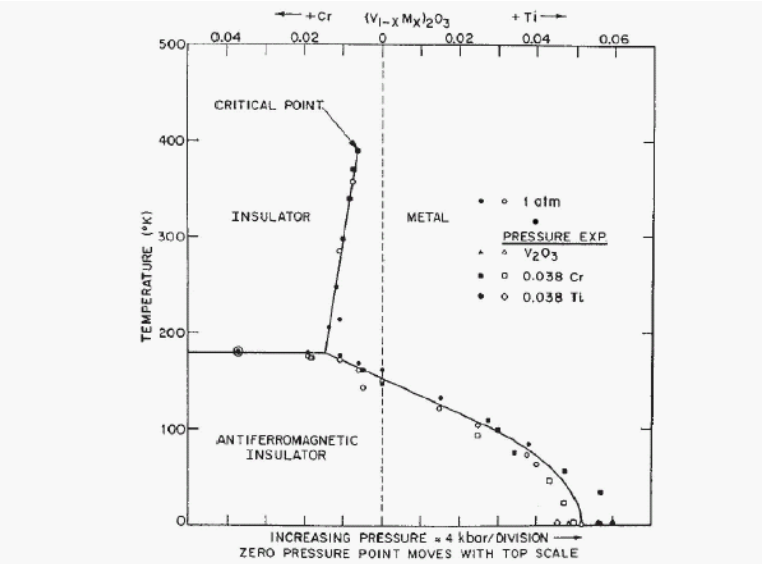


Figure: McWhan, PRB 1970; Limelette, Science 2003

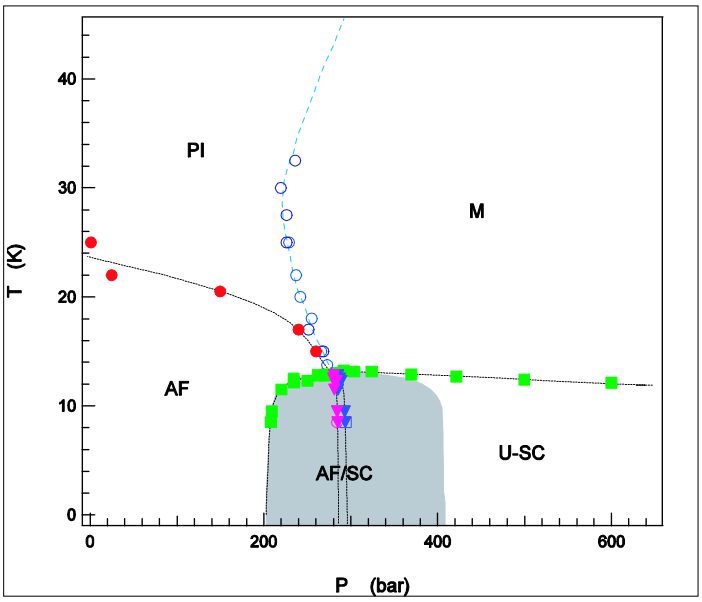
is an antiferromagnetic phase at low temperature, suggesting the importance of electron-electron interactions.

Simple pictures of the Mott transition have been proposed. In the Brinkman-Rice scenario, the effective mass becomes infinite at the Mott transition. In the Mott picture, at large interaction and half-filling, the non-interacting band splits in two and there is an empty and a filled band, so no conduction. As the interaction strenght decreases, a metallic phase occurs when the bands overlap.

The modern view of this transition contains a bit of both of the above ideas. That view emerges from dynamical mean-field theory, that we explain in this Chapter. This theory was discovered after Vollhardt and Metzner proposed and exact solution for the Hubbard model in infinite dimension. Georges and Kotliar and independently Jarrell arrived at the same theory. I begin by an example in classical statistical mechanics where mean-field theory is exact. Before the contribution of Metzner and Vollhardt, there was no known limit where a mean-field theory for a quantum system becomes exact. The mean-field in that case is a function of frequency, not a single number. We will argue that in infinite dimension the self-energy depends only on frequency. This allows a mapping to the co-called Anderson impurity model, where a single site with a Hubbard interaction is connected to a bath of non-interacting electrons. When this model can be solved, dynamical mean-field theory establishes a self-consistency relation with the infinite system.

60.1 A simple example of a model exactly soluble by mean-field theory

Let us forget momentarily about quantum mechanics and consider a simpler problem of classical statistical mechanics. Mean-field theory is often taken as an ap-



proximate solution to a model. It can also be formulated as an exact solution of a different model. That helps understand the content of mean-field theory.

Mean-field theory is the exact solution of the following infinite-range Ising model

$$H = -\frac{1}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 - h\sum_i S_i. \tag{60.1}$$

with $S_i = \pm 1$. We have chosen the exchange $J = 1$. The range of the interaction is extremely weak in the thermodynamic limit. The $1/N$ normalisation is necessary to have an energy that is extensive, i.e. proportional to the number of sites. In the usual Ising model, a given site interacts only with its neighbors so the energy is clearly extensive.

To compute the partition function, we use the Hubbard-Stratonovich transformation that represents $e^{-\beta H}$ as a Gaussian integral

$$e^{\left[\frac{\beta}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 + \beta h \sum_i S_i\right]} = \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{\left[-\frac{\beta N}{2}\lambda^2 + \beta(\lambda+h)\sum_i S_i\right]}. \tag{60.2}$$

The result can be checked by completing the square. Then, the partition function can be computed easily

$$\begin{aligned} Z &= \sum_{\{S_i\}} e^{-\beta H} \\ &= \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-\frac{\beta N}{2}\lambda^2} \left[2\cosh\left(\beta\left(\lambda+h\right)\right)\right]^N \\ &= \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-N\beta F(\lambda)} \end{aligned} \tag{60.3}$$

where

$$F\left(\lambda\right) = \frac{\lambda^2}{2} - \frac{1}{\beta}\ln\left[2\cosh\left(\beta\left(\lambda+h\right)\right)\right]. \tag{60.4}$$

Because $N \to \infty$, we can evaluate the integral by steepest descent and the free energy per site is given by

$$f(h) = \min_{\lambda} F(\lambda) + O\left(\frac{1}{N}\right). \tag{60.5}$$

The value of λ which minimizes F has the meaning of magnetization density. Indeed, $\partial F/\partial\lambda = 0$ leads to

$$\lambda = \tanh[\beta(\lambda + h)] \tag{60.6}$$

and using the previous result,

$$m = \left(\frac{\partial F}{\partial h}\right)_{\lambda} = \tanh[\beta(\lambda + h)] = \lambda. \tag{60.7}$$

This is what is found in mean-field theory.

60.2 Mean-field theory in classical physics

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60.3 The self-energy is independent of momentum in infinite dimension

It took a long time to find a variant of the Hubbard model that could be solved by a mean-field theory. That the Hubbard model was exactly soluble in infinite dimension was discovered by Metzner and Vollhardt [160]. Georges and Kotliar [77] and Jarrell [107] found that is was possible to formulate a mean-field theory based on these ideas. The key result is that in infinite dimension, the self-energy depends only on frequency. This is sharp contrast with the TPSC results where we saw that in two dimensions, the spatial dependence of the self-energy is very important. Hot spots appear along the Fermi surface. However, we also saw that the imaginary part of the self-energy at the hot spots vanishes at $T = 0$ in four or more dimensions since we found $\Sigma''(\mathbf{k}_F, 0) \sim T\xi^{3-d}/v_F$. So, since the hot spots disappear, it is likely that the self-energy is not momentum dependent anymore. That is what I proceed to show more rigorously here.

First we need to formulate the Hubbard model in such a way that in infinite dimension it gives a non-trivial and physical result, somewhat in the way that we did for the Ising model above. The possibly troublesome term is the kinetic energy. Consider the value of $\left\langle c^{\dagger}_{i\sigma} c_{j\sigma} \right\rangle$ for nearest neighbors. In the ground state, that quantity can be interpreted as the matrix element $\langle \psi_{i\sigma} | \psi_{j\sigma} \rangle$ where $|\psi_{j\sigma}\rangle$ is the ground state with one less particle at site j and $\langle \psi_{i\sigma}|$ the ground state where we remove a particle at site i (think of $c^{\dagger}_{i\sigma}$ acting to the left bra). Hence $|\langle \psi_{i\sigma} | \psi_{j\sigma} \rangle|^2$ is the probability for a particle to go from j to i. It has to scale like $1/d$ if we want particle-number to be conserved. This means that $\left\langle c^{\dagger}_{i\sigma} c_{j\sigma} \right\rangle$ scales as $1/\sqrt{d}$

so if we want a finite number for the kinetic energy, we need to multiply t by $\sqrt{d}$. Taking into account that there are Z neighbors, with $Z = 2d$ for a hypercubic lattice, we need an additional factor of $1/d$. The kinetic energy in the end is thus written as

$$E_{kin} = -\left(t^*\sqrt{d}\right)\frac{1}{d}\sum_{\langle i,j\rangle}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right). \tag{60.8}$$

The interaction term does not need to be scaled since it is local. The quantity $t^*/\sqrt{d}$ thus plays the role of the usual t entering the kinetic energy, with t^* finite in the $d \to \infty$ limit

We can find the same result by requiring that the bandwidth remains finite in the infinite dimensional limit. Consider the single-particle density of states

$$N(\omega) = \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\ldots\int_{-\pi}^{\pi}\frac{dk_d}{2\pi}\delta\left(\omega - \varepsilon_1 - \varepsilon_2 - \ldots\varepsilon_d\right) \tag{60.9}$$

with $\varepsilon_i = -2t\cos k_i$. This has the structure of a probability density for a variable that is the sum of identically distributed statistically independent variables. One can make the change of variables from $P(k_i) = 1/(2\pi)$ to $P(\varepsilon_i)$ so that

$$N(\omega) = \int d\varepsilon_1\int d\varepsilon_2\ldots\int d\varepsilon_d P(\varepsilon_1)P(\varepsilon_2)\ldots P(\varepsilon_d)\,\delta\left(\omega - \varepsilon_1 - \varepsilon_2 - \ldots\varepsilon_d\right). \tag{60.10}$$

The resulting probability density is a Gaussian with mean zero since $\int d\varepsilon_1 P(\varepsilon_1)\varepsilon_1 = 0$ and variance $2t^2d$ because $\int d\varepsilon_1 P(\varepsilon_1)\varepsilon_1^2 = \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\left(2t\cos(k_1)\right)^2 = (2t)^2/2$. More specifically,

$$N(\omega) = \frac{1}{\sqrt{2\pi(2t)^2 d}}\exp\left[-\left(\frac{\omega}{2t\sqrt{d}}\right)^2\right]. \tag{60.11}$$

This means that in the limit $d \to \infty$, we need to choose

$$t = t^*/\sqrt{d}$$

with t^* finite if we want a density of states with a finite width in that limit. In the same way that we had to take an effective exchange interaction smaller in our Ising model example, here we need to take an effective hopping that is smaller, $t^*/\sqrt{d}$, in the infinite dimensional limit.

The fact that $\left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle$ scales as $1/\sqrt{d}$ in the $d \to \infty$ limit has important consequences on the self energy. Indeed, $\mathcal{G}$ will also scale as $1/\sqrt{d}$. Hence, if we consider the real space expression for Σ_{12} where 1 and 2 are near-neighbor sites, then apart from the Hartree-Fock term that arises in first order perturbation theory, we find from second order that the contribution is proportional to $\mathcal{G}^3_{1,2}$ which is proportional to $1/d^{3/2}$. There is an additional factor $1/\sqrt{d}$ in the Green's function every time the distance increases by one so Σ_{ij} for more distant ij is even smaller. In the end, this means that the self-energy depends only on frequency.

60.4 The dynamical mean-field self-consistency relation, derivation 1

Suppose we start from the premise that the self-energy is purely local, namely that it is calculated with diagrams where only the local self-consistent Green's function

comes in the calculation. Suppose we can solve this problem, either by summing all diagrams or by some other method. Since we have proven that in infinite dimension the exact self-energy for the lattice has only frequency dependence, we take the impurity self-energy as the self-energy for the lattice. In other words, the Green's function on the infinite lattice reads in Fourier-Matsubara space

$$\mathcal{G}\left(\mathbf{k},ik_n\right)=\frac{1}{ik_n-\left(\varepsilon_{\mathbf{k}}-\mu\right)-\Sigma\left(ik_n\right)}. \tag{60.12}$$

It is clear that with the appropriate Fourier transform of the lattice Green's function we obtain the Green's function on a single site:

$$\begin{aligned}\mathcal{G}_{ii}\left(ik_n\right) &= \int\frac{d^d\mathbf{k}}{\left(2\pi\right)^d}\frac{1}{ik_n-\left(\varepsilon_{\mathbf{k}}-\mu\right)-\Sigma\left(ik_n\right)}\\ &= \int\frac{d^d\mathbf{k}}{\left(2\pi\right)^d}\int d\varepsilon\delta\left(\varepsilon-\left(\varepsilon_{\mathbf{k}}-\mu\right)\right)\frac{1}{ik_n-\varepsilon-\Sigma\left(ik_n\right)}\\ &= \int d\varepsilon N\left(\varepsilon\right)\frac{1}{ik_n-\varepsilon-\Sigma\left(ik_n\right)}.\end{aligned} \tag{60.13}$$

That is the only Green's function that is involved in the calculation of the self-energy. Suppose now that we compute the self-energy with that Green's function. When we substitute that self-energy back into the Green's function for the infinite lattice and project it back on a single site, as in Eq. (60.13) above, it is possible that we do not find the $\mathcal{G}_{ii}\left(ik_n\right)$ that we started with. This means that we need to modify it until self-consistency is achieved. This is not the way it is done in practice, although new methods exist to obtain the self-energy directly from $\mathcal{G}_{ii}\left(ik_n\right)$, so it could be done in principle.

The question we have not answered, is how, given $\mathcal{G}_{ii}\left(ik_n\right)$, do we find the self-energy if we do not have these recent methods available to us? Suppose we can write the new $\mathcal{G}_{ii}\left(ik_n\right)$ obtained with the self-energy in the following form

$$\mathcal{G}_{ii}^{-1}\left(ik_n\right)=\left(\mathcal{G}_{ii}^{0}\left(ik_n\right)\right)^{-1}-\Sigma\left(ik_n\right). \tag{60.14}$$

In this form, it is $\mathcal{G}_{ii}^{0}\left(ik_n\right)$ that we need to modify before starting the next iteration. If we want to use perturbative methods in terms of an unperturbed Green's function, it is $\mathcal{G}_{ii}^{0}\left(ik_n\right)$ that we need. It is not clear at this point that this last equation is correct or that we can do that.

And in practice, how do we do we find the self-energy and how do we do this iteration? The answer is that it suffices to solve a single-impurity Anderson model with the same U as the Hubbard model. That allows us to take advantage of a whole set of methods that have been developed to solve that model. But what is the Anderson impurity model? This is the subject of the next section.

Remark 329 *The DMFT equations may also be found by looking for a lattice propagator with a frequency-dependent self-energy Σ that is such that the effective medium self-energy is zero. The effective medium self-energy will be calculated from all diagrams that involve only propagators beginning and ending on the same site. This is like mean-field but going beyond Hartree-Fock for the calculation of the self-energy of the residual interactions. That self-energy is like that of a quantum-impurity problem with a $\mathcal{G}_{ff}$ obtained from the lattice. See the discussion in the section on Eliashberg equations.*

Remark 330 *There are many methods to find the solution to the single-impurity Anderson model. Here is a partial list (To come ???)*

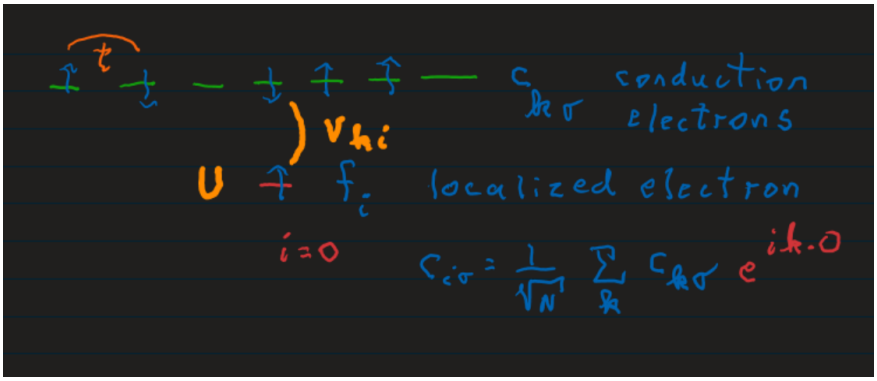


Figure 60-1 Anderson impurity model. There is a conduction band of non-interacting electrons, a localized site located at $i = 0$ that is hybridized to the conduction band.

60.5 Quantum impurities: The Anderson impurity model

The problem of a single site with a Hubbard interaction, connected to a bath of non-interacting electrons is the so-called Anderson impurity model. It is a generalization of the static single-impurity problem that we saw in an exercice. Its self-energy depends only on frequency. Since in infinite dimension the self-energy depends only on frequency, this will allow us to find a mapping between the single-impurity Anderson model and the DMFT approximation to the lattice problem. I will only set up the problem of quantum impurities without solving it. The Numerical Renormalization Group approach (NRG) Density Matrix Renormalization Group and continuous-time quantum Monte-Carlo methods are examples of approaches that can be used to solve this problem.

Including the chemical potential, the model is defined by

$$K_I = H_f + H_c + H_{fc} - \mu N \tag{60.15}$$

$$K_f \equiv \sum_\sigma (\varepsilon - \mu) f^\dagger_{i\sigma} f_{i\sigma} + U \left(f^\dagger_{i\uparrow} f_{i\uparrow}\right)\left(f^\dagger_{i\downarrow} f_{i\downarrow}\right) \tag{60.16}$$

$$K_c \equiv \sum_\sigma \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{60.17}$$

$$H_{fc} \equiv \sum_\sigma \sum_{\mathbf{k}} \left(V_{\mathbf{k}i} c^\dagger_{\mathbf{k}\sigma} f_{i\sigma} + V^*_{\mathbf{k}i} f^\dagger_{i\sigma} c_{\mathbf{k}\sigma}\right) \tag{60.18}$$

To physically motivate this model, think of a single f level on an atom where the on-site interaction is very large. That site is hybridized through $V_{\mathbf{k}i}$ with conduction electrons around it. The sum over $\mathbf{k}$ in the hybridization part of the Hamiltonian H_{fc} basically tells us that it is the local overlap of the conduction band with the impurity that produces the coupling.

Suppose we want to know the properties of the impurity, such as the local density of states. It can be obtained from the Green function

$$\mathcal{G}_{ff}(\tau) = -\left\langle T_\tau f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. \tag{60.19}$$

We will proceed with the equations of motion method, following steps analogous to those in the exercise on non-interacting impurities. We first write the equations

of motion for $c_{\mathbf{k}\sigma}$ and $f_{i\sigma}$

$$\begin{aligned}
\frac{\partial}{\partial\tau}c_{\mathbf{k}\sigma} &= [K_I, c_{\mathbf{k}\sigma}] && (60.20)\\
&= -(\varepsilon_{\mathbf{k}}-\mu)\,c_{\mathbf{k}\sigma} - V_{\mathbf{k}i}f_{i\sigma} && (60.21)\\
\frac{\partial}{\partial\tau}f_{i\sigma} &= [K_I, f_{i\sigma}] && (60.22)\\
&= -(\varepsilon-\mu)\,f_{i\sigma} - Uf^{\dagger}_{i-\sigma}f_{i-\sigma}f_{i\sigma} - \sum_{\mathbf{k}} V^{*}_{\mathbf{k}i}c_{\mathbf{k}\sigma} && (60.23)
\end{aligned}$$

Proceeding like our in our earlier derivation of the equations of motion we have

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{ff}(\tau) &= -\delta(\tau)\left\langle\left\{f_{i\sigma}(\tau), f^{\dagger}_{i\boldsymbol{\sigma}}\right\}\right\rangle\\
&\quad -\left\langle T_\tau\left(-(\varepsilon-\mu)\,f_{i\sigma}(\tau) - Uf^{\dagger}_{i-\sigma}(\tau)\,f_{i-\sigma}(\tau)\,f_{i\sigma}(\tau) - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}i}c_{\mathbf{k}\sigma}\right)f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle \quad (60.24)\\
&= -\delta(\tau) - (\varepsilon-\mu)\,\mathcal{G}_{ff}(\tau) + U\left\langle T_\tau f^{\dagger}_{i-\sigma}(\tau)\,f_{i-\sigma}(\tau)\,f_{i\sigma}(\tau)\,f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}i}\mathcal{G}_{cf}(\mathbf{k},i,\tau)
\end{aligned}$$

where we defined

$$\mathcal{G}_{cf}(\mathbf{k},i,\tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau)\,f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle. \quad (60.25)$$

To eliminate this quantity, we write its equations of motion

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{cf}(\mathbf{k},i,\tau) &= -\delta(\tau)\left\langle\left\{c_{\mathbf{k}\sigma}(\tau), f^{\dagger}_{i\boldsymbol{\sigma}}\right\}\right\rangle\\
&\quad -\left\langle T_\tau\left(-(\varepsilon_{\mathbf{k}}-\mu)\,c_{\mathbf{k}\sigma}(\tau) - V_{\mathbf{k}i}f_{i\sigma}(\tau)\right)f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle\\
&= -(\varepsilon_{\mathbf{k}}-\mu)\,\mathcal{G}_{cf}(\mathbf{k},i,\tau) - V_{\mathbf{k}i}\mathcal{G}_{ff}(\tau) && (60.26)
\end{aligned}$$

that follows because $\left\{c_{\mathbf{k}\boldsymbol{\sigma}}, f^{\dagger}_{i\boldsymbol{\sigma}}\right\} = 0$. It can be solved by going to Matsubara frequencies

$$\mathcal{G}_{cf}(\mathbf{k},i,ik_n) = \frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}\mathcal{G}_{ff}(ik_n). \quad (60.27)$$

Substituting in the equation for $\mathcal{G}_{ff}(ik_n)$ we obtain

$$\begin{aligned}
&\left[ik_n-(\varepsilon-\mu) - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}i}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}\right]\mathcal{G}_{ff}(ik_n)\\
&= 1 - U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f^{\dagger}_{i-\sigma}(\tau)\,f_{i-\sigma}(\tau)\,f_{i\sigma}(\tau)\,f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle. \quad (60.28)
\end{aligned}$$

The last term on the right-hand side is related to the self-energy as usual by

$$\Sigma_{ff}(ik_n)\,\mathcal{G}_{ff}(ik_n) \equiv -U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f^{\dagger}_{i-\sigma}(\tau)\,f_{i-\sigma}(\tau)\,f_{i\sigma}(\tau)\,f^{\dagger}_{i\boldsymbol{\sigma}}\right\rangle \quad (60.29)$$

Except for the self-energy, the equation to be solved has exactly the same Dyson equation structure as that which we would find for a single impurity,

$$\begin{aligned}
\mathcal{G}^0_{ff}(ik_n)^{-1}\,\mathcal{G}_{ff}(ik_n) &= 1 + \Sigma_{ff}(ik_n)\,\mathcal{G}_{ff}(ik_n) && (60.30)\\
\mathcal{G}_{ff}(ik_n) &= \mathcal{G}^0_{ff}(ik_n) + \mathcal{G}^0_{ff}(ik_n)\,\Sigma_{ff}(ik_n)\,\mathcal{G}_{ff}(ik_n), && (60.31)
\end{aligned}$$

with the "non-interacting" Green function's

$$\begin{aligned}
\mathcal{G}^0_{ff}(ik_n)^{-1} &= ik_n-(\varepsilon-\mu) - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}i}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}. && (60.32)\\
&= ik_n-(\varepsilon-\mu)-\Delta_{ff}(ik_n). && (60.33)
\end{aligned}$$

This is in fact exactly the non-interacting Green's function that we would find with $U = 0$. The significance of $\Delta_{ff}(ik_n)$ is that over the imaginary-time interval β, it takes into account that one can propagate from the impurity site back to the impurity site by going through the bath. This function $\Delta_{ff}(ik_n)$, defined by

$$\begin{aligned}\Delta_{ff}(ik_n) &= \sum_{\mathbf{k}} V^*_{\mathbf{k}i} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i} \\ &= \sum_{\mathbf{k}} V^\dagger_{i\mathbf{k}} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i} \end{aligned} \tag{60.34}$$

is called the hybridization function.

What is important to remember is that the self-energy affects only the site where there is an interaction U. Equations (85.29) and (85.31) for the Green's functions, written in Matsubara frequency, read:

$$\begin{pmatrix} ik_n - (\varepsilon - \mu) - \Sigma_{ff}(ik_n) & -V^*_{\mathbf{k}i} \\ -V_{\mathbf{k}i} & ik_n - (\varepsilon_{\mathbf{k}} - \mu) \end{pmatrix} \begin{pmatrix} \mathcal{G}_{ff}(ik_n) \\ \mathcal{G}_{cf}(\mathbf{k}, i, ik_n) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

In this equation, the sum over $\mathbf{k}$ is implicit**.** This problem is analogous to the one we encountered with the harmonic oscillator in Eq.(4.7). Except that we now have a self-energy to compute. Correspondingly, the column vector has $N+1$ elements if there are N possible values of $\mathbf{k}$**.** Explicitly, for three values of $\mathbf{k}$, the matrix is that acts on the Green's function column is

$$\begin{pmatrix} ik_n - (\varepsilon - \mu) - \Sigma_{ff}(ik_n) & -V^*_{\mathbf{k}i} & -V^*_{\mathbf{k}'i} & -V^*_{\mathbf{k}''i} \\ -V_{\mathbf{k}i} & ik_n - (\varepsilon_{\mathbf{k}} - \mu) & 0 & 0 \\ -V_{\mathbf{k}'i} & 0 & ik_n - (\varepsilon_{\mathbf{k}'} - \mu) & 0 \\ -V_{\mathbf{k}''i} & 0 & 0 & ik_n - (\varepsilon_{\mathbf{k}''} - \mu) \end{pmatrix}.$$

What we have done, is to use the second block of this equation to eliminate $\mathcal{G}_{cf}(\mathbf{k}, i, ik_n)$ i.e. the bath, completely. We are left with a single-site problem where the bath is replaced by a hybridization function. We are left with Dyson's equation for $\mathcal{G}_{ff}$ and and a new $\mathcal{G}^0_{ff}(ik_n)^{-1}$ which contains the bath as a hybridization function Eq.(60.34).

As mentionned above, the structure of this last equation is not too different from what we saw with the harmonic oscillator in Eq. (4.6).

Remark 331 *To see that we are left with Dyson's equation for $\mathcal{G}_{ff}$ and and a new $\mathcal{G}^0_{ff}(ik_n)^{-1}$ which contains the bath as a hybridization function Eq.(60.34), let us write the problem as follows*

$$\begin{pmatrix} \mathcal{G}^0_{ff}(ik_n)^{-1} & -V^\dagger \\ -V & \mathbf{G}^0(ik_n)^{-1} \end{pmatrix} \begin{pmatrix} \mathcal{G}^0_{ff}(ik_n) & \mathcal{G}^0_{cf}(ik_n) \\ \mathcal{G}^0_{fc}(ik_n) & \mathbf{G}^0_{cc}(ik_n) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \mathcal{I} \end{pmatrix}$$

where V is a column vector with as many entries as there are values of $\mathbf{k}$ and $V^\dagger$the corresponding row vector. The general matrix form is

$$\begin{pmatrix} \mathcal{A} & B \\ C & D \end{pmatrix} \begin{pmatrix} \mathcal{E} & F \\ G & H \end{pmatrix} = I. \tag{60.35}$$

where $\mathcal{A}$ and D are square matrices while B and C are rectangular matrices. Then simple algebra leads to $\mathcal{E} = \left(\mathcal{A} - \mathcal{B}\mathcal{D}^{-1}C\right)^{-1}$. This is called the inverse of Shur's complement. The other components of the matrix can be obtained by similar manipulations.

The solution to this impurity problem is complicated. The structure in imaginary time is highly non-trivial. Contrary to the atomic limit, the number of electrons on a site is not conserved, i.e. it is time-dependent, and the simplicity of the problem is lost. There is a complicated dynamics where electrons move in and out of the impurity site and what happens at a given time depends on what happened at earlier ones. For example, if there is a down electron on the impurity site, another down electron will not be able to come on the site unless the previous one comes out. This problem, when U is large, contains the rich Physics that goes under the name of Kondo and could be the subject of many chapters in this book. It has been the focus of much attention in Condensed Matter Physics for decades. We will not for now expand further on this.

Remark 332 *The self-energy will influence the value of* $\mathcal{G}_{cf}(\mathbf{k}, ik_n)$, *as we can see by inverting the matrix in the last equation. Nevertheless, the self-energy comes only from the site that has interactions. When particles propagate in the bath, they can step on the interacting site and that is where the effect of interactions show up.*

Remark 333 *Note that the hybridization function is analog to our source field* ϕ *in the Schwinger formalism, but in the latter case, the fields* $\psi^\dagger$ *and* ψ *in* $\psi^\dagger \phi \psi$ *were evolving in the interaction representation with the full Hamiltonian. Now, assume we do something analogous with* $\psi^\dagger \Delta \psi$. *Perturbation theory can the be formulated in terms of a* $\mathcal{G}_\Delta$ *as we discuss below in Sec.60.7. We can also generate high-order correlation functions as functional derivatives with respect to* Δ. *In the functional integral formalism with Grassmann variables, this comes out more naturally.*

Remark 334 *The hybridization function can be understood in the Feynman path-integral formalism as representing the amplitude to come back to the starting site after a certain time* τ.

60.6 The dynamical mean-field self-consistency relation, derivation 2

In the next section, I will show that perturbation theory for the impurity Anderson model is identical to perturbation theory for the Hubbard model on a lattice when the self-energy is calculated using only local Green's functions.

For now, suppose the self-energy for the Anderson model can be obtained. For example, one can solve the Anderson impurity problem from exact diagonalization if the bath is finite. Then, we can solve the DMFT self-consistency problem iteratively as follows. Take a $\left(\mathcal{G}^0_{ff}(ik_n)\right)^{-1}$ and a self-energy to write down $\mathcal{G}_{ff}(ik_n)$. From that quantity, compute $\Sigma(ik_n)$ for the single-site Anderson impurity problem. Substitute that self-energy in the expression for the infinite lattice Green's function and ask that the projected Green's function found from Eq.(60.13) be equal to the impurity Green's function Eq.(60.14). If this is not the case, change $\mathcal{G}^0_{ff}(ik_n)$ until the condition is satisfied. One can think of the hybridization function as the self-consistent dynamical mean-field, as we will see.

Remark 335 *It is not enough to say that one is working with dynamical mean-field theory. One also has to specify the "impurity solver", in other words to specify with what approximation the Anderson impurity model is solved. Exact*

diagonalization, as mentioned above, is an example. Solving the single-site Anderson impurity model is analog to solving the model of a single spin in an effective field as a mean-field solution to the Ising model. It is much more complicated for the quantum impurity, but it can be done, mostly with numerical methods.

Let me do explain this in more detail. Suppose we have a way to solve the Anderson impurity problem, a so-called impurity solver. Then we can achieve the DMFT self-consistency by the following iterative procedure. I use the Anderson impurity notation here, but we are really talking about the same objects as before. For example, $\mathcal{G}_{ff}(ik_n)$ is what I called $\mathcal{G}_{ii}(ik_n)$ in the first derivation of the DMFT self-consistency.

Since we do not know the self-energy from the start, we need to begin with a trial $\Delta_{ff}^{(n)}(ik_n)$ that can be obtained for example from projecting the lattice Green's function with zero self energy. Then,

1. From $\Delta_{ff}^{(n)}(ik_n)$ obtain $\mathcal{G}_{ff}^{0(n)}(ik_n)$

2. $\mathcal{G}_{ff}^{0(n)}(ik_n)$ and the value of U is used by the impurity solver to compute $\Sigma^{(n+1)}(ik_n)$.

3. The above self-energy should be the self-energy for the lattice Green's function. Project that Green's function on a single site using

$$\mathcal{G}_{ff}^{(n+1)}(ik_n) = \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu) - \Sigma^{(n+1)}(ik_n)}. \tag{60.36}$$

4. Obtain a new hybridization function $\Delta_{ff}^{(n+1)}(ik_n) = ik_n - (\varepsilon - \mu) - \left[\mathcal{G}_{ff}^{(n+1)}(ik_n)\right]^{-1} - \Sigma^{(n+1)}(ik_n)$.

5. If $\Delta_{ff}^{(n)}(ik_n)$ and $\Delta_{ff}^{(n+1)}(ik_n)$ are not equal, go back to 1 with $\Delta_{ff}^{(n)}(ik_n) \to \Delta_{ff}^{(n+1)}(ik_n)$.

We still need to show that summing all diagrams of the original problem, but using only the local Green's function $\mathcal{G}_{ff}(ik_n)$, is equivalent to solving exactly a single-impurity Anderson model. In the next section then, I will show that perturbation theory, or more generally the many-body problem for the Anderson impurity model, has the same structure as the original problem when the self-energy of the original problem is calculated using $\mathcal{G}_{ff}^{(0)}(ik_n)$ that contains the hybridization function.

Remark 336 *When the Anderson model is solvved using exact diagonalization, the hybridization function at each cycle is obtained by adjusting the parameters $V_{\mathbf{k}i}$ and $\varepsilon_{\mathbf{k}}$ so that the value of the hybridization function is as closed as possible to the one we want.[46].*

60.7 Perturbation theory for the Anderson impurity model is the same as before but with a Green's function that contains the hybridization function.

In this section, I want to show that perturbation theory for the impurity site of f electrons has the same structure as the perturbation theory we have done up to now, except that what plays the role of the "unperturbed" Green's function is the Green's function that includes the hybridization function, namely Eq.(85.37) or if you want

$$\mathcal{G}^0_{ff}\left(ik_n\right)^{-1} = ik_n - (\varepsilon - \mu) - \Delta\left(ik_n\right) \tag{60.37}$$

where $\Delta\left(ik_n\right)$ is the hybridization function Eq.(60.34).

There are several possible proofs as usual. I start from the linked-cluster theorem. First we use $K_f + K_c$ as "unperturbed" Hamiltonian in the interaction representation. Since $[K_f, K_c] = 0$ we have that

$$\begin{aligned} Z &= \mathrm{Tr}\left[e^{-\beta K_f} e^{-\beta K_c} T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right] \\ &= Z_0 \mathrm{Tr}\left[e^{-\beta K_f}\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0\right] \end{aligned} \tag{60.38}$$

with Z_0 defined by $\mathrm{Tr}\left[e^{-\beta K_c}\right]$, the partition function of the the bath of non-interacting electrons alone, and where we also defined the average over that bath by

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 \equiv \frac{\mathrm{Tr}\left[e^{-\beta K_c} T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right]}{\mathrm{Tr}\left[e^{-\beta K_c}\right]}. \tag{60.39}$$

Since we can manipulate exponentials inside time-ordered products as if they were ordinary numbers, this has precisely the structure of the linked-cluster theorem Eq.(33.60) that can be rewritten as

$$\left\langle e^{-f(\mathbf{x})}\right\rangle = \exp\left[\left\langle e^{-f(\mathbf{x})}\right\rangle_c - 1\right]. \tag{60.40}$$

Thus, applying this theorem, we have

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 = \exp\left[\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_{oc} - 1\right]. \tag{60.41}$$

The cumulant average is easy to evaluate because the average is over non-interacting electrons. Since in $\left\langle T_\tau\left(-\int_0^\beta H_{fc}\left(\tau\right)d\tau\right)\right\rangle_{oc}$ there is a single creation or annihilation operator for the conduction electrons, this first order term vanishes. Then, because of Wick's theorem, the only term that cannot be factored in lower-order correlations is the second order one.[1] Thus

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 = \exp\left[\frac{1}{2}\left\langle T_\tau \int_0^\beta H_{fc}\left(\tau\right)d\tau \int_0^\beta H_{fc}\left(\tau'\right)d\tau'\right\rangle_{oc}\right]. \tag{60.42}$$

Using the explicit expression for H_{fc} in Eq.(60.15) and the fact that the bath is diagonal in $\mathbf{k}$, we are left with the following non-vanishing terms

[1] Note that f electrons evolve with K_f while c electrons evolve with K_c because $\left[K_c, K_f\right] = 0$.

$$\begin{aligned}
&\frac{1}{2}\left\langle T_\tau \int_0^\beta H_{fc}(\tau)\,d\tau \int_0^\beta H_{fc}(\tau')\,d\tau' \right\rangle_{oc} \\
= \;& \frac{1}{2}\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k}} \left\langle T_\tau V_{\mathbf{k}i} c^\dagger_{\mathbf{k}\sigma}(\tau) f_{i\sigma}(\tau) V^*_{\mathbf{k}i} f^\dagger_{i\sigma}(\tau') c_{\mathbf{k}\sigma}(\tau') \right. \quad (60.43)\\
& \left. + V^*_{\mathbf{k}i} f^\dagger_{i\sigma}(\tau) c_{\mathbf{k}\sigma}(\tau) V_{\mathbf{k}i} c^\dagger_{\mathbf{k}\sigma}(\tau') f_{i\sigma}(\tau') \right\rangle_{0c}. \quad (60.44)
\end{aligned}$$

The two terms on the right-hand side give identical results, simplifying the factor of 2. We can use the fact that the average does not affect the f electrons and substitute in our equation for the full average, Eq.(60.42) to write

$$\begin{aligned}
&\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau} \right\rangle_0 \quad (60.45)\\
= \;& T_\tau \exp\left[\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') \left(\sum_{\mathbf{k}} V^*_{\mathbf{k}i} \left\langle T_\tau \left[c_{\mathbf{k}\sigma}(\tau') c^\dagger_{\mathbf{k}\sigma}(\tau) \right] \right\rangle_{0c} V_{\mathbf{k}i} \right) f_{i\sigma}(\tau) \right] \\
= \;& T_\tau \exp\left[-\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') \sum_{\mathbf{k}} V^\dagger_{i\mathbf{k}} \mathcal{G}_{\sigma\mathbf{k}}(\tau',\tau) V_{\mathbf{k}i} f_{i\sigma}(\tau). \right] \quad (60.46)
\end{aligned}$$

The Green's function is that of the bath. Using the fact that it depends only on time differences, we can find its value in Matsubara frequency,

$$\sum_{\mathbf{k}} V^\dagger_{i\mathbf{k}} \mathcal{G}_{\sigma\mathbf{k}}(ik_n) V_{\mathbf{k}i} = \sum_{\mathbf{k}} V^*_{\mathbf{k}i} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i}. = \Delta(ik_n). \quad (60.47)$$

We recognize the hybridation function.

Substituting our final result

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau} \right\rangle_0 = T_\tau \exp\left[-\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') \Delta(\tau' - \tau) f_{i\sigma}(\tau) \right] \quad (60.48)$$

back in the partition function, we see that

$$Z = Z_0 \mathrm{Tr}\left[e^{-\beta K_f} T_\tau \exp\left[-\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') \Delta(\tau - \tau') f_{i\sigma}(\tau) \right] \right]. \quad (60.49)$$

This has the same structure as our generating function in the Schwinger formalism, but for a single-site problem that depends only on imaginary time. The imaginary time evolution of the f fermions is through K_f that contains interactions. The equation of motion will be precisely that which we found in Eqs.(85.36) and (85.37). The perturbation series that can be generated by adding a source term will have precisely the same structure as before, except that the hybridation function will enter in the function that plays the role of the non-interacting Green's function, namely Eq.(60.37) is our non-interacting part.

Remark 337 *The link between the hybridization function and $\mathcal{G}_{\sigma\mathbf{k}}(\tau,\tau')$ makes it clear that it is as if the non-interacting Green's function now contained all the ways to evolve in imaginary time going through the bath, as in the Feynman path integral formalism. This evolution is retarded.*

Remark 338 *Another way to think about this result is that if we do perturbation theory for the interaction U, all the diagrams where the Green functions go in the bath can be resummed into the hybridization function.*

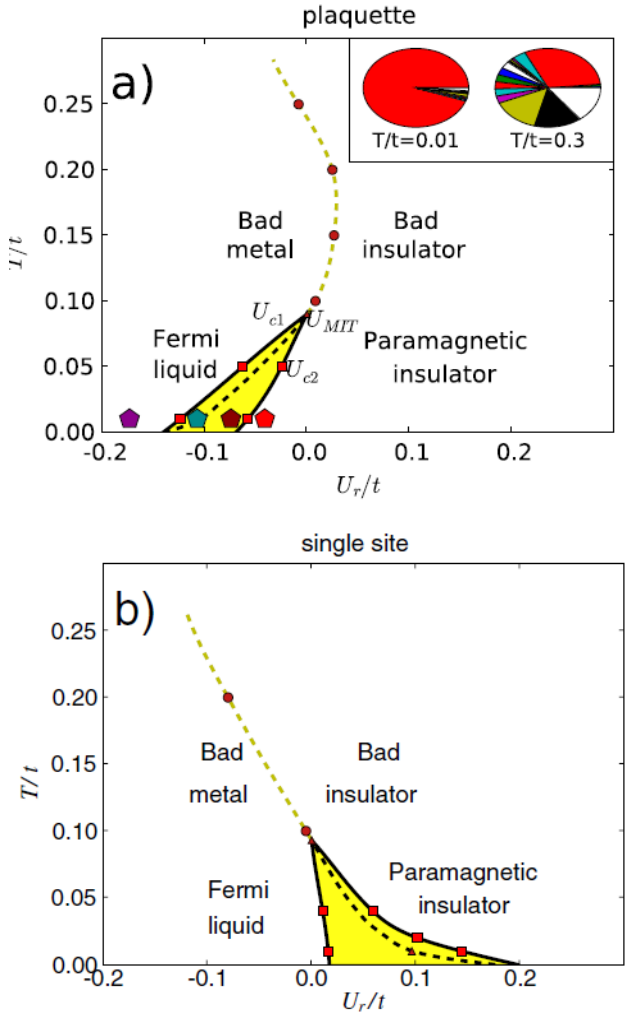


Figure 60-2 First order transition for the Mott transition. (a) shows the result fro two dimensions obtained for a 2×2 plaquette in a bath. In (b), the result obtained for a single site. The horizontal axis is $U_r = (U - U_{MIT})/U_{MIT}$ with $U_{MIT} = 6.05t$ in the plaquette case and $U = 9.35t$ in the single site case.

60.8 The Mott transition

Clausius-Clapeyron

$$dE = TdS + \mu dN + DdU \tag{60.50}$$

$$d(E - TS - \mu N) = -SdT - Nd\mu + DdU \tag{60.51}$$

Set $d\mu = 0$,then along the phase boundary

$$-S_M dT_c + D_M dU_c = -S_I dT_c + D_I dU_c. \tag{60.52}$$

Hence

$$\frac{dT_c}{dU_c} = \frac{D_I - D_M}{S_I - S_M} \tag{60.53}$$

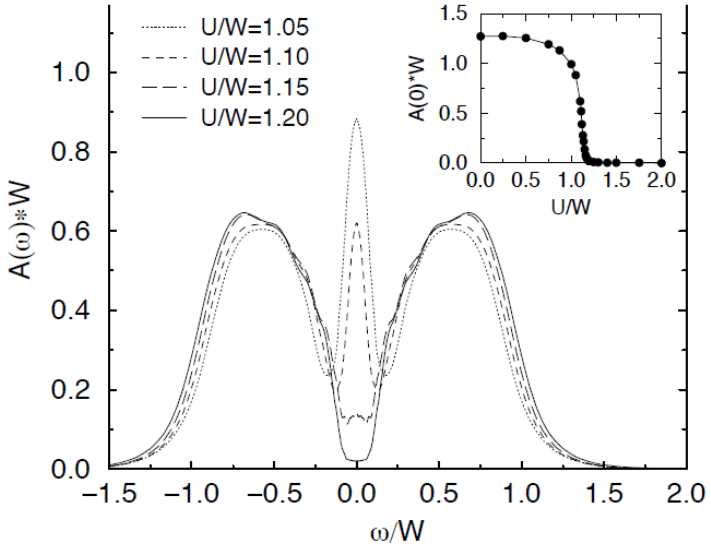
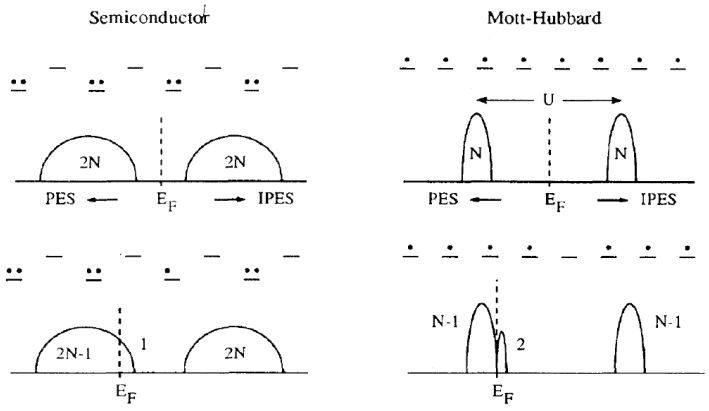


Figure 60-3 decrease for U 1:1 W; from Ref. [78] in Vollhardt in Mancini.



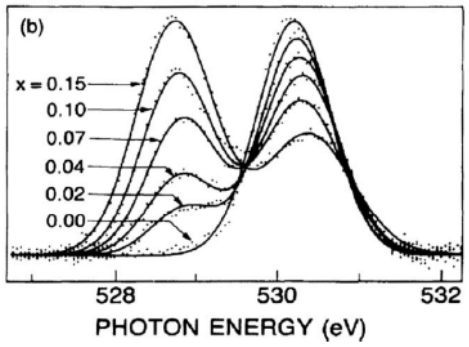
60.9 Doped Mott insulators

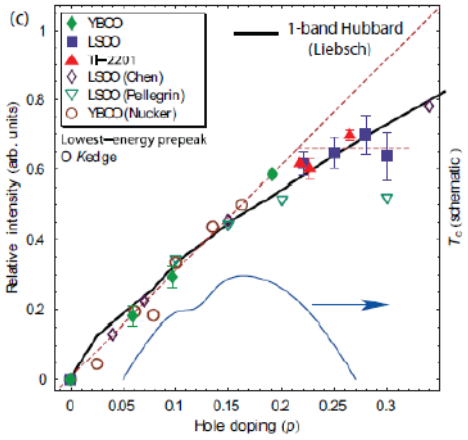
$$\frac{dT_c}{d\mu_c} = \frac{n_{\mathrm{UD}} - n_{\mathrm{OD}}}{S_{\mathrm{OD}} - S_{\mathrm{UD}}}. \tag{60.54}$$

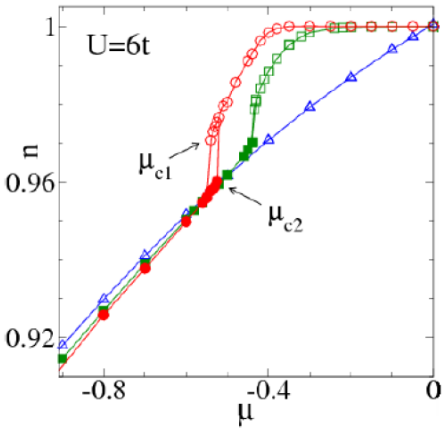
The calculation shows that T_c increases as μ_c increases (i.e. the first-order line bends toward the Mott insulator). This implies that the UD phase has a lower entropy than the OD phase. In an analogous way, by taking a constant T plane, one obtains

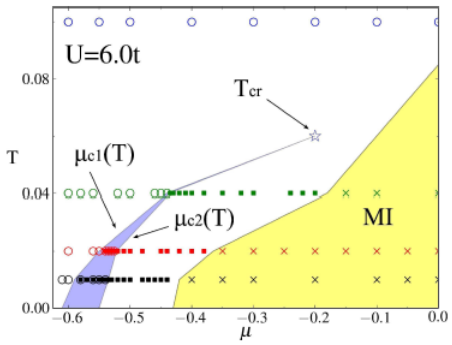
$$\frac{dU_c}{d\mu_c} = \frac{n_{\mathrm{UD}} - n_{\mathrm{OD}}}{D_{\mathrm{UD}} - D_{\mathrm{OD}}}. \tag{60.55}$$

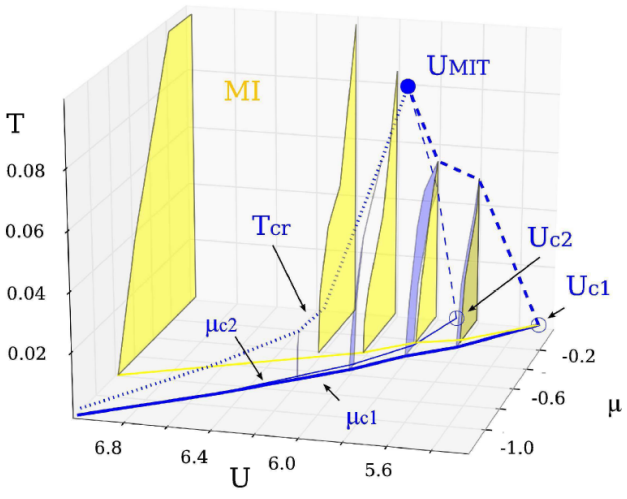
The calculations show that μ_c decreases as U_c increases. Hence, the UD phase has lower double occupancy than the OD phase. This is as expected and suggests again that in the UD phase the correlations are stronger.


(b)
x = 0.15
0.10
0.07
0.04
0.02
0.00
528
530
532
PHOTON ENERGY (eV)


(c)
YBCO
LSCO
LSCO (Chen)
LSCO (Pellegrin)
YBCO (Nücker)
1-band Hubbard
(Liebsch)
Lowest-energy prepeak
O K edge
Relative intensity (arb. units)
T_c (schematic)
Hole doping (p)


U=6t
n
1
0.96
0.92
μ_{c1}
μ_{c2}
-0.8
-0.4
0
μ


U=6.0t
Tcr
μc1(T)
μc2(T)
MI
T
μ
0.08
0.04
0.00
−0.6
−0.5
−0.4
−0.3
−0.2
−0.1
0.0


MI
UMIT
T
Tcr
Uc2
Uc1
μc2
μc1
μ
0.08
0.06
0.04
0.02
6.8
6.4
6.0
5.6
U
-0.2
-0.6
-1.0

61. A SHORT HISTORY

61.1 Model Hamiltonians

61.1.1 Early work

In parallel to DFT efforts to understand properties of materials, the study of simple Hamiltonians revealed very rich physics. One of the first difficult problems that was tackled was that of the Kondo Hamiltonian. That Hamiltonian was suggested by Nobel Prize winner PW Anderson in his study of a model, now known as the Anderson impurity model, that introduced a double occupancy cost U for electrons on an impurity with localized orbital [10]. In the Kondo problem, an isolated impurity with a local moment is hybridized antiferromagnetically with a conduction-electron sea. At high temperature, this local moment is free. At low temperature, there is a crossover to a state where the localized moment essentially disappears by forming a highly entangled singlet state with the conduction sea. A full solution of that problem had to wait for the renormalization group of Nobel Prize winner Ken Wilson [253]. The solution to this problem explained in particular the resistivity minimum found in dilute alloys.

Another important model was proposed independently in 1964 by Hubbard, Kanamori and Gutwiller. Known today as the Hubbard model, this model has two non-commuting terms. A term that represents electrons moving on a lattice with one orbital per site. That term is diagonal in a plane-wave basis. The other term represents the energy cost U associated with double occupancy and is diagonal in the site basis. This model was proposed to understand emergent phases of matter such as ferromagnetism. But in the end, it revealed itself as a way to explain antiferromagnetism and the metal-insulator transition, or Mott transition. The latter problem was by far the most difficult one. The interaction-induced metal insulator transition was proposed by Peierls and Mott around 1937 as an explanation for the discrepancy between the band picture of solids and observation in materials sur as NiO.

Early explanations of the Mott transition at half-filling, all based on the Hubbard model, included a) Hubbard who proposed that the original density of states is split in two by U so that when U is small enough, a metal is recovered [98] b) Brinkmann and Rice who suggested that the effective mass of electrons diverges at the transition [44], a result recovered by the modern slave-boson approach of Kotliar and Ruckenstein [122] c) Slater who associated the transition to an emergent long-range antiferromagnetic order [220]. The latter explanation is invalid for what are called today Mott insulators in a paramagnetic state.

61.1.2 Solving the Hubbard Hamiltonian in infinite dimension

The Hubbard model is the paradygmatic model for electrons that interact strongly. Apart from an exact solution in zero and one dimension, there was no simple tractable case where the model could be solved. Metzner and Vollhardt [160]

made the first important contribution by showing that it was possible to scale the hopping amplitude of the model in such a way that there was an interesting non-trivial limit in infinite dimension where perturbation theory became completely local, *i.e.* depended only on frequency. Müller-Hartmann [169] also proved the locality of perturbation theory. A number of authors, Brandt, Mielsch, Janiš, van Dongen, among others, applied these ideas to a simpler but related model, the Falicov-Kimball model.

61.2 Dynamical Mean-Field Theory (DMFT)

61.2.1 Single-Site Dynamical Mean-Field Theory

Following the seminal paper of Metzner and Vollhardt [160], the breakthrough came in the 1992 seminal paper of Georges and Kotliar [77]. In that paper, they showed that the functional equations could be interpreted as an Anderson impurity model in a self-consistent bath. They established a correspondence with classical mean-field theory and identified the quantum analog of the Weiss effective field. Their approach captured both the itinerant and localized nature of electrons that interact strongly. They could show how Hubbard bands appear. They solved the Lorentzian model exactly. This allowed to understand the high-temperature spin-fluctuation dominated regime and the low-temperature Fermi liquid regime. It opened the way to the study of broken symmetry phases of strongly interacting systems. Importantly, the mean-field interpretation meant that the method would be useful in finite dimension, even though it was exact only in infinite dimension or for large coordination number, in the same way that the mean-field solution of the Ising model is useful in low dimension, even if it is exact only in the same limits as above. Since a number of methods had been developed to understand the Anderson-impurity model in the context of Kondo physics, all these methods became available for the study of the Hubbard model.

A few months later, in an apparently independent paper, Jarrell [107], using a Quantum Monte Carlo method, provided an essentially exact numerical solution of the DMFT equations that demonstrated the metal-insulator Mott transition in the paramagnetic state as well as the antiferromagnetic transition. Georges and Krauth [79] later, but independently, obtained similar results. The paper demonstrating the three peak structure of the spectral weight near the Mott transition by Kotliar and collaborators [260] is a classic.

One should note that the DMFT equations had appeared in print before in the 1987 paper by Kuramoto and Watanabe [125] that focused on the periodic Anderson model and in the 1991 paper by Ohkawa [104] who studied the antiferromagnetic ground state and who also argued that solving the DMFT equations amounts to finding the exact solution to the Hubbard model in infinite dimension. These authors however failed to recognize the depth, importance and the wide applicability of these ideas and to pursue their consequences.

A number of reviews of DMFT have appeared [198, 78, 120, 123, 187]. They explain some of this history in detail. Vollhardt has continued to contribute to DMFT by, for example, developing an accurate method of solution [45]. Metzner moved in another directions, in particular developing the functional renormalization group method.

Single-site DMFT applied to model Hamiltonians has shed light on a number of problems, in particular the metal-insulator Mott transition, revealing the for-

mation of both Hubbard bands and of the Fermi liquid that, in this picture, is a highly entangled state of matter [248].

But Kotliar and collaborators have also found applications of DMFT in biology, for example in elucidating the importance of many-body effects in the kernel of hemoglobin for ligand binding [251]. In fact, many enzymes contain transition metal elements where DMFT could go beyond DFT to predict properties.

61.2.2 Cluster generalizations of DMFT

While the self-energy can be considered to depend only on frequency in infinite dimension, momentum dependence becomes important in lower dimension. This is obvious in angle-resolved photoemission experiments on cuprate superconductors for example, that are quasi-two dimensional. There are several ways to add momentum dependence to dynamical mean-field theory. Clearly, one can extend the concept to clusters. The exact result would be obtained for an infinite cluster. A first generalization to clusters, the so-called Dyanmical Cluster Approximation (DCA) was introduced in 1998 by Jarrell and collaborators [93]. It discretized momentum space. A real space version, the Cellular Dynamical Mean-Field theory (CDMFT), was introduced in 2001 by Kotliar and collaborators [121]. Early reviews appeared in Refs. [145, 120, 236]. In CDMFT, a finite cluster is embedded in an infinite medium and extended to the infinite lattice using Cluster Perturbation Theory [84, 213].

Functional formulations of DMFT and its cluster generalization by Chitra and Kotliar [53] and Potthoff [194, 196, 193] have suggested several other variants of DCA and CDMFT [195]. Extensions of single-site DMFT to the infinite lattice have also been done using diagrammatic methods by the Vienna group [201] and also using so-called dual fermions [203, 182] or dual bosons [204] by Rubtsov and collaborators.

The Hubbard model is commonly used to understand the physics of high-temperature superconductors, one of the great challenges of twentieth century physics. In my opinion, one of the main achievements of these cluster extensions of dynamical mean-field theory has been to show that the most prominent phases of the temperature-doping phase diagram, namely antiferromagnetism and d-wave superconductivity, occur in calculations basically for the doping and temperature range where they are found experimentally. What is special, is that these emergent phases of matter are obtained without any static mean-field approximation on the clusters. The symmetry is broken dynamically in the infinite bath only [144, 143], even in the doped Mott insulator regime [215, 49, 54, **?**, 86, 76]. The pseudogap also finds a natural explanation.

61.2.3 Impurity solvers

The difficult part of any DMFT or cluster DMFT calculation is to solve the problem of the correlated site or cluster in an infinite bath of electrons. A number of methods have been devised, but the breakthrough occured when continuous-time Monte Carlo methods allowed solutions that were exact to within small statistical errors. Rubstov, Werner and Millis and Haule were the main contributors in the development of these methods that are reviewed in this Ref. [85].

61.3 Merging DFT and Dynamical Mean-Field Theory

Just five years after the discovery of DMFT, Kotliar, with Anisimov and collaborators [14] began to lead the effort to combine this approach with DFT to develop general computational tools that start from first principles to predict the properties of correlated electron materials. With his postdoc Savrasov, Kotliar developed the first code that combined DMFT with DFT and obtained remarkable results for the delta phase of plutonium [207]. He began to consider functionals of the spectral weight as the general conceptual framework within which DFT and DMFT could be understood within the same formalism. This was clearly formulated in his 2006 review [120] using the constraining field approach in conjunction with the Kadanoff-Baym et Luttinger Ward functionals.

Georges and Kotliar also developed ways to extract frequency-dependent interactions from electronic structure calculations [21] These interactions enter the DMFT part of LDA+DMFT calculations. Georges also extended the LDA+DMFT approach by showing how to introduce the longer-range part of interactions with the GW approach in the LDA+DMFT calculations (where DMFT treats mostly the short-range part of the interaction) [33].

The successes of the LDA+DMFT approach are already numerous. For example, no other method can explain the Mott transition observed in V_2O_3. Similarly, plutonium was actually not understood by any other electronic structure method before the LDA+DMFT calculations that also predicted a lot of experimentally relevant properties, such as the neutron scattering spectra, and various form factors [207]. With Haule, Kotliar predicted that plutonium hexaboride is a correlated topological insulator [66] and made ground-breaking studies of iron arsenide superconductors that unveiled the fundamental role of Hund's coupling in these materials [254]. Georges on the other hand developed the ideas of orbital-selective Mott transition [65] that had been proposed before by Anisimov et al. [13] and also showed the role of Hund's coupling in leading to strong correlations, what is now known as Hund's metals [61, 80]. Kotliar and Georges both contributed to the understanding of iron pnictide superconductors [4, 254]. They not only developed the DMFT methodology, they used it to solve a number of outstanding problems. The list of achievements is really very long. LDA+DMFT is by now routinely used to explain ARPES, optical conductivity and many other types of experiments on correlated materials.

Open source software packages such AbInit and TRIQS, have been developed to make the latest DFT approaches that include many-body perturbation theory and DMFT widely accessible. Kotliar and Georges made some of their software publicly available early on [78].

62. EXERCICES FOR PART VI

62.0.1 Symétrie particule-trou pour Hubbard

Soit le modèle de Hubbard sur un réseau carré bi-dimensionnel. On pose une intégrale de saut t pour les premiers voisins et t' pour les seconds voisins.

a) Montrez que la relation de dispersion prend la forme suivante lorsque le pas du réseau est pris égal à l'unité:

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 2t' \left(\cos\left(k_x + k_y\right) + \cos\left(k_x - k_y\right)\right). \tag{62.1}$$

b) Montrez que la transformation canonique suivante

$$\begin{aligned} d_{\mathbf{k}\sigma} &= c^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma} \\ d^{\dagger}_{\mathbf{k}\sigma} &= c_{\mathbf{k}+\mathbf{Q}\sigma} \end{aligned} \tag{62.2}$$

où $\mathbf{Q} = (\pi, \pi)$, transforme $H - \mu N$ en un Hamiltonien ayant la même forme mais avec des paramètres différents. Sachant ce résultat, montrez que la solution obtenue avec $t' > 0$ pour le modèle original est reliée à la solution qu'on obtiendrait pour ce modèle avec $t' < 0$ à un potentiel chimique différent. Quelle est la relation entre la densité évaluée à ces deux potentiels chimiques? Finalement, lorsque $t' = 0$, montrez que $\mu = U/2$ correspond au demi-remplissage.

62.0.2 Règle de somme f

En utilisant la définition exacte de χ_{ch} et de χ_{sp} et l'expression pour leurs parties imaginaires comme des commutateurs, montrez que pour le modèle de Hubbard, la règle de somme f devient

$$\int \frac{d\omega}{\pi} \omega \chi''_{ch,sp}\left(\mathbf{q},\omega\right) = \frac{1}{N} \sum_{\mathbf{k}\sigma} \left(\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}} - 2\epsilon_{\mathbf{k}}\right) n_{\mathbf{k}\sigma} \tag{62.3}$$

où $n_{\mathbf{k}\sigma} = \left\langle c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle$.

62.0.3 Impureté quantique dans le cas sans interaction

Soit le hamiltonien

$$K_I = H_f + H_c + H_{fc} - \mu N \tag{62.4}$$

$$K_f \equiv \sum_{\sigma} \left(\varepsilon - \mu\right) f^{\dagger}_{i\sigma} f_{i\sigma} \tag{62.5}$$

$$K_c \equiv \sum_{\sigma} \sum_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \mu\right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{62.6}$$

$$H_{fc} \equiv \sum_{\sigma} \sum_{\mathbf{k}} \left(V_{\mathbf{k}i} c^{\dagger}_{\mathbf{k}\sigma} f_{i\sigma} + V^{*}_{i\mathbf{k}} f^{\dagger}_{i\sigma} c_{\mathbf{k}\sigma} \right). \tag{62.7}$$

On peut motiver ce modèle en pensant à un seul niveau d'énergie f hybridé avec une bande de conduction par le terme $V_{i\mathbf{k}}$. La somme sur $\mathbf{k}$ dans la partie de l'hamiltonien représentant l'hybridation H_{fc} nous dit que c'est le recouvrement local entre l'impureté et la bande de conduction qui compte.

Supposons que nous désirions savoir les propriétés de l'impureté, comme par exemple la densité d'états locale. Celle-ci peut s'obtenir de la fonction de Green

$$\mathcal{G}_{ff}(\tau) = -\left\langle T_\tau f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. \tag{62.8}$$

En procédant par la méthode des équations du mouvement, montrez que

$$\frac{\partial}{\partial\tau}\mathcal{G}_{ff}(\tau) = -\delta(\tau) - (\varepsilon-\mu)\mathcal{G}_{ff}(\tau) - \sum_{\mathbf{k}} V^*_{i\mathbf{k}}\mathcal{G}_{cf}(\mathbf{k},i,\tau)$$

où nous avons défini

$$\mathcal{G}_{cf}(\mathbf{k},i,\tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. \tag{62.9}$$

Pour éliminer cette dernière quantité, montrez que

$$\frac{\partial}{\partial\tau}\mathcal{G}_{cf}(\mathbf{k},i,\tau) = -(\varepsilon_{\mathbf{k}}-\mu)\mathcal{G}_{cf}(\mathbf{k},i,\tau) - V_{\mathbf{k}i}\mathcal{G}_{ff}(\tau)$$

dont la solution en fréquance de Matsubara est:

$$\mathcal{G}_{cf}(\mathbf{k},i,ik_n) = \frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)} V_{\mathbf{k}i}\mathcal{G}_{ff}(ik_n). \tag{62.10}$$

Montrez ensuite que

$$\mathcal{G}_{ff}(ik_n) = \left[ik_n - (\varepsilon-\mu) - \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)} V_{\mathbf{k}i} \right]^{-1}.$$

On définit la fonction d'hybridation par $\Delta_{ff}(ik_n)$

$$\Delta_{ff}(ik_n) \equiv \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)} V_{\mathbf{k}i}. \tag{62.11}$$

62.0.4 Screening of spin fluctuations by the Coulomb interaction:

Show with the help of diagrams, but without any lenghty calculations, that for a spin-rotation invariant system, the diagrams for spin fluctuations that are reducible with respect to the Coulomb interaction, (that is spin independent), all vanish. This is different from the Hubbard model where the spins do not interact with spins of the same species, a manifestaton of the Pauli exclusion principle.

62.0.5 Generalized RPA:

Going back to the original Coulomb interaction, it is possible to sum bubbles and ladders at the same time. This is like taking ladders for the vertex that is irreducible with respect to the Coulomb interaction. Do this calculation for the

Hubbard model, but starting with the version Eq.(54.10) where the Pauli exclusion principle has not been used yet, and up electrons still interact with up electrons. You will show that there are a lot of cancellations so that the final result for spin and charge fluctuations is the same as the one found starting from the model where there are interactions only between up and down electrons.

62.0.6 Atomic limit $(t = 0)$:.

a) Using elementary arguments in the grand canonical ensemble, find the value of $\langle n_\downarrow \rangle$.

b) Then, using the definition of the evolution operators in imaginary time compute the spectral weight directly using the Lehmann representation.

62.0.7 Limite atomique $(t = 0)$:

a) Utilisant des arguments élémentaires d'ensemble grand canonique, trouvez la valeur de $\langle n_\downarrow \rangle$.

b) Calculez le poids spectral directement en utilisant la représentation de Lehmann.

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Part VII

Broken Symmetry

From now on, these are very sketchy notes that will evolve towards a more structured text with time.

In this chapter we encounter the limits of our first principle of *adiabatic continuity,* mentioned in the introduction. That principle is in competition with another one. Indeed. interactions may lead to divergent perturbation theory that cannot be resummed in any way. This breakdown reflects a deep fact of nature, that interactions may lead to new phases of matter, and these phases may be characterized sometimes by broken symmetries. This is the principle of *broken symmetry.* It is a principle because it is an empirically observed fact of very broad applicability. This is a very important concept that applies throughout the theory of condensed matter physics, or quantum materials. This idea was even taken by elementary-particle physics to unify forces for example. At high energy, or high temperature, the forces are identical. The symmetry between the forces is broken at low energy.

We will see how it arises in the simplest manner in a model of ferromagnetism proposed many years ago by Stoner. Original ideas go back to Weiss. This will allow us to develop most of the concepts and approaches we will need to study superconductivity. One of the lessons of this chapter will be that it is impossible to reach a broken symmetry phase from the phase without the broken symmetry by using perturbation theory. And vice-versa. The transition point, whether as a function of interaction strength or as a function of temperature, is a singularity. Our main example will be ferromagnetism. At the end of the chapter we will touch upon many problems of mean-field theories.

63. SOME GENERAL IDEAS ON THE ORIGIN OF BROKEN SYMMETRY

Interactions will often lead to broken symmetries. As a simple example, I will shortly discuss the ferromagnet. Suppose that in some model I find that the uniform spin susceptibility ($\mathbf{q} = \mathbf{0}$) diverges at some temperature. This means that below that temperature, perturbation theory does not converge any more. The paramagnetic state is not adiabatically connected to the state below that temperature. We can guess what is happening. If there is in the Hamiltonian a near-neighbor interaction that favors spin alignment, spins will be aligned in the ground state. In what direction? If the Hamiltonian is symmetric under rotation, there is no prefered direction. Nevertheless, it suffices to assume that there is some small stray magnetic field to see that this will determine the direction in which the spins will align. The stray field breaks the symmetry. The trick then is to make our computations in the presence of an infinitesimal stray field and then to let that field go to zero at the end. In practice, it suffices to choose an arbitrary direction in which the spins will point.

While the expectation value of a spin on a site is zero in the paramagnetic state, in the broken symmetry state it does not vanish. It becomes an "order parameter". That is also another key concept for broken symmetry states.

64. INSTABILITY OF THE NORMAL STATE

In this Chapter, I will show that there are signs of the ferromagnetic instability in the normal state itself. We will find a divergence of the $\mathbf{q} = \mathbf{0}$ spin susceptibility. That divergence is physical, but it also signals a breakdown of perturbation theory. Starting from the normal state, we cannot go below the transition temperature, or below the critical value of U.We first treat the $U = 0$ case and then include the effect of interactions.

As a preamble, we recall why it is the connected function that we are interested in

$$\left.\frac{\partial \langle S_z \rangle}{\beta \partial h}\right|_{h=0} = \left.\frac{\partial}{\beta \partial h}\frac{\mathrm{Tr}\left[e^{-\beta(K-hS_z)}S_z\right]}{\mathrm{Tr}\left[e^{-\beta(K-hS_z)}\right]}\right|_{h=0} \tag{64.1}$$

$$= \langle S_z S_z \rangle - \langle S_z \rangle \langle S_z \rangle \equiv \langle S_z S_z \rangle_c . \tag{64.2}$$

64.1 The noninteracting limit and rotational invariance

The spin susceptibility is obtained from the spin-spin correlation function. Very schematically, consider the connected part of the time-ordered product,

$$\langle T_\tau S_z S_z \rangle_c = \langle T_\tau \left(n_\uparrow - n_\downarrow\right)\left(n_\uparrow - n_\downarrow\right)\rangle_c \tag{64.3}$$

$$= \langle T_\tau n_\uparrow n_\uparrow \rangle_c + \langle T_\tau n_\downarrow n_\downarrow \rangle_c - \langle T_\tau n_\uparrow n_\downarrow \rangle_c - \langle T_\tau n_\downarrow n_\uparrow \rangle_c \tag{64.4}$$

We have assumed $\hbar/2 = 1$ here for the purposes of this discussion. As illustrated in Fig.(?), only the first two terms have non-zero contractions. Hence, for the noninteracting system, the charge and spin susceptibilities are identical when expressed in units $\hbar/2 = 1$ since

$$\langle T_\tau \rho\rho \rangle_c = \langle T_\tau \left(n_\uparrow + n_\downarrow\right)\left(n_\uparrow + n_\downarrow\right)\rangle_c \tag{64.5}$$

$$= \langle T_\tau n_\uparrow n_\uparrow \rangle_c + \langle T_\tau n_\downarrow n_\downarrow \rangle_c + \langle T_\tau n_\uparrow n_\downarrow \rangle_c + \langle T_\tau n_\downarrow n_\uparrow \rangle_c . \tag{64.6}$$

Since the last two terms do not contribute, we are left for both spin and charge with

$$\chi_0(\mathbf{q}, iq_n) = -\frac{1}{N}\sum_{\mathbf{p},\sigma} T\sum_n G^0_\sigma(\mathbf{p}+\mathbf{q}, ip_n + iq_n)\, G^0_\sigma(\mathbf{p}, ip_n) \tag{64.7}$$

$$= -\frac{2}{N}\sum_{\mathbf{p}} \frac{f\left(\zeta_{\mathbf{p}}\right) - f\left(\zeta_{\mathbf{p}+\mathbf{q}}\right)}{iq_n + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}. \tag{64.8}$$

Rotational invariance should give us in general, even in the presence of interactions and again with $\hbar/2 = 1$,

$$\begin{aligned}
\left\langle T_\tau S^+ S^- \right\rangle_c + \left\langle T_\tau S^- S^+ \right\rangle_c &= \frac{1}{4} \left\langle T_\tau \left(S_x + iS_y\right)\left(S_x - iS_y\right)\right\rangle_c && (64.9)\\
&\quad + \frac{1}{4} \left\langle T_\tau \left(S_x - iS_y\right)\left(S_x + iS_y\right)\right\rangle_c && (64.10)\\
&= \frac{1}{2}\left(\left\langle T_\tau S_x S_x\right\rangle_c + \left\langle T_\tau S_y S_y\right\rangle_c\right)\\
&= \left\langle T_\tau S_z S_z\right\rangle_c . && (64.11)
\end{aligned}$$

This comes out indeed from considering the diagrams in Fig.(). At the outer vertices, the spin must now flip as indicated because of the presence of the operators S^+S^-.

64.2 Effect of interactions for ferromagnetism, the Schwinger way

We have seen in Eq.(56.33) how to compute the spin fluctuations for the Hubbard model, either through RPA, or in Eq.(57.6) with the more accurate TPSC method. The simple RPA result suffices to illustrate the main principles. In Sec.(66.3), I will address a more subtle point where TPSC is useful.

64.3 *Effect of interactions for ferromagnetism, the Feynman way

You can read the next section immediately if you have read the previous part.

In the Hubbard model, we took into account the Pauli principle so that up electrons interact only with down electrons. If we return to the original problem where up can interact with down, we need to sum at the same time ladders and bubbles in the way indicated in Fig.(?) to recover rotational invariance in an RPA-like approximation. Since the interaction U is independent of momentum, the two diagrams in Fig.(?a) cancel each other exactly and we are left only with Fig.(?b) which corresponds to the theory where up interacts only with down.

In that theory, the set of diagrams that contributes to $\left\langle T_\tau S_z S_z\right\rangle_c$ is given in Fig.(?). It is different from the set of diagrams that contributes to $\left\langle T_\tau S^+ S^-\right\rangle_c + \left\langle T_\tau S^- S^+\right\rangle_c$ but the final answer is the same in the paramgnetic state with no broken symmetry. Bubbles only contribute to $\left\langle T_\tau S_z S_z\right\rangle_c$ but the odd terms have one extra minus sign because the minus sign in $-\left\langle T_\tau n_\uparrow n_\downarrow\right\rangle_c - \left\langle T_\tau n_\downarrow n_\uparrow\right\rangle_c$. Hence, the result is exacly the same as for $\left\langle T_\tau S^+ S^-\right\rangle_c + \left\langle T_\tau S^- S^+\right\rangle_c$ that we compute with the ladder sum in Fig.(?). Consider for example $\left\langle T_\tau S^+ S^-\right\rangle_c$. There is one minus sign for each order in perturbation theory, hence a factor $(-U)$ and since there are no extra fermion loops included and U is momentum independent, it is the quantity $-\chi_0/2$ that is multiplied when we increase the order by one. More

specifically, we obtain

$$\left\langle T_\tau S^+ S^- \right\rangle_c = \frac{\chi_0}{2} + \frac{\chi_0}{2}(-U)\left(-\frac{\chi_0}{2}\right) + \frac{\chi_0}{2}(-U)^2\left(-\frac{\chi_0}{2}\right)^2 + \ldots \quad (64.12)$$

$$= \frac{\chi_0/2}{1-\frac{U}{2}\chi_0}. \quad (64.13)$$

We thus obtain in Fourier space where the above equation is algebraic,

$$\chi = \left\langle T_\tau S^+ S^- \right\rangle_c + \left\langle T_\tau S^- S^+ \right\rangle_c = \left\langle T_\tau S_z S_z \right\rangle_c = \frac{\chi_0}{1-\frac{U}{2}\chi_0}. \quad (64.14)$$

64.4 The thermodynamic Stoner instability

At finite frequency, a retarded response function can be positive or negative because of resonances. But at zero frequency, we are looking at thermodynamics, hence a susceptibility must be positive. One can show that any $\chi(\mathbf{q}, iq_n)$ is positive when $\chi_0''(\mathbf{q},\omega) = -\chi_0''(\mathbf{q},-\omega)$, since

$$\chi(\mathbf{q}, iq_n) = \int \frac{d\omega}{\pi}\frac{\chi''(\mathbf{q},\omega)}{\omega - iq_n} = \int \frac{d\omega}{\pi}\frac{\omega\chi''(\mathbf{q},\omega)}{(\omega)^2 + (q_n)^2} \quad (64.15)$$

hence *a fortiori* $\chi(\mathbf{q},0)$ is positive. Hence, the RPA result Eq.(64.14) is non-physical when $1 < \frac{U}{2}\chi_0(\mathbf{q},0)$. There is a phase transition when the generalized Stoner criterion

$$\boxed{1 = \tfrac{U}{2}\chi_0(\mathbf{q},0)} \quad (64.16)$$

is satisfied. Note that the first wave vector for which the above result is satisfied is the one that becomes unstable. It does not necessarily correspond to a uniform ferromagnet ($\mathbf{q} = \mathbf{0}$). We will see a specific example below with the antiferromagnet. In the special ferromagnetic case

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi_0(\mathbf{q},0) = \lim_{\mathbf{q}\to\mathbf{0}} -\frac{2}{N}\sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} = -\frac{2}{N}\sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \quad (64.17)$$

which reduces to $2N(\varepsilon_{p_F})$ in the zero temperature limit. So we recover a simple special case that I will discuss below in Eq.(65.6).

64.5 Magnetic structure factor and paramagnons

The transition to the ferromagnetic state is a continuous transition (or second order transition in the mean-field language). It is signaled by a diverging susceptibility, as we saw above. The correlation length is diverging at the transition point. We can see this by expanding $\chi(\mathbf{q},0)$ near the transition point so that it becomes asymptotically equal to

$$\chi(\mathbf{q},0) \approx \frac{\chi_0(\mathbf{0},0)}{1-\frac{U}{2}\chi_0(\mathbf{q},0) - \frac{1}{2}\left(\frac{U}{2}\right)\frac{\partial^2\chi_0(\mathbf{q},0)}{\partial^2 q^2}q^2} \sim \frac{A}{\xi^{-2}+q^2} \quad (64.18)$$

which shows an exponential decrease in real space with correlation length $\xi^{-2} \sim 1 - \frac{U}{2}\chi_0(\mathbf{q},0)$. The above functional form is known by the name of Ornstein-Zernicke. At the transition point, the system becomes "critical". The transition point itself is called a critical point. The presence of this long correlation length also manifests itself in the existence of "critical slowing down". In the present case, we will discover an overdamped collective mode whose typical frequency decreases as we approach the critical point.

Consider for example, the zero temperature transverse magnetic structure factor

$$S_\perp(\mathbf{q},\omega) = \frac{2}{1-e^{-\beta\omega}}\chi''_\perp(\mathbf{q},\omega). \tag{64.19}$$

In the paramagnetic state there is rotational invariance so there is in fact no difference between longitudinal and transverse. We see that $T=0$, $S_\perp(\mathbf{q},\omega) = 2\chi''_\perp(\mathbf{q},\omega)$ for $\omega > 0$. The RPA prediction is thus,

$$S_\perp(\mathbf{q},\omega) = 2\,\mathrm{Im}\left[\frac{\chi_0^R}{1-\frac{U}{2}\chi_0^R}\right] = \frac{2\chi''_0(\mathbf{q},\omega)}{\left(1-\frac{U}{2}\chi'_0(\mathbf{q},\omega)\right)^2 + \left(\frac{U}{2}\chi''_0(\mathbf{q},\omega)\right)^2} \tag{64.20}$$

$$\approx \frac{2\chi''_0(\mathbf{q},\omega)}{\left(1-UN(\varepsilon_{p_F})\right)^2 + \left(\frac{U}{2}\chi''_0(\mathbf{q},\omega)\right)^2}. \tag{64.21}$$

To evaluate $\chi''_0(\mathbf{q},\omega)$, it suffices to analytically continue our general result for the non-interacting spin susceptibility Eq.(64.8) in the small $\mathbf{q}$ limit

$$\chi_0^R(\mathbf{q},\omega) = -\frac{2}{N}\sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p+q}})}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p+q}}} \tag{64.22}$$

$$\approx -\frac{2}{N}\sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \frac{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p+q}}}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p+q}}} \tag{64.23}$$

and to use

$$\zeta_{\mathbf{p}} - \zeta_{\mathbf{p+q}} = -\frac{\mathbf{p}\cdot\mathbf{q}}{m} - \frac{q^2}{2m}$$

as well as the fact that $\mathbf{p}$ in the integrand is constrained to lie near the Fermi surface and that $v_F \gg q/m$ so that $\zeta_{\mathbf{p}} - \zeta_{\mathbf{p+q}} \approx -\mathbf{v}_F\cdot\mathbf{q}$

$$\chi_0^R(\mathbf{q},\omega) = 2\int d\varepsilon N(\varepsilon) \int_{-1}^{1} \frac{d(\cos\theta)}{2} \frac{\partial f(\varepsilon-\mu)}{\partial\varepsilon} \frac{v_F q\cos\theta}{\omega + i\eta - v_F q\cos\theta} \tag{64.24}$$

$$\chi''_0(\mathbf{q},\omega) = -2\pi\int d\varepsilon N(\varepsilon) \int_{-1}^{1} \frac{d(\cos\theta)}{2} \frac{\partial f(\varepsilon-\mu)}{\partial\varepsilon} v_f q\cos(\theta)\,\delta(\omega - v_F q\cos\theta)$$

$$= \pi N(\varepsilon_{p_F}) \frac{\omega}{v_F q} \equiv C\frac{\omega}{v_F q} \tag{64.25}$$

Substituting in the RPA expression Eq.(64.20) we find

$$S_\perp(\mathbf{q},\omega) = 2\chi''_\perp(\mathbf{q},\omega) = \frac{2C\frac{\omega}{v_F q}}{\left(1-UN(\varepsilon_{p_F})\right)^2 + \left(C\frac{\omega}{v_F q}\right)^2}. \tag{64.26}$$

This function is plotted in Fig.(?) as a function of ω for two small values of $\mathbf{q}$ and for $U=0$ and $UN(\varepsilon_{p_F}) = 0.8$ along with $2\chi''_\perp(\mathbf{q},\omega)/\omega$. Clearly this mode is in the particle-hole continuum, in other words it is overdamped. Also its characteristic frequency is becoming smaller as the correlation length $\xi^{-2} \approx 1 - UN(\varepsilon_{p_F})$ increases, to eventually diverge at the critical point. We have a "soft

mode". In the presence of a small uniform magnetic field h, the low-frequency small q limit takes the form

$$\chi_{\perp}(\mathbf{q},\omega)=\frac{A}{\xi^{-2}+aq^{2}+bh^{2/3}-c\frac{i\omega}{v_{F}q}}. \tag{64.27}$$

To see what is meant by critical slowing down, it suffices to note that the effect of the frequency becomes important when ω becomes of order $\xi^{-2}v_{F}q/C$, which is a small number.

65. WEAK INTERACTIONS AT LOW FILLING, STONER FERROMAGNETISM AND THE BROKEN SYMMETRY PHASE

Consider the case of an almost empty band where the dispersion relation is quadratic. And take U/t small so that we may think *a priori* that perturbation theory is applicable. Stoner showed using simple arguments that if U is large enough, the system has a tendency to become ferromagnetic. This is easy to understand in the ground state by an energy balance argument. When U is very large, it is energetically favourable to populate the states with only spins with the same orientation, say up. Indeed, there is then no potential energy since $Un_\uparrow n_\downarrow$ then vanishes. This costs kinetic energy since the Fermi energy of the up spins needs to be larger to accomodate more spins than if the spin down band was also occupied. The balance determines whether the symmetry will be broken or not. There is thus a simple energetic argument that tells us why it is preferable to break a symmetry (choose up spins for example). It is often possible to "guess" which symmetry will be broken using that type of arguments, but it is not always possible.

We will look at ferromagnetism from many points of view. And then we will see that so-called Stoner argument has some problems and that ferromagnetism is much harder to find than what Stoner first thought.

65.1 Simple arguments, the Stoner model

In the Hartree Fock approximation,

$$\widetilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle \tag{65.1}$$

The idea of Stoner, illustrated in Figs.() and () for two and three dimensions, is best illustrated in the limiting case where U is very large. Then by taking all the spins to be up, one increases the kinetic energy, but there is no potential energy. Clearly, if U is large enough (Nagaoka ferromagnetism) it seems that this will always be the lowest energy solution since the kinetic energy is the same whatever the value of U .

The above solution breaks the rotational symmetry of the original Hamiltonian, yet it is a lower energy state. The proper way to consider this problem is to put an infinitesimal magnetic field pointing in one direction in the original Hamiltonian, then take the infinite volume limit, then take the field to zero. In pratical situations, this is how symmetry is broken anyway.

At the threshold for the instability, when the two wave vectors become different, the energies for up and down spins are still identical, so

$$\varepsilon_{\mathbf{k}_{F\uparrow}} - \varepsilon_{\mathbf{k}_{F\downarrow}} = U \left(\langle n_\downarrow \rangle - \langle n_\uparrow \rangle \right). \tag{65.2}$$

Expanding the left-hand side in powers of $\langle n_\downarrow \rangle - \langle n_\uparrow \rangle$ we have, using that $\left| \frac{\partial \varepsilon_{k_{F\sigma}}}{\partial k_{F\sigma}} \frac{\partial k_{F\sigma}}{\partial n_\sigma} \right|$ is independent of spin,

$$\begin{aligned} \frac{\partial \varepsilon_{k_F}}{\partial k_F} \frac{\partial k_F}{\partial n} \left(\langle n_\downarrow \rangle - \langle n_\uparrow \rangle \right) &= U \left(\langle n_\downarrow \rangle - \langle n_\uparrow \rangle \right) && (65.3) \\ \frac{\partial \varepsilon_{k_F}}{\partial n} &= U && (65.4) \\ 1 &= U \frac{\partial n}{\partial \varepsilon_{k_F}} = U \frac{\partial}{\partial \varepsilon_{k_F}} \int^{\varepsilon_{k_F}} N(\varepsilon)\, d\varepsilon && (65.5) \\ 1 &= U N(\varepsilon_{k_F}) && (65.6) \end{aligned}$$

where $N(E)$ is the density of states for a given spin species. The last formula is the celebrated Stoner criterion for ferromagnetism (or antiferromagnetism).

65.2 Variational wave function

If we take a non-interacting solution but with two different Fermi wave vectors for up and down electrons, then we can write a variational wave function

$$|\Psi\rangle = \prod_{\mathbf{k}\uparrow} \theta(k_{F\uparrow} - |\mathbf{k}|) \prod_{\mathbf{k}\downarrow} \theta(k_{F\downarrow} - |\mathbf{k}|)\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\downarrow} |0\rangle . \tag{65.7}$$

Using Ritz's variational principle, we need to minimize

$$\langle \Psi | H - \mu N | \Psi \rangle = \sum_{\mathbf{k},\boldsymbol{\sigma}} (\varepsilon_{\mathbf{k}} - \mu) \langle n_{\mathbf{k},\boldsymbol{\sigma}} \rangle + NU \langle n_{-\sigma} \rangle \langle n_\sigma \rangle . \tag{65.8}$$

We will not proceed further since this is a special case ($T = 0$) of the more general equations treated in the following section.

65.3 Feynman's variational principle for variational Hamiltonian. Order parameter and ordered state

We start from one-body a trial Hamiltonian where the symmetry between up and down spins can be broken. In other words we postulate

$$\widetilde{H}_0 \equiv \sum_{\mathbf{k},\boldsymbol{\sigma}} \widetilde{\zeta}_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{65.9}$$

where $\widetilde{\zeta}_{\mathbf{k}\sigma} = \widetilde{\varepsilon}_{\mathbf{k}\sigma} - \mu$ can be different for up and down spins.

The calculation then proceeds as usual by using Feynman's variational principle

$$-T \ln Z \leq -T \ln Z_{\widetilde{0}} + \left\langle \left(H - \widetilde{H}_0 \right) \right\rangle_{\widetilde{0}} \tag{65.10}$$

to minimize the right-hand side, which can be evaluated as

$$-T\ln\left[\prod_{\mathbf{k}\sigma}\left(1+e^{-\beta\widetilde{\zeta}_{\mathbf{k}\sigma}}\right)\right]+\sum_{\mathbf{k},\sigma}\left(\zeta_{\mathbf{k}\sigma}-\widetilde{\zeta}_{\mathbf{k}\sigma}\right)\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}$$
$$+U\sum_{i}\left\langle c^{\dagger}_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^{\dagger}_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}\ . \tag{65.11}$$

where the last term can also be written by translational invariance as $UN\left\langle n_{\sigma}\right\rangle_{\widetilde{0}}\left\langle n_{-\sigma}\right\rangle_{\widetilde{0}}$ with, as usual, N the number of sites. To evaluate $\langle H\rangle_{\widetilde{0}}$ we have used Wick's theorem since $\widetilde{H}_0$ is non-interacting. Our variational parameters are $\widetilde{\zeta}_{\mathbf{k}\sigma}$. We thus set to zero the derivative of the above expression with respect to $\widetilde{\zeta}_{\mathbf{k}\sigma}$, recalling that the values $\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}$ taken with the trial Hamiltonian also depend on $\widetilde{\zeta}_{\mathbf{k}\sigma}$. Using translational invariance and the definition of Fourier transforms we have the following equalities

$$N\left\langle c^{\dagger}_{i\sigma}c_{i\sigma}\right\rangle_{\widetilde{0}}=\sum_{i}\left\langle c^{\dagger}_{i\sigma}c_{i\sigma}\right\rangle_{\widetilde{0}}=\sum_{\mathbf{k},\sigma}\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} \tag{65.12}$$

so that for the spin σ,

$$U\sum_{i}\left\langle c^{\dagger}_{i\sigma}c_{i\sigma}\right\rangle_{\widetilde{0}}\left\langle c^{\dagger}_{i-\sigma}c_{i-\sigma}\right\rangle_{\widetilde{0}}=U\left\langle c^{\dagger}_{i-\sigma}c_{i-\sigma}\right\rangle_{\widetilde{0}}\sum_{\mathbf{k},\sigma}\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}.$$

This leads to the spin-dependent equation

$$\begin{aligned}0 &= -T\frac{e^{-\beta\widetilde{\zeta}_{\mathbf{k}\sigma}}}{1+e^{-\beta\widetilde{\zeta}_{\mathbf{k}\sigma}}}(-\beta)-\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}\\ &\quad+\left(\zeta_{\mathbf{k}\sigma}+U\left\langle c^{\dagger}_{i-\sigma}c_{i-\sigma}\right\rangle_{\widetilde{0}}-\widetilde{\zeta}_{\mathbf{k}\sigma}\right)\frac{\partial\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}}{\partial\widetilde{\zeta}_{\mathbf{k}\sigma}}.\end{aligned} \tag{65.13}$$

Note that $\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}$ depends only on $\widetilde{\zeta}_{\mathbf{k}\sigma}$ with the same $\mathbf{k},\sigma$ index. Given that for the trial Hamiltonian

$$\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}=\frac{1}{1+e^{\beta\widetilde{\zeta}_{\mathbf{k}\sigma}}}, \tag{65.14}$$

the first two terms cancel and the minimization equation is satisfied if we require the coefficient of $\partial\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}}/\partial\widetilde{\zeta}_{\mathbf{k}\sigma}$ to vanish. This leads to

$$\widetilde{\zeta}_{\mathbf{k}\sigma} = \zeta_{\mathbf{k}\sigma}+U\left\langle c^{\dagger}_{i-\sigma}c_{i-\sigma}\right\rangle_{\widetilde{0}} \tag{65.15}$$
$$= \zeta_{\mathbf{k}\sigma}+U\left\langle n_{-\sigma}\right\rangle_{\widetilde{0}} \tag{65.16}$$

Defining

$$n=\left\langle n_{\uparrow}\right\rangle_{\widetilde{0}}+\left\langle n_{\downarrow}\right\rangle_{\widetilde{0}} \tag{65.17}$$

and the "order parameter"

$$m=\left\langle n_{\uparrow}\right\rangle_{\widetilde{0}}-\left\langle n_{\downarrow}\right\rangle_{\widetilde{0}} \tag{65.18}$$

that measures the magnetization, or spin polarization that can occur because the number of up spins is not restricted to be equal to the number of down spins, we obtain from this equation and from the equation for the occupation number

Eq. (65.14) the self-consistency equation Eq. (65.15) and the relation between $\left\langle c^\dagger_{i-\sigma} c_{i-\sigma} \right\rangle_{\widetilde{0}}$ and $\left\langle c^\dagger_{\mathbf{k}-\sigma} c_{\mathbf{k}-\sigma} \right\rangle_{\widetilde{0}}$ Eq. (65.12)

$$\boxed{\frac{1}{N}\sum_{\mathbf{k}} f\left(\zeta_{\mathbf{k}} + U\left\langle n_{\downarrow}\right\rangle_{\widetilde{0}}\right) - \frac{1}{N}\sum_{\mathbf{k}} f\left(\zeta_{\mathbf{k}} + U\left\langle n_{\uparrow}\right\rangle_{\widetilde{0}}\right) = \left\langle n_{\uparrow}\right\rangle_{\widetilde{0}} - \left\langle n_{\downarrow}\right\rangle_{\widetilde{0}}.} \tag{65.19}$$

This equation is called the "gap equation", as we will understand in the following sections. It must be solved simultaneously with the equation for the chemical potential

$$\boxed{\left\langle n_{\downarrow}\right\rangle_{\widetilde{0}} + \left\langle n_{\uparrow}\right\rangle_{\widetilde{0}} = \frac{1}{N}\sum_{\mathbf{k}}\left(f\left(\zeta_{\mathbf{k}} + U\left\langle n_{\uparrow}\right\rangle_{\widetilde{0}}\right) + f\left(\zeta_{\mathbf{k}} + U\left\langle n_{\downarrow}\right\rangle_{\widetilde{0}}\right)\right).} \tag{65.20}$$

Remark 339 *If we add a constant to the trial Hamiltonian Eq. (65.9), it drops out from* $-T\ln Z_{\widetilde{0}} + \left\langle \left(H - \widetilde{H}_0\right)\right\rangle_{\widetilde{0}}$ *and from the minimization equation. See the remark in the next section, Sec. 65.4 about the calculation of the total energy or free energy.*

65.4 The mean-field Hamiltonian can be obtained by a method where the neglect of fluctuations is explicit

It is possible to "guess" the form of the best one-body Hamiltonian by a simple procedure where the neglect of fluctuations is more explicit. Let us define

$$c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} = \left(c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\right\rangle\right) + \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\right\rangle\ , \tag{65.21}$$

so that

$$\begin{aligned} n_{i\sigma} &= \left(n_{i\sigma} - \left\langle n_{i\sigma}\right\rangle\right) + \left\langle n_{i\sigma}\right\rangle & (65.22)\\ &\equiv \delta n_{i\sigma} + \left\langle n_{i\sigma}\right\rangle. & (65.23)\end{aligned}$$

The expectation values are with respect to a yet unspecified one-body Hamiltonian. With the above definitions, the original Hamiltonian can be rewritten as follows:

$$H = \sum_{\mathbf{k},\boldsymbol{\sigma}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U\sum_i \left(\delta n_{i\uparrow} + \left\langle n_{i\uparrow}\right\rangle\right)\left(\delta n_{i\downarrow} + \left\langle n_{i\downarrow}\right\rangle\right). \tag{65.24}$$

So far there is no approximation. If we neglect terms that are quadratic in fluctuations, namely proportional to $\delta n_{i\uparrow}\delta n_{i\downarrow}$, we are left with the following one-body Hamiltonian

$$\widetilde{H}_0 = \sum_{\mathbf{k},\boldsymbol{\sigma}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U\sum_i \left(\delta n_{i\uparrow}\left\langle n_{i\downarrow}\right\rangle + \left\langle n_{i\uparrow}\right\rangle \delta n_{i\downarrow} + \left\langle n_{i\downarrow}\right\rangle\left\langle n_{i\uparrow}\right\rangle\right). \tag{65.25}$$

Subtituting back $\delta n_{i\sigma} = n_{i\sigma} - \left\langle n_{i\sigma}\right\rangle$ and *imposing self-consistency* by requiring that expectation values appearing on the right-hand side of this equation be the same as those obtained from $\widetilde{H}_0$, namely replacing $\left\langle n_{i\sigma}\right\rangle$ by $\left\langle n_{i\sigma}\right\rangle_{\widetilde{0}}$ we obtain

$$\widetilde{H}_0 = \sum_{\mathbf{k},\boldsymbol{\sigma}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U\sum_i \left(n_{i\uparrow}\left\langle n_{i\downarrow}\right\rangle_{\widetilde{0}} + \left\langle n_{i\uparrow}\right\rangle_{\widetilde{0}} n_{i\downarrow} - \left\langle n_{i\downarrow}\right\rangle_{\widetilde{0}}\left\langle n_{i\uparrow}\right\rangle_{\widetilde{0}}\right). \tag{65.26}$$

Applying Wick's theorem for expectation values computed with $\widetilde{H}_0$, this one-body Hamiltonian has the property that

$$\langle H\rangle_{\widetilde{0}} = \left\langle \widetilde{H}_0 \right\rangle_{\widetilde{0}}. \tag{65.27}$$

Remark 340 *The above steps could be repeated in position space without assuming translational invariance simply by starting from the beginning with*

$$c^\dagger_{i\sigma}c_{j\sigma} = \left(c^\dagger_{i\sigma}c_{j\sigma} - \left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle\right) + \left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle \tag{65.28}$$

and making replacements such that when Wick's theorem is applied the expectations values of the full Hamiltonian and of the mean-field Hamiltonian are equal, as in Eq. (65.27). In the above example there is no exchange term. In general there will be.

Remark 341 $\widetilde{H}_0$ *in this section differs by a constant from* $\widetilde{H}_0$ *in the previous section 65.3. In that previous section, the partition function, or ground state energy in the zero temperature limit, is* $-T\ln Z_{\widetilde{0}} + \left\langle \left(H - \widetilde{H}_0\right)\right\rangle_{\widetilde{0}}$ *and not* $\left\langle \widetilde{H}_0\right\rangle_{\widetilde{0}}$. *Indeed, in the* $T\to 0$ *limit we evaluate*

$$-T\ln\left[\prod_{\mathbf{k}\sigma}\left(1+e^{-\beta\widetilde{\zeta}_{\mathbf{k}\sigma}}\right)\right] = {\sum_{\mathbf{k},\boldsymbol{\sigma}}}' \widetilde{\zeta}_{\mathbf{k}\sigma}, \tag{65.29}$$

where the sum is restricted to $\widetilde{\zeta}_{\mathbf{k}\sigma} < 0$. *On the other hand,*

$$\begin{aligned}&\sum_{\mathbf{k},\boldsymbol{\sigma}}\left(\zeta_{\mathbf{k}\sigma} - \widetilde{\zeta}_{\mathbf{k}\sigma}\right)\left\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} + U\sum_i \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}\\ &= -U\sum_i \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}.\end{aligned} \tag{65.30}$$

Combining the two previous results and using $\left\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} = 0$ *for* $\widetilde{\zeta}_{\mathbf{k}\sigma} > 0$ *and* $\left\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} = 1$ *for* $\widetilde{\zeta}_{\mathbf{k}\sigma} < 0$, *leads to*

$$\begin{aligned}&{\sum_{\mathbf{k},\boldsymbol{\sigma}}}'\widetilde{\zeta}_{\mathbf{k}\sigma} - U\sum_i \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}\\ =\ &\sum_{\mathbf{k},\boldsymbol{\sigma}}\left(\zeta_{\mathbf{k}} + U\langle n_{-\sigma}\rangle_{\widetilde{0}}\right)\left\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} - U\sum_i \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}\\ =\ &\sum_{\mathbf{k},\boldsymbol{\sigma}}\zeta_{\mathbf{k}}\left\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle_{\widetilde{0}} + U\sum_i \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle_{\widetilde{0}}\left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle_{\widetilde{0}}.\end{aligned} \tag{65.31}$$

This is the correct expression for the mean-field ground-state energy.

65.5 The gap equation and Landau theory in the ordered state

Using our definition of the magnetization Eq.(65.18) and the equation for the minimum Eq.(65.19), we obtain an equation (also called the gap equation) for the

order parameter m,

$$m = \frac{1}{N}\sum_{\mathbf{k}} \left(f\left(\zeta_{\mathbf{k}} + U\frac{n}{2} - U\frac{m}{2}\right) - f\left(\zeta_{\mathbf{k}} + U\frac{n}{2} + U\frac{m}{2}\right)\right). \tag{65.32}$$

Suppose we are close to the transition where m is small. Expanding the right-hand side, we have

$$\begin{aligned} m &= \frac{1}{N}\sum_{\mathbf{k}} \frac{\partial f\left(\zeta_{\mathbf{k}} + U\frac{n}{2}\right)}{\partial \zeta_{\mathbf{k}}} \left(-Um\right) + O\left(m^3\right) & (65.33)\\ &= UN\left(\varepsilon_{k_F}\right) m + O\left(m^3\right), & (65.34) \end{aligned}$$

where we have used that as $T \to 0$ the derivative of the Fermi function becomes minus a delta function. Here, ε_{k_F} is defined by $\left(\varepsilon_{k_F} - \mu\right) + U\frac{n}{2} = 0$.

The last equation may also be written

$$\left(1 - UN\left(\varepsilon_{k_F}\right)\right) m = bm^3 \tag{65.35}$$

where a more detailed calculation gives that

$$b = \frac{N''\left(\varepsilon_{k_F}\right)}{24} - \frac{\left(N'\left(\varepsilon_{k_F}\right)\right)^2}{8N\left(\varepsilon_{k_F}\right)}. \tag{65.36}$$

That quantity is generally negative, although one must watch in two dimensions for example where the second derivative of the density of state is positive. The calculation of b is tedious since one must also take into account the dependence of the chemical potential on m^2.

The last form of the equation for m Eq.(65.35) is the so-called Landau-Ginzburg equation for the magnetization. If we had expanded the trial free energy in powers of m, we would have obtained the Landau-Ginzburg free energy. That free energy would have been of the form of a polynomial in powers of m^2 given the structure of its first derivative in m, m^3 etc... It could have been guessed based purely on general symmetry arguments. The free energy must be a scalar so given that m is a vector, one has to take its square. The difference here is that we have explicit expression for the coefficients of m^2 in terms of a microscopic theory. In the absence of a microscopic theory, one can make progress anyway with the Landau-Ginzburg strategy.

What are the consequences of the equation for the magnetisation Eq.(65.35)? First of all we recover the Stoner criterion, $m = 0$ when $1 = UN\left(E_F\right)$ and takes a finite value $m^2 = \left(1 - UN\left(E_F\right)\right)/b$ if U is sufficiently large. This is the broken symmetry state. Here that state breaks rotational invariance.

Broken symmetry is an empirically observed property of matter. Ferromagnets, solids, antiferromagnets, superconductors are all broken symmetry states. The fact the broken symmetry is a general result that is empirically observed makes it a principle. Landau-Ginzburg type theories are theories of principle. The free energy is a scalar, the broken symmetry is described by an order parameter so the free energy is a function of all scalars that can be built with this order parameter.

Remark 342 *It should be clear that the phase transition can occur at fixed temperature by increasing U, or at fixed U by decreasing T. Indeed, in general the equation for the order parameter Eq.(65.33) is temperature dependent. In Eq.(65.34) we have taken the zero temperature limit.*

65.6 The Green function point of view (effective medium)

We can obtain the same results from the effective medium point of view. We proceed exactly as with Hartree-Fock theory for the normal state except that this time, our trial Hamiltonian $\widetilde{H}_0$ is spin dependent

$$\widetilde{H}_0 = \sum_{\mathbf{k},\boldsymbol{\sigma}} \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \tag{65.37}$$

Starting from the diagrams in Fig.(42-3) and recalling that only the Hartree diagram survives because up electrons interact only with down, the effective medium equations are obtained for each spin component

$$\widetilde{\Sigma}_\sigma = U \langle n_{-\sigma} \rangle + \varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} = 0 \tag{65.38}$$

so that we recover the Stoner result $\widetilde{\zeta}_{\mathbf{k}\sigma} = \zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle$. The gap equation is obtained from

$$G_\sigma (\mathbf{k}, ik_n) = \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} + \mu} \tag{65.39}$$

from which we extract the spin-dependent density

$$\begin{aligned} \langle n_\sigma \rangle &= T \sum_n e^{ik_n \eta} \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} + \mu} && (65.40) \\ &= \frac{1}{N} \sum_{\mathbf{k}} f \left(\varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle - \mu \right) && (65.41) \\ &= \frac{1}{N} \sum_{\mathbf{k}} f \left(\zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle \right). && (65.42) \end{aligned}$$

Adding the previous equations to that for $\langle n_\downarrow \rangle + \langle n_\uparrow \rangle$, we recover all the previous results for the magnetization etc.

65.7 There are residual interactions

The full Hamiltonian we need to work with is

$$\begin{aligned} H &= \widetilde{H}_0 + \left(H - \widetilde{H}_0 \right) && (65.43) \\ H - \mu N &= \widetilde{H}_0 - \mu N + \sum_i U n_{i\downarrow} n_{i\uparrow} + \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(\varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} \right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. && (65.44) \end{aligned}$$

The second term $\left(H - \widetilde{H}_0 \right)$ in the first line is our residual interaction. The term $\sum_{\mathbf{k},\boldsymbol{\sigma}} \left(\varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} \right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ in the last line is known as a counter term. Its role is to cancel all Hartree-Fock diagrams that could appear from $\sum_i U n_{i\downarrow} n_{i\uparrow}$ when we do perturbation theory. The perturbation theory in U will be in terms of an unperturbed Green's function obtained from $\widetilde{H}_0$. It will not contain any Hartree-Fock terms.

66. COLLECTIVE GOLDSTONE MODE, STABILITY AND THE MERMIN-WAGNER THEOREM

What do the collective modes look like in the ordered state? The minimal energy to excite a particle with an up spin to a state with down spin is $\varepsilon_{\mathbf{p}_{F\downarrow}} - \varepsilon_{\mathbf{p}_{F\uparrow}} = U\left(\langle n_{\uparrow}\rangle - \langle n_{\downarrow}\rangle\right) = Um$. This tells us, with $m > 0$, that there is a single-particle gap

$$\Delta = Um. \tag{66.1}$$

This same gap exists for particle-hole excitations in the ordered state that flip a spin. There is thus a gap in the particle-hole continuum for what is called the "longitudinal susceptibility". We see in passing that the equation for m is also the equation for the gap Δ. But that is not the whole story. We also need to look at all the collective modes, in particular those of the transverse spin susceptibility. It is a general result (Goldstone's theorem) that when there is a *continuous* symmetry that is broken, such as rotational symmetry, then there is a collective mode whose frequency vanishes at long wave lengths and whose role is to "restore" the symmetry. In the case of the ferromagnet, it does not cost any energy to rotate the overall magnetization of the system. This is the mode that restores the symmetry. At small q the frequency is very small by continuity.

66.1 Tranverse susceptibility

The longitudinal susceptibility is always gapped in the ordered state since it corresponds to changing the magnetization. The transverse susceptibility on the other hand is given by a RPA formula analogous to above Eq.(64.14). Being careful that $\chi_{\perp}^{R-+}(\mathbf{q},\omega) \equiv \langle T_\tau S^- S^+\rangle_c$ has one less factor of two in its definition we find,

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \tag{66.2}$$

with, given the new excitation spectrum in the ordered state, a new definition of the "non-interacting" susceptibility $\chi_{0\perp}^{R-+}(\mathbf{q},\omega)$

$$\chi_{0\perp}^{R-+}(\mathbf{q},\omega) = -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta + \widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow}}. \tag{66.3}$$

that corresponds to the diagram in Fig.(?).

To simplify the calculations, we assume that $\Delta << E_F$ so that we can neglect the energy dependence of the density of states and take the Fermi velocities for up and down electrons to be identical. Expanding as before in the small $\mathbf{q}$ limit, we then have, for small wave vector

$$\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow} \approx \mathbf{v}_F\cdot\mathbf{q} + U\left(\langle n_{\downarrow}\rangle - \langle n_{\uparrow}\rangle\right) = \mathbf{v}_F\cdot\mathbf{q} - \Delta \tag{66.4}$$

so that for $\mathbf{v}_F \cdot \mathbf{q} \ll \Delta$ we can expand,

$$\chi_{0\perp}^{R-+}(\mathbf{q},\omega) \approx -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta - \Delta} \tag{66.5}$$

$$\times \left[1 - \frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta}\right)^2 + \cdots\right] \tag{66.6}$$

$$\approx -\frac{\left(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle\right)}{\omega + i\eta - \Delta}\left(1 + O\left(q^2\right)\right) = \frac{-\Delta/U}{\omega + i\eta - \Delta}\left[1 + \frac{C}{\Delta^2}q^2\right]$$

At then end of this section, we prove that $C < 0$, which is necessary for stability as we will show. Note that the above formula immediately gives that at $q = 0$ the imaginary part is vanishing for $\omega < \Delta$, *i.e.* there is a gap in the particle-hole continuum.

To see the effect of *residual interactions* in the ordered state, in other words the effect of the interactions that are not taken care of by the mean field, we consider the corresponding RPA result in the additional limit $|\omega| < \Delta$

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \approx \frac{\frac{-\Delta/U}{\omega+i\eta-\Delta}}{1 - \frac{(-\Delta)}{\omega+i\eta-\Delta} - \frac{(-\Delta)C}{(\omega+i\eta-\Delta)\Delta^2}q^2} \tag{66.7}$$

$$\approx \frac{-\Delta/U}{\omega + i\eta - Dq^2}, \tag{66.8}$$

with $D = -C/\Delta > 0$. The complete transverse spin susceptibility is obtained by combining the two results

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega) + \chi_{\perp}^{R+-}(\mathbf{q},\omega) = \frac{-\Delta/U}{\omega + i\eta - Dq^2} + \frac{\Delta/U}{\omega + i\eta + Dq^2} \tag{66.9}$$

$$= -\frac{\Delta}{U}\frac{2Dq^2}{(\omega + i\eta)^2 - (Dq^2)^2}. \tag{66.10}$$

In these expressions we have used that the calculation of $\chi_{0\perp}^{R-+}(\mathbf{q},\omega)$ amounts to changing $\Delta \to -\Delta$ as can be seen by repeating the steps above with up and down spins interchanged. Note also that the last form is that of the propagator for a single boson of frequency Dq^2. There is thus a collective mode at $\omega = \pm Dq^2$.

This mode, a Goldstone mode, appears in the particle-hole continuum gap. We can also see this from the imaginary part

$$\mathrm{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega) + \chi_{\perp}^{R+-}(\mathbf{q},\omega)\right) = \pi\frac{\Delta}{U}\delta\left(\omega - Dq^2\right) - \pi\frac{\Delta}{U}\delta\left(\omega + Dq^2\right). \tag{66.11}$$

It is thus a propagating mode and here it has a quadratic dispersion relation, just like we find in the $1/S$ expansion of ferromagnetic spin models. Stability requires that D be positive, otherwise the condition for positivity of dissipation $\mathrm{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega) + \chi_{\perp}^{R+-}(\mathbf{q},\omega)\right)\omega > 0$ is violated.

To show that $D = -C/\Delta$ is positive, it suffices to show that C in the expression for the non-interacting transverse susceptibility, Eq.(66.5), is negative. Note first that in the small q limit, i.e. $q \ll k_F$, we are justified to have neglected $q^2/2m$ compared with $\mathbf{v}_F \cdot \mathbf{q}$. There are two terms of order q^2 that contribute. The first

obvious one is given by,

$$\begin{aligned} & -\frac{1}{N}\sum_{\mathbf{p}}\frac{f(\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow})-f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega+i\eta-\Delta}\left[\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega+i\eta-\Delta}\right]^2 \\ \approx & -\frac{1}{N}\sum_{\mathbf{p}}\frac{f(\widetilde{\zeta}_{\mathbf{p}\uparrow})-f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega+i\eta-\Delta}\left[\frac{\mathbf{v}_F\cdot\mathbf{q}}{\Delta}\right]^2=-\frac{\langle n_\uparrow\rangle-\langle n_\downarrow\rangle}{\omega+i\eta-\Delta}\frac{1}{3}\frac{(v_Fq)^2}{\Delta^2} \\ = & -\frac{\Delta/U}{\omega+i\eta-\Delta}\frac{1}{3}\frac{(v_Fq)^2}{\Delta^2}. \end{aligned} \tag{66.12}$$

The other contribution comes from the expansion of $\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}$ in the argument of the Fermi function, combined with the first order expansion of the denominator

$$-\frac{1}{N}\sum_{\mathbf{p}}\frac{\partial f(\widetilde{\zeta}_{\mathbf{p}\uparrow})}{\partial\widetilde{\zeta}_{\mathbf{p}\uparrow}}\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega+i\eta-\Delta}\left[-\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega+i\eta-\Delta}\right] \tag{66.13}$$

$$=\frac{N(\varepsilon_{p_F})}{\omega+i\eta-\Delta}\frac{1}{3}\frac{(v_Fq)^2}{\Delta}, \tag{66.14}$$

where, as mentioned above, we assume $N(\varepsilon_{p_F})=N(\varepsilon_{p_F\uparrow})=N\left(\varepsilon_{p_F\downarrow}\right)$. Note that the contribution from $\left(\partial^2 f(\widetilde{\zeta}_{\mathbf{p}\uparrow})/\partial^2\widetilde{\zeta}_{\mathbf{p}\uparrow}\right)(\mathbf{v}_F\cdot\mathbf{q})^2$ vanishes when we can neglect the ε dependence of the density of states at the Fermi surface, as we can see by integrating by parts. The two non-zero contributions add up to

$$-\frac{\Delta/U}{\omega+i\eta-\Delta}\left[\frac{1}{3}\frac{(v_Fq)^2}{\Delta^2}\left(1-UN(\varepsilon_{p_F})\right)\right]. \tag{66.15}$$

We have thus shown that

$$C=\frac{1}{3}(v_Fq)^2\left(1-UN(\varepsilon_{p_F})\right)<0 \tag{66.16}$$

because we are in the ferromagnetic state, which means that U is larger than the critical value $U_c=1/N(\varepsilon_{p_F})$.

Remark 343 *Critical slowing down: Note that as U is decreased, approaching the transition from the ferromagnetic state, the diffusion constant, $D=-C/\Delta$, decreases, until it reaches zero. This means that the typical frequencies (Dq^2 in our case) become small, showing that the critical slowing down phenomenon that we encountered in the paramagnetic state also occurs in the ferromagnetic state. Critical slowing down is a very general phenomenon.*

66.2 Thermodynamics and the Mermin-Wagner theorem

The thermodynamic transverse susceptibility is obtained from the usual thermodynamic sum rule (Note that $\mathrm{Im}\left(\chi_\perp^{R-+}(\mathbf{q},\omega')+\chi_\perp^{R+-}(\mathbf{q},\omega')\right)$ is odd but not each of the terms individually).

$$\chi_\perp^{R-+}(\mathbf{q},\omega=0)+\chi_\perp^{R+-}(\mathbf{q},\omega=0)=\int\frac{d\omega'}{\pi}\frac{\mathrm{Im}\left(\chi_\perp^{R-+}(\mathbf{q},\omega')+\chi_\perp^{R+-}(\mathbf{q},\omega')\right)}{\omega'} \tag{66.17}$$

The contribution of the Goldstone mode to that susceptibility is easy to obtain from our previous results, either from the imaginary part or from the full susceptibility Eq.(66.9),

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega=0)+\chi_{\perp}^{R+-}(\mathbf{q},\omega=0)=\frac{\Delta}{U}\frac{2}{Dq^2}. \tag{66.18}$$

Again we see that D must be positive if we want a positive susceptibility. Note however that the divergence of the susceptibility at $q=0$ is physical and does not denote an instability of the system. It just reflects the fact that the orientation of the magnetization can be changed at will, without energy cost, since the broken rotation symmetry is a continuous symmetry. It is a consequence of so-called Bogoliubov inequalities [**?**]. Physically, in the original position space it means that there are long-range correlations in S_x and in S_y.

Despite the singular behavior in the long-wave length fluctuations, the local quantities, such as $\langle S_x^2\rangle$ on one site for example, should be finite. This may be obtained from the correlation function for $\langle S^+S^-\rangle$ since we still have rotation symmetry around the z axis, so that $\langle S_x^2\rangle=\langle S_y^2\rangle$, and inversion symmetry, so that $\langle S_xS_y\rangle=0$. This means that the following quantity

$$T\sum_{iq_n}\frac{1}{N}\sum_{\mathbf{q}}\chi_{\perp}^{-+}(\mathbf{q},iq_n)\,e^{\pm iq_n\eta} \tag{66.19}$$

must be finite. Since S^+ and S^- do not commute, we must specify the convergence factor, as usual, but either one must give a finite result. But we know from the previous section Eq.(66.8) that the spin-wave contribution to that susceptibility is

$$\chi_{\perp}^{-+}(\mathbf{q},iq_n)=\frac{-\Delta/U}{iq_n-Dq^2}. \tag{66.20}$$

Substituting this in our previous condition and using the usual result

$$\lim_{\eta\to 0}T\sum_{n}\frac{e^{iq_n\eta}}{iq_n-x}=\frac{-1}{e^{\beta x}-1} \tag{66.21}$$

for performing the sum over bosonic Matsubara frequencies, we obtain in the long wavelength limit

$$T\sum_{iq_n}\frac{1}{N}\sum_{\mathbf{q}}\frac{-\Delta/U}{iq_n-Dq^2}e^{iq_n\eta} = \frac{\Delta}{U}\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{e^{\beta Dq^2}-1} \tag{66.22}$$

$$\sim \frac{\Delta}{U}\int\frac{d^dq}{(2\pi)^d}\frac{T}{Dq^2} \tag{66.23}$$

a quantity that diverges logarithmically in $d=2$. That is a manifestation of the Mermin-Wagner theorem, a much more general result that says that a continuous symmetry cannot be broken in two dimension at finite temperature. In other words, if we assume that a continuous symmetry is broken at finite temperature, we find that the thermal fluctuations of the Goldstone modes destroy it.

Remark 344 *A classical way to obtain the last result is to see that the free energy functional should contains a term $C(\nabla S_x)^2$ as a restoring force for deviations from the perfectly aligned state. In Fournier space, this means $q^2CS_{x\mathbf{q}}S_{x-\mathbf{q}}$, so that by the equipartition theorem, $q^2C\langle S_{x\mathbf{q}}S_{x-\mathbf{q}}\rangle\propto T$. Since the local value of $\langle S_x^2\rangle$ is obtained from $\int\frac{d^dq}{(2\pi)^d}\langle S_{x\mathbf{q}}S_{x-\mathbf{q}}\rangle$ we recover the previous result Eq.(66.23) concerning the divergence of local fluctuations in two dimensions.*

66.3 Kanamori-Brückner screening: Why Stoner ferromagnetism has problems

Very early on, Kanamori in the context of Solid State Physics and Brückner in the context of nuclear matter, found in the low density limit that interactions U are renormalized by quantum fluctuations. Said in a less mysterious manner, the cross section for two electrons scattering off each other should be calculated beyond the Born approximation. As we have seen in the problem of one electron scattering off and impurity in Fig.(?), in the case of only two electrons scattering off each other, summing the Born series, or the analog of the Lipmann-Schwinger equation, corresponds to summing the ladder diagrams in Fig. (?). This means that in the calculation of the diagram in Fig.(?) that contributes to the transverse spin susceptibility, we should use instead the diagram in Fig.(?). By flipping the lines, one also sees that this is identical to computing the "fan diagrams" illustrated in Fig.(?). In other words, everywhere U appears in the summationn of the ladder diagrams to compute the transverse susceptibility, we should instead use

$$U_{eff}\left(\mathbf{Q},iQ_n\right)=\frac{U}{1+U\Lambda\left(\mathbf{Q},iQ_n\right)} \tag{66.24}$$

where Λ is given by the diagram in Fig.(?). To recover a simple momentum independent U_{eff}, we average the above expression over $\mathbf{Q}$. In addition, we assume that the $iQ_n = 0$ piece dominates. It was shown by Chen *et al.* (1991) by comparing the results of the above approximation with essentially exact quantum Monte Carlo calculations, that this is a good approximation. It does not seem to work however for the charge fluctuations.

The consequences of this effect are important. Indeed, there is a maximum value of U_{eff} given by the average of $1/\Lambda\left(\mathbf{Q},0\right)$. This gives roughly the bandwidth since physically this effect comes about from making the two-body wave function small where U is large. This is more or less like making a strong depression in the two-body wave function when the two electrons are on top of each other. The maximum kinetic energy that can cost is the bandwidth W. Hence, the maximum of U_{eff} is W. On the other hand, the density of states $N\left(\varepsilon_{p_F}\right)$ is proportional to $1/W$. So at best the product $U_{eff}N\left(\varepsilon_{p_F}\right)$ can become equal to unity with difficulty at large U. In more exact calculations, one sees that ferromagnetism does not generally occur in the one-band Hubbard model, because of this effect, except perhaps in special cases where there is a Van Hove singularity in the density of states that is not located at half-filling (otherwise antiferromagnetism dominates), a possibility that arises when $t' \neq 0$. (Hankevych et al. 2004).

A more systematic way of taking these effects into account, including the charge channel and the absence of ferromagnetism unless one is close to the Van Hove singularity, is the TPSC that we introduced in the previous part.

66.4 Exercices

66.4.1 Antiferromagnétisme itinérant

La fonction de Green dans l'état Hartree-Fock d'un antiferroaimant itinérant est donnée par la matrice deux par deux suivante

$$\widetilde{\mathcal{G}}_0(\mathbf{k},\tau) = -\left\langle T_\tau \Psi_{\mathbf{k}}(\tau)\, \Psi_{\mathbf{k}}^\dagger(0)\right\rangle \tag{66.25}$$

où le spineur $\Psi_{\mathbf{k}}$ est défini par

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}+\mathbf{Q}\downarrow} \end{pmatrix} \tag{66.26}$$

avec $\mathbf{Q} = (\pi,\pi)$. La forme explicite de la fonction de Green est,

$$\widetilde{\mathcal{G}}_0(\mathbf{k}, ik_n) = \frac{ik_n\tau_0 + \varepsilon_{\mathbf{k}}\tau_3 + \Delta\tau_1}{(ik_n)^2 - (\varepsilon_{\mathbf{k}}^2 + \Delta^2)} \tag{66.27}$$

où $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ alors que les τ_i sont les matrices de Pauli et la matrice identité et où Δ obéit à l'équation d'autocohérence suivante

$$\Delta = \frac{U}{N}\sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}}\left(1 - 2f(E_{\mathbf{k}})\right) \tag{66.28}$$

$$E_{\mathbf{k}}^2 \equiv \varepsilon_{\mathbf{k}}^2 + \Delta^2 \tag{66.29}$$

Exprimez

$$\mathcal{G}(\mathbf{k},\tau) \equiv -\left\langle T_\tau c_{\mathbf{k}\uparrow}(\tau)\, c_{\mathbf{k}\uparrow}^\dagger(0)\right\rangle - \left\langle T_\tau c_{\mathbf{k}\downarrow}(\tau)\, c_{\mathbf{k}\downarrow}^\dagger(0)\right\rangle \tag{66.30}$$

en fonction de $\widetilde{\mathcal{G}}_0(\mathbf{k},\tau)$ seulement, (*i.e.* en négligeant les termes d'interactions résiduelles) puis obtenez le poids spectral correspondant à $\mathcal{G}(\mathbf{k}, ik_n)$. Interprétez votre résultat en utilisant les idées de quasiparticules. Comment expliquez-vous le fait que les opérateurs $c_{\mathbf{k}\uparrow}(\tau)$ semblent être des combinaisons linéaires d'autres quasiparticules?

67. *ADDITIONAL REMARKS: HUBBARD-STRATONOVICH TRANSFORMATION AND CRITICAL PHENOMENA

68. ELECTRON-PHONON INTERACTIONS IN METALS (JELLIUM)

BCS theory is based on two important concepts, Cooper pairs and broken $U(1)$ symmetry. Whatever the superconductor, these two "emergent" properties are always present. Several mechanisms can lead to the same kind of Cooper pair and associated broken symmetry. The one put forward at the beginning by Bardeen, Cooper and Schrieffer was based on electron-phonon interactions. The fact that the transition temperature dependend on the isotopic content of the material had suggested that phonons were important. So we will first discuss these interactions.

68.1 Beyond the Born-Oppenheimer approximation, electron-phonon interaction, Kohn anomaly

We add the kinetic energy of the ions.

They become quantized.

There is an interaction between electrons and phonons. Phonons can create electron-hole pairs. That modifies the bare phonon frequencies. This is going beyond Born Oppenheimer.

The polarization bubble to lowest order contains Kohn anomalies.

Migdal Theorem allows one to neglect vertex corrections.

Integrating out the phonons leads to an effective electron-electron interaction.

$M*/M = 1 + \lambda$

68.2 Hamiltonian and matrix elements for interactions in the jellium model

Up to now we have considered a fixed lattice. If we let the lattice have its own dynamics we need to solve the problem of two interspersed jellium models. It is quite amazing that in the end, if we take into account the heavy mass of the ions, this simple model gives us phonons with a linear dispersion relation at long wavelengths along with a retarded electron-phonon interaction that is attractive at low frequencies. This is the basis for the standard electron-phonon theory of superconductivity. We will see in the following sections and chapters why the normal metal is unstable at low temperature in the presence of an effective attraction between electrons.

We want an expression for an effective potential $U(\mathbf{r})$ that takes into account the Coulomb interaction and the retardation effects. In the *jellium* model, we consider a system of n electrons per cm^3 of mass m and charge $-e$ and ions

of mass M and charge $+Ze$. Charge neuterality imposes n/Z ions per cm^3. We only take electrostatic interactions into account and suppose that the ions form a continuous fluid. That model neglects

a) Short range repulsion effects coming from the Pauli exclusion principle.

b) The fact that wave functions must be orthogonal to those of valence electrons.

c) Transverse phonons.

In this simple model, the effective interaction between electrons takes the form,

$$\frac{e^2}{\varepsilon\left(\mathbf{q},\omega\right)q^2}. \tag{68.1}$$

Our objective is to compute the dielectric constant. Clearly, there should not be a frequency in a Hamiltonian. It is preferable to think in terms of perturbation theory where there are energy denominators, or to use an action formalism. The calculation of the dielectric constant is as follows

68.2.1 Place holder

68.2.2 Dielectric constant for mobile ions

The Poisson equation is

$$\nabla\cdot\mathbf{E}=\frac{1}{\varepsilon_0}\rho \tag{68.2}$$

where ρ is the charge density. Using $\mathbf{E}=-\boldsymbol{\nabla}\phi$, the equation for the scalar potential induced by all deviations from electroneutrality is

$$\nabla^2\phi=-\frac{1}{\varepsilon_0}\left(\delta\left\langle\rho_i\right\rangle+\delta\left\langle\rho_e\right\rangle+\rho_{ext}\right) \tag{68.3}$$

where $\delta\left\langle\rho_i\right\rangle$ is the fluctuation in the ion density, $\delta\left\langle\rho_e\right\rangle$ is the fluctuation in the electronic density, both induced by the electrostatic potential, and ρ_{ext} is an "external" charge that depends on both space and time. The dielectric constant that we are looking for is defined by

$$\nabla^2\phi=-\frac{1}{\varepsilon}\rho_{ext}. \tag{68.4}$$

Proceeding as in Sec. (40.3) where we explain that the dielectric constant can be calculated with irreducible susceptibility, I can write

$$q^2\phi\left(\mathbf{q},\omega\right)=\frac{1}{\varepsilon_0}\left(-\chi^{irr,R}_{\rho_i\rho_i}\left(\mathbf{q},\omega\right)\phi\left(\mathbf{q},\omega\right)-\chi^{irr,R}_{\rho_e\rho_e}\left(\mathbf{q},\omega\right)\phi\left(\mathbf{q},\omega\right)+\rho_{ext}\left(\mathbf{q},\omega\right)\right). \tag{68.5}$$

There is no cross term $\chi^{irr,R}_{\rho_i\rho_e}$ because such a term is necessarily reducible with respect to the Coulomb interaction. With the definition $V_{\mathbf{q}}=e^2/\left(\varepsilon_0q^2\right)$, we are left with

$$\phi\left(\mathbf{q},\omega\right)\left[1+V_{\mathbf{q}}\chi^{irr,R}_{n_in_i}\left(\mathbf{q},\omega\right)+V_{\mathbf{q}}\chi^{irr,R}_{n_en_e}\left(\mathbf{q},\omega\right)\right]=\frac{\rho_{ext}}{\varepsilon_0q^2}. \tag{68.6}$$

This gives the dielectric function

$$\varepsilon\left(\mathbf{q},\omega\right)=\varepsilon_0\left[1+V_{\mathbf{q}}\chi^{irr,R}_{n_in_i}\left(\mathbf{q},\omega\right)+V_{\mathbf{q}}\chi^{irr,R}_{n_en_e}\left(\mathbf{q},\omega\right)\right].$$

The Lindhard function in the case of the ions $\chi^{irr,R}_{n_i n_i}(\mathbf{q},\omega)$ is calculated the same way as in the case of the electrons, $\chi^{irr,R}_{n_e n_e}(\mathbf{q},\omega)$, but the masses are different in the two cases. In the case of the ions, we are at frequencies well above the ion plasma frequency, whereas the opposite is true for the electrons. This means that for ions we can use the limiting case for the Lindhard function that we found for the plasmon in Sec.41.2.4,

$$1 + V_{\mathbf{q}} \chi^{irr,R}_{n_i n_i}(\mathbf{q},\omega) = 1 - \frac{\omega_i^2}{\omega^2} \tag{68.7}$$

whereas for the electrons we can use the limiting case in Sec.**??** appropriate for Thomas-Fermi screening, namely

$$1 + V_{\mathbf{q}} \chi^{irr,R}_{n_e n_e}(\mathbf{q},\omega) = \left(1 + \frac{q_{TF}^2}{q^2}\right). \tag{68.8}$$

We thus have the final result

$$\varepsilon(\mathbf{q},\omega) = \varepsilon_0 \left(1 - \frac{\omega_i^2}{\omega^2} + \frac{q_{TF}^2}{q^2}\right). \tag{68.9}$$

68.3 The plasmon frequency of the ions is replaced by an acoustic mode due to screening

The phonon frequencies correspond to the case where there are spontaneous oscillations of the system in the absence of external charges, namely when $\varepsilon(\mathbf{q},\omega) = 0$. This happens when

$$\begin{aligned} \omega^2 q^2 &= \omega_i^2 q^2 - \omega^2 q_{TF}^2 \\ \omega^2 &= \omega_i^2 \frac{q^2}{q_{TF}^2 + q^2} \equiv \omega_{\mathbf{q}}^2. \end{aligned} \tag{68.10}$$

The Thomas Fermi wavelength is very short, of the order of the inverse Fermi wave vector. This means that at long wavelength,

$$\omega_{\mathbf{q}} \simeq c_s q \tag{68.11}$$

where the speed of sound is given approximatively by

$$c_s = \frac{\omega_i}{q_{TF}}. \tag{68.12}$$

This is the Bohm-Staver relation, that gives a good approximation for the speed of sound in metals that are not transition metals when for Z one uses the number of valence electrons.

68.4 Effective electron-electron interaction mediated by phonons

The effective interaction between electrons is obtained from the dielectric constant,

$$\begin{aligned}\frac{e^2}{\varepsilon(\mathbf{q},\omega)\,q^2} &= \frac{e^2}{\varepsilon_0 q^2}\frac{\omega^2 q^2}{\omega^2 q^2-\omega_i^2 q^2+\omega^2 q_{TF}^2} \\ &= \frac{e^2}{\varepsilon_0}\frac{1}{q^2+q_{TF}^2}\frac{\omega^2}{\omega^2-\omega_{\mathbf{q}}^2} \\ &= \frac{e^2}{\varepsilon_0}\frac{1}{q^2+q_{TF}^2}\left(1+\frac{\omega_{\mathbf{q}}^2}{\omega^2-\omega_{\mathbf{q}}^2}\right). \end{aligned} \tag{68.13}$$

The first term is the screened Coulomb interaction that we obtained in the absence of phonons ($\omega_{\mathbf{q}}=0$). The second term comes from the electron-phonon interaction. It can be negative for frequencies smaller than phononic frequencies. It can even be very negative close to the reconnance. As a first approximation, we take the interaction as attractive for the frequencies smaller than the Debye frequency. It is retardation (ω small) that leads to an attractive interaction, despite the strong direct Coulomb repulsion.

68.5 RPA approximation

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68.6 Effective mass, quasiparticle renormalization, Kohn anomaly and Migdal's theorem

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69. INSTABILITY OF THE NORMAL PHASE IN THE SCHWINGER FORMALISM

In the same way that the divergence of the spin susceptibility in the normal state signaled the emergence of a new ordered state, ferromagnetism and antiferromagnetism providing examples of such a situation, the divergence of the pair susceptibility in the normal state signals the appearance of superconductivity. But what is the pair susceptibility? Let us go back to the spin susceptibility: we measure the spin at a certain point in space and imaginary time and then at a second space-time point later we measure again, checking whether the zero Matsubara frequency component at a certain wave-vector diverges. Phase transitions are thermodynamic quantities and hence we see them coming at zero frequency. For the pair susceptibility, we replace spin in the above reasoning by measurement of the operator that corresponds to adding a pair of electrons $\psi_\downarrow^\dagger(\mathbf{r}_2,0)\,\psi_\uparrow^\dagger(\mathbf{r}_2,0)$. These extra electrons must be destroyed later since the normal state conserves the number of particle. The corresponding zero-Matsubara frequency susceptibility (in the so-called s-wave channel)

$$\int_0^\beta d\tau \int d^3(\mathbf{r}_1-\mathbf{r}_2)\,\left\langle T_\tau \psi_\uparrow(\mathbf{r}_1,\tau)\,\psi_\downarrow(\mathbf{r}_1,\tau)\,\psi_\downarrow^\dagger(\mathbf{r}_2,0)\,\psi_\uparrow^\dagger(\mathbf{r}_2,0)\right\rangle$$

will diverge at the transition. Historically, Cooper considered a single pair of electrons and found that in the presence of a Fermi surface, a bound state always exists at low temperature. Here we do the full problem where both electrons or holes can be injected and are antisymmetrized with all other electrons.

We first begin by introducing the Nambu representation. It is sort of an overkill in the normal state but then the superconducting state will be easy to treat. To compute the pair susceptibility we will need the functional derivative of the self-energy as usual, so we need to first find the equations of motion before we compute the pair susceptibility.

69.1 Nambu space and generating functional

Define the spinor

$$\mathbf{\Psi}=\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow^\dagger\end{pmatrix};\mathbf{\Psi}^\dagger=\begin{pmatrix}\psi_\uparrow^\dagger & \psi_\downarrow\end{pmatrix}.$$

This is a canonical transformation since it is easy to verify that

$$\left\{\Psi_\alpha,\Psi_\beta^\dagger\right\}=\delta_{\alpha,\beta} \tag{69.1}$$

where we take Ψ and $\Psi^\dagger$ at the same space-time point. Greek indices like α take the values $1,2$ to indicate the two components of the spinor.

The ground state that is annihilated by Ψ has all down-spin electron states filled. It is clear that instead of working with ψ_σ we can work with Ψ_α. We have exactly the same number of operators. In this case, the Green function takes the form

$$\begin{aligned}\mathbf{G}(1,2) &= -\left\langle T_\tau \mathbf{\Psi}(1)\mathbf{\Psi}^\dagger(2)\right\rangle \\ &= \begin{pmatrix} -\left\langle T_\tau \psi_\uparrow(1)\psi_\uparrow^\dagger(2)\right\rangle & -\left\langle T_\tau \psi_\uparrow(1)\psi_\downarrow(2)\right\rangle \\ -\left\langle T_\tau \psi_\downarrow^\dagger(1)\psi_\uparrow^\dagger(2)\right\rangle & -\left\langle T_\tau \psi_\downarrow^\dagger(1)\psi_\downarrow(2)\right\rangle \end{pmatrix}.\end{aligned}$$

In the normal state, the off-diagonal terms vanish, but they don't in the superconducting state. To compute the susceptibility, it is useful to introduce an off-diagonal source field in the presence of which the off-diagonal Green function does not vanish even in the normal state:

$$G_{\alpha\beta}(1,2) = -\frac{\delta \ln Z[\phi]}{\delta\phi_{\beta\alpha}(2,1)} \tag{69.2}$$

$$Z[\phi] = \mathrm{Tr}\left[e^{-\beta K} T_\tau e^{-\mathbf{\Psi}^\dagger(\overline{1})\boldsymbol{\phi}(\overline{1},\overline{2})\mathbf{\Psi}(\overline{2})}\right]. \tag{69.3}$$

In the last expression, the argument of the exponential should be thought of as row-vector, matrix, column-vector product. Clearly, in the presence of off -diagonal components of ϕ, it is possible for the off-diagonal components of G to survive.

69.2 Equations of motion

Given that we preserve the structure that we had before, the equations of motion will give us

$$\mathbf{G}^{-1}(1,2) = \mathbf{G}_0^{-1}(1,2) - \boldsymbol{\phi}(1,2) - \mathbf{\Sigma}(1,2). \tag{69.4}$$

To find out the expression for Σ, we need to first find out what happens to all the terms in the Hamiltonian when it is expressed in terms of the Nambu field operators. For the quadratic terms of the Hamiltonian, the creation and destruction operators come now in the wrong order for down spins. Namely, $\psi_\downarrow^\dagger(1)\psi_\downarrow(2) \to \Psi_2(1)\Psi_2^\dagger(2)$. We had no such trouble for the up spins: $\psi_\uparrow^\dagger(1)\psi_\uparrow(2) \to \Psi_1^\dagger(1)\Psi_1(2)$. We can get away with this by using anticommutation, $\Psi_2(1)\Psi_2^\dagger(2) \to -\Psi_2^\dagger(2)\Psi_2(1)$. There is a constant term that can be generated, but since we will not compute the free energy itself, we can forget about it.[1]

Take the kinetic energy in momentum space for example. We have,

$$\begin{aligned}\sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \Psi_{\mathbf{k}1}^\dagger \Psi_{\mathbf{k}1} - \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \Psi_{\mathbf{k}2}^\dagger \Psi_{\mathbf{k}2} \\ &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \mathbf{\Psi}_{\mathbf{k}}^\dagger \tau^3 \mathbf{\Psi}_k. \end{aligned} \tag{69.5}$$

In the last line, we just used the third Pauli matrix. For memory, we write the three of them here

$$\tau^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \tau^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};\ \tau^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{69.6}$$

[1] In practice, when we return to the original operators in the end, the constant terms disappear.

For the potential energy, we recall that if we anticommute operators to put them in the form of a density-density interaction, we introduce quadratic terms that modify the chemical potential. This is not important since, anyway, we will determine the chemical potential by requiring that we obtain the correct total number of particles. Each of the two density operators may be written in Nambu space at the price of introducing a τ^3 matrix. So, we have the following modification of the potential energy

$$\frac{1}{2}\sum_{\sigma,\sigma'}\psi_\sigma^\dagger\left(\overline{1}\right)\psi_\sigma\left(\overline{1}\right)V\left(\overline{1}-\overline{2}\right)\psi_{\sigma'}^\dagger\left(\overline{2}\right)\psi_{\sigma'}\left(\overline{2}\right)\rightarrow\frac{1}{2}\mathbf{\Psi}^\dagger\left(\overline{1}\right)\tau^3\mathbf{\Psi}\left(\overline{1}\right)V\left(\overline{1}-\overline{2}\right)\mathbf{\Psi}^\dagger\left(\overline{2}\right)\tau^3\mathbf{\Psi}\left(\overline{2}\right).$$

What can be thought of as an identity matrix sandwiched between the $\psi^\dagger$ and ψ spinor in the usual notation now becomes a τ^3 matrix. The equations of motion will thus lead to the following equation for the self-energy. First, we introduce $\left(\mathbf{\Sigma G}\right)\left(1,3\right)_{\alpha\beta}$ as the element $(1,3)$ in space time and $\alpha\beta$ in Nambu space of the generalized matrix product $(\mathbf{\Sigma G})$

$$\left(\mathbf{\Sigma G}\right)\left(1,3\right)_{\alpha\beta}=-V\left(1-\overline{2}\right)\left\langle T_\tau\mathbf{\Psi}^\dagger\left(\overline{2}\right)\tau^3\mathbf{\Psi}\left(\overline{2}\right)\left(\tau^3\mathbf{\Psi}\left(1\right)\right)_\alpha\mathbf{\Psi}^\dagger\left(3\right)_\beta\right\rangle.$$

Note that $\tau^3\mathbf{\Psi}\left(1\right)$ is a vector and recall that the right hand-side comes from computing the commutator of $\Psi_\alpha\left(1\right)$ with the interaction and appending $\mathbf{\Psi}^\dagger\left(3\right)_\beta$ to the right. It is easier to draw a diagram. It will take the same form as in the ordinary notation. The only difference is the presence of τ^3 at each of the two vertices of the Coulomb interaction. Also, the Green functions are matrix Green function in Nambu space that are not necessarily diagonal.

The equation for the self-energy will be given by Fig.?? which is very similar to what was obtained before. The main differences are that the Green's functions are now in Nambu space and are not necessarily diagonal. The irreducible vertices have a Nambu index at each entry or exit point. In addition, each vertex of the interaction has a Pauli matrix τ^3 associated with it, linking incoming and outgoing Green functions. In the normal state, the Nambu Green functions become diagonal. But the irreducible vertex can nevertheless be written in terms of $\delta\Sigma_{12}/\delta G_{12}$ if we wish instead of $\delta\Sigma_\sigma/\delta G_{\sigma'}$.

69.3 Pair susceptibility

The diagram in Fig.?? illustrates the susceptibility we want to compute. We have an incoming up electron and an incoming down electron. The diagram looks as if we have a spin-up hole on the right but if we take the component 2 of the Nambu spinor, we really have a down electron. The susceptibility we are after, using our usual trick of differentiating $\left(\mathbf{G}\mathbf{G}^{-1}=1\right)$ is thus

$$\begin{aligned}\frac{\delta G_{12}\left(1,1\right)}{\delta\phi_{12}\left(2,2\right)} &= -G_{1\overline{\alpha}}\left(1,\overline{2}\right)\left[-\frac{\delta\phi_{\overline{\alpha}\overline{\beta}}\left(\overline{2},\overline{3}\right)}{\delta\phi_{12}\left(2,2\right)}\right]G_{\overline{\beta}2}\left(\overline{3},1\right)\\ &\quad -G_{1\overline{\alpha}}\left(1,\overline{2}\right)\left[-\frac{\delta\Sigma_{\overline{\alpha}\overline{\beta}}\left(\overline{2},\overline{3}\right)}{\delta G_{\overline{\gamma}\overline{\delta}}\left(\overline{4},\overline{5}\right)}\frac{\delta G_{\overline{\gamma}\overline{\delta}}\left(\overline{4},\overline{5}\right)}{\delta\phi_{12}\left(2,2\right)}\right]G_{\overline{\beta}2}\left(\overline{3},1\right). \quad (69.7)\end{aligned}$$

Since we will evaluate the derivatives with off-diagonal components of ϕ that vanish, only $\frac{\delta G_{12}\left(\overline{4},\overline{5}\right)}{\delta\phi_{12}\left(2,2\right)}$ is non-vanishing. Indeed, the other components will give

four-point functions that viiolate particle-number conservation. Similarly, $G_{1\overline{\alpha}}$ is non-zero only for $\overline{\alpha}=1$ and $G_{\overline{\beta}2}$ for $\overline{\beta}=2$. We are thus left with

$$\begin{aligned}\frac{\delta G_{12}(1,1)}{\delta\phi_{12}(2,2)} &= G_{11}(1,2)\,G_{22}(2,1)\\ &\quad +G_{11}\left(1,\overline{2}\right)\left[\frac{\delta\Sigma_{12}\left(\overline{2},\overline{3}\right)}{\delta G_{12}\left(\overline{4},\overline{5}\right)}\frac{\delta G_{12}\left(\overline{4},\overline{5}\right)}{\delta\phi_{12}(2,2)}\right]G_{22}\left(\overline{3},1\right). \quad (69.8)\end{aligned}$$

To compute the functional derivative of the irreducible vertex, we use the Hartree-Fock approximation for the self-energy in Fig.??. The Hartree term contains only diagonal components of the Nambu Green function, so it drops out. For the Hartree term, since we have indices $1,2$, the two τ^3 matrices give a net minus sign that cancels the minus sign in front of the Fock term. Consequently, the irreducible vertex is

$$\frac{\delta\Sigma_{12}\left(\overline{2},\overline{3}\right)}{\delta G_{12}\left(\overline{4},\overline{5}\right)}=V\left(\overline{2},\overline{3}\right)\delta\left(\overline{2}-\overline{4}\right)\delta\left(\overline{3}-\overline{5}\right). \quad (69.9)$$

We can thus rewrite our integral equation for the pair susceptibility as using this previous result as well as $G_{22}\left(\overline{3},1\right)=-G_{\downarrow}\left(1,\overline{3}\right)$

$$\begin{aligned}\frac{\delta G_{12}(1,1)}{\delta\phi_{12}(2,2)} &= -G_{\uparrow}(1,2)\,G_{\downarrow}(1,2)\\ &\quad -G_{\uparrow}\left(1,\overline{2}\right)\left[V\left(\overline{2},\overline{3}\right)\frac{\delta G_{12}\left(\overline{2},\overline{3}\right)}{\delta\phi_{12}(2,2)}\right]G_{\downarrow}\left(1,\overline{3}\right). \quad (69.10)\end{aligned}$$

The result is illustrated in Fig. ??

Remark 345 *This integral equation in the particle-particle channel is known as the Bethe-Salpeter equation. It is a natural generalization, in the many-body context, of the integral equation that also occurs naturally in the theory of two-particle scattering in a vacuum.*

For illustrative purposes, take contact interaction, i.e. $V\left(\overline{2},\overline{3}\right)=V\delta\left(\overline{2}-\overline{3}\right)$ like in an attractive Hubbard model. Then, Fig.?? which draws the diagram in momentum space using the four-momentum conservation law at vertices gives

$$-\chi_p(q)=-\chi_p^0(q)+\chi_p^0(q)\,V\chi_p(q) \quad (69.11)$$

where we have defined the pair susceptibility $\chi_p(q)$ as the Fourier transform of $-\frac{\delta G_{12}(1,1)}{\delta\phi_{12}(2,2)}$. The solution is

$$\chi_p(q)=\frac{\chi_p^0(q)}{1+V\chi_p^0(q)}.$$

The pair susceptibility will diverge, signaling an instability, if there is a solution to $1+V\chi_p^0(q)=0$. So let us evaluate $\chi_p^0(q)$. From the diagram, it is clear that

$$\begin{aligned}\chi_p^0(q) &= \frac{T}{N}\sum_{\mathbf{k}}\sum_{ik_n}\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\frac{1}{-ik_n-\zeta_{-\mathbf{k}}}\\ &= \frac{T}{N}\sum_{\mathbf{k}}\sum_{ik_n}\left[\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}-\frac{1}{ik_n+\zeta_{-\mathbf{k}}}\right]\frac{1}{iq_n-\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{-\mathbf{k}}} \quad (69.12)\\ &= \frac{1}{N}\sum_{\mathbf{k}}\frac{f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)-f\left(-\zeta_{-\mathbf{k}}\right)}{iq_n-\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{-\mathbf{k}}}. \quad (69.13)\end{aligned}$$

To look for a thermodynamic instability, we need to take $iq_n = 0$. The most diverging wave vector will be $\mathbf{q} = \mathbf{0}$ also. It will become clear why when you see the final form

$$\chi_p^0(0) = \int \frac{d^3k}{(2\pi)^3} \frac{1 - 2f(\zeta_{\mathbf{k}})}{2\zeta_{\mathbf{k}}}, \tag{69.14}$$

where we have used $f(-\zeta) = 1 - f(\zeta)$ and assumed inversion symmetry, $\zeta_{-\mathbf{k}} = \zeta_{\mathbf{k}}$. The equation for the diverging pair susceptibility, $1 + V\chi_p^0(q) = 0$, thus reads

$$1 = -V \int \frac{d^3k}{(2\pi)^3} \frac{1 - 2f(\zeta_{\mathbf{k}})}{2\zeta_{\mathbf{k}}}. \tag{69.15}$$

If V is negative, there will always be a solution at sufficiently low temperature because

$$\int \frac{d^3k}{(2\pi)^3} \frac{1 - 2f(\zeta_{\mathbf{k}})}{2\zeta_{\mathbf{k}}} = \int d\zeta N(\zeta) \frac{\tanh\left(\frac{\beta\zeta}{2}\right)}{2\zeta} \tag{69.16}$$

is positive and logarithmically divergent at low temperature. Indeed, take a constant density of state $N(\zeta)$, then we integrate $1/\zeta$ up to a lower energy cutoff of order T given by the tanh and an upper energy cutoff of the order of the Fermi energy. It looks like the antiferromagnet with perfect nesting. This gives the BCS equation for T_c. We now move to the superconducting state.

70. BCS THEORY

The phenomenological Ginzburg-Landay theory, based on an order parameter with $U(1)$ symmetry, just as a wave function, allows one to understand many phenomenological aspects of the superconducting state: The Meissner effect, the existence of two critical fields, associated to the existence of two critical magnetic fields, the relation between critical field and condensation energy, persistent currents in a torus, flux quantization, jump of specific heat. BCS theory will allow us to understand how the effective attraction leads to phase rigidity and will give us a theory where there is a gap that appears in several observable quantities, like the specific heat, ultrasonic attenuation, finite frequency infrared conductivity. It explains naturally the isotopic effect and allows one to compute the ratio between the $T = 0$ gap and T_c. The BCS theory is based on an effective interaction between electrons V that is attractive in a range of wave vectors located within a shell of energy equal to the Debye frequency. This is clearly an approximation, but it gives remarkable agreement with experiment. This comes about because the Cooper pair size is so large, that the mean-field approximation is a good approximation.

70.1 Broken symmetry, analogy with the ferromagnet

Having more spins up and spin down is like having a bound state of up spins with down holes. That is the analog of the Cooper pair. Having the same bound state on all sites is the analog of having phase coherence in BCS. But the analogy is even closer with itinerant antiferromagnet because, as in the case of superconductivity, the order parameter does not commute with the Hamiltonian, whereas it does in the case of the ferromagnet.

70.2 The BCS equation the Green's function way (effective medium)

The broken symmetry state has to be guessed. It cannot be reached by perturbation theory since there is a phase transition. However, the divergence of perturbation theory at the phase transition gives us a hint of what symmetry we should break. Here, it seems that the pair field takes a non-zero expectation value, in the same way that the spin at a given wave vector took a non-zero expectation value in the magnetic case. In modern treatments, the BCS theory of superconductivity in the presence of electromagnetic fields is a theory with topological order instead of broken symmetry. We give the standard treatment here. We take for our trial

Hamiltonian in the Nambu notation

$$\widetilde{K}_0 = \sum_{\mathbf{k}} \mathbf{\Psi}_{\mathbf{k}}^{\dagger} \left[\left(\widetilde{\varepsilon}_{\mathbf{k}} - \mu \right) \tau^3 + \Delta_{\mathbf{k}}^1 \tau^1 + \Delta_{\mathbf{k}}^2 \tau^2 \right] \mathbf{\Psi}_{\mathbf{k}}. \tag{70.1}$$

In this expression the off-diagonal components Δ violate total charge conservation. Our off-diagonal field ϕ entering the generating function now has a finite expectation value.

The Green's function is

$$\mathbf{G}\left(\mathbf{k}, ik_n\right) = \begin{pmatrix} -\left\langle T_\tau c_{\mathbf{k}\uparrow}\left(\tau\right) c_{\mathbf{k}\uparrow}^{\dagger} \right\rangle & -\left\langle T_\tau c_{\mathbf{k}\uparrow}\left(\tau\right) c_{-\mathbf{k}\downarrow} \right\rangle \\ -\left\langle T_\tau c_{-\mathbf{k}\downarrow}^{\dagger}\left(\tau\right) c_{\mathbf{k}\uparrow}^{\dagger} \right\rangle & -\left\langle T_\tau c_{-\mathbf{k}\downarrow}^{\dagger}\left(\tau\right) c_{-\mathbf{k}\downarrow} \right\rangle \end{pmatrix} \tag{70.2}$$

or rewriting the lower-right matrix element in terms of a more usual Green's function using anti-commutation properties under a time-ordered product, the above takes the form

$$\mathbf{G}\left(\mathbf{k}, ik_n\right) = \begin{pmatrix} -\left\langle T_\tau c_{\mathbf{k}\uparrow}\left(\tau\right) c_{\mathbf{k}\uparrow}^{\dagger} \right\rangle & -\left\langle T_\tau c_{\mathbf{k}\uparrow}\left(\tau\right) c_{-\mathbf{k}\downarrow} \right\rangle \\ -\left\langle T_\tau c_{-\mathbf{k}\downarrow}^{\dagger}\left(\tau\right) c_{\mathbf{k}\uparrow}^{\dagger} \right\rangle & \left\langle T_\tau c_{-\mathbf{k}\downarrow}\left(-\tau\right) c_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle \end{pmatrix}. \tag{70.3}$$

With the above trial Hamiltonian, the trial inverse Green's function then is

$$\widetilde{\mathbf{G}}^{-1}\left(\mathbf{k}, ik_n\right) = \left[ik_n I - \left(\widetilde{\varepsilon}_{\mathbf{k}} - \mu \right) \tau^3 - \Delta_{\mathbf{k}}^1 \tau^1 - \Delta_{\mathbf{k}}^2 \tau^2 \right] \tag{70.4}$$

where I is the identity matrix in Nambu space and where $\widetilde{\varepsilon}_{-\mathbf{k}} = \widetilde{\varepsilon}_{\mathbf{k}}$ has been used in the equation of motion of $\left\langle T_\tau c_{-\mathbf{k}\downarrow}\left(-\tau\right) c_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle$. The overall sign of that last quantity combined with the $-ik_n$ instead of ik_n coming from the Fourier transform of $c_{-\mathbf{k}\downarrow}\left(-\tau\right)$ allows ik_n in the equation for $\widetilde{\mathbf{G}}^{-1}\left(\mathbf{k}, ik_n\right)$ to appear with the identity matrix. The absence of minus sign in front of $\left\langle T_\tau c_{-\mathbf{k}\downarrow}\left(-\tau\right) c_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle$ leads to the τ^3 matrix.

To invert this equation, it suffices to use the fact that Pauli matrices anticommute when their index is different while their square is the identity matrix. In other words, we can use the result

$$\left(aI - \mathbf{b}\cdot\boldsymbol{\sigma}\right)\left(aI + \mathbf{b}\cdot\boldsymbol{\sigma}\right) = \left(a^2 - \mathbf{b}\cdot\mathbf{b}\right) I.$$

With this identity, we find

$$\widetilde{\mathbf{G}}\left(\mathbf{k}, ik_n\right) = \frac{ik_n I + \left(\widetilde{\varepsilon}_{\mathbf{k}} - \mu \right) \tau^3 + \Delta_{\mathbf{k}}^1 \tau^1 + \Delta_{\mathbf{k}}^2 \tau^2}{\left(ik_n\right)^2 - E_{\mathbf{k}}^2} \tag{70.5}$$

where $E_{\mathbf{k}}$ will be the quasiparticle energy

$$E_{\mathbf{k}} = \sqrt{\left(\widetilde{\varepsilon}_{\mathbf{k}} - \mu \right)^2 + \left(\Delta_{\mathbf{k}}\right)^2} \tag{70.6}$$

with

$$\left(\Delta_{\mathbf{k}}\right)^2 = \left(\Delta_{\mathbf{k}}^1\right)^2 + \left(\Delta_{\mathbf{k}}^2\right)^2. \tag{70.7}$$

Now we move to mean-field theory the Green function way. The total Hamiltonian with quadratic part $K_0 = H_0 - \mu N$, and attractive potential energy V having the properties described at the beginning of this section, is

$$K_0 + V = K = \widetilde{K}_0 + \left(H_0 - \widetilde{H}_0 + V \right) \tag{70.8}$$

where $\widetilde{K}_0$ is our trial quadratic part $\widetilde{H}_0 - \mu N$. The term in parenthesis represents the residual interactions. Evaluating the effect of these residual interactions within

Hartree-Fock, onlyu the Fock terme contributing, and requiring that the resulting self-energy $\widetilde{\Sigma}$ of the effective medium vanish, we obtain

$$\begin{aligned}\Sigma\left(\mathbf{k}, ik_n\right) &= 0 = \left(\varepsilon_{\mathbf{k}}-\mu\right)\tau^3 - \left[\left(\widetilde{\varepsilon}_{\mathbf{k}}-\mu\right)\tau^3 + \Delta^1_{\mathbf{k}}\tau^1 + \Delta^2_{\mathbf{k}}\tau^2\right] \\ &\quad -\frac{T}{N}\sum_{\mathbf{k}'}\sum_{ik'_n} V_{\mathbf{k}-\mathbf{k}'}\tau^3 \frac{ik'_n I + \left(\widetilde{\varepsilon}_{\mathbf{k}'}-\mu\right)\tau^3 + \Delta^1_{\mathbf{k}'}\tau^1 + \Delta^2_{\mathbf{k}'}\tau^2}{\left(ik'_n\right)^2 - E^2_{\mathbf{k}'}}\tau^3.\end{aligned}$$

Note the τ^3 matrices from the interaction. Since the Pauli matrices and I form a basis, the coefficient of each of the matrices must vanish separately. The terms with the identity matrix and the τ^3 Pauli matrix give the Hartree-Fock contribution of the normal state, slightly modified by the presence of the gap. The new equation involves the off-diagonal components. The equation for $\Delta^1_{\mathbf{k}'}$ is identical to that of $\Delta^2_{\mathbf{k}'}$. Let us thus look at one of them, recalling that $\tau^3\tau^1\tau^3 = -\tau^1$.

$$\Delta^1_{\mathbf{k}} = \frac{T}{N}\sum_{\mathbf{k}'}\sum_{ik'_n} V_{\mathbf{k}-\mathbf{k}'}\frac{\Delta^1_{\mathbf{k}'}}{\left(ik'_n\right)^2 - E^2_{\mathbf{k}'}} \tag{70.9}$$

$$= \frac{T}{N}\sum_{\mathbf{k}'}\sum_{ik'_n} V_{\mathbf{k}-\mathbf{k}'}\left[\frac{1}{ik'_n - E_{\mathbf{k}'}} - \frac{1}{ik'_n + E_{\mathbf{k}'}}\right]\frac{\Delta^1_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tag{70.10}$$

$$= \frac{1}{N}\sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}\frac{f\left(E_{\mathbf{k}'}\right) - f\left(-E_{\mathbf{k}'}\right)}{2E_{\mathbf{k}'}}\Delta^1_{\mathbf{k}'} \tag{70.11}$$

$$= -\int \frac{d^3k}{\left(2\pi\right)^3} V_{\mathbf{k}-\mathbf{k}'}\frac{1-2f\left(E_{\mathbf{k}'}\right)}{2E_{\mathbf{k}'}}\Delta^1_{\mathbf{k}'}. \tag{70.12}$$

This is the BCS gap equation. When we take a momentum independent interaction, it clearly reduces at T_c to Eq.(69.15) that we found before.

Note that since $\Delta^1_{\mathbf{k}'}$ and $\Delta^2_{\mathbf{k}'}$ obey the same equation, we can always choose an overall phase factor and work with one of them only.

Remark 346 *The normal-state part of the calculation in the presence of a frequency-dependent interaction, i.e. phonon-mediated interactions, gives non-trivial results. In particular, the effective mass is strongly influenced by electron-phonon interactions.*

70.3 Phase coherence

One of the most important results from a conceptual point of view that BCS teaches us is that even when the interaction depends on $\mathbf{k}-\mathbf{k}'$, the phase of the gap must be $\mathbf{k}$ independent. Indeed, the gap equation (70.12) can be written in the form

$$\left[C_{\mathbf{k}}\Delta_{\mathbf{k}}\right] = -\frac{1}{2\mathcal{V}}\sum_{\mathbf{k}'} C_{\mathbf{k}}V_{\mathbf{k}-\mathbf{k}'}C_{\mathbf{k}'}\left[C_{\mathbf{k}'}\Delta_{\mathbf{k}'}\right]. \tag{70.13}$$

where

$$C_{\mathbf{k}} = \left(\frac{\left(1-2f\left(E_{\mathbf{k}}\right)\right)}{E_{\mathbf{k}}}\right)^{1/2}. \tag{70.14}$$

Everything within the square root is positive since with $E_{\mathbf{k}}$ positive, $f\left(E_{\mathbf{k}}\right)$ is less than $1/2$. The BCS gap equation can then be interpreted as an eigenvalue equation. The eigenvectors are in the square brackets and the eigenvalue is unity.

Since the matrix $-C_{\mathbf{k}}U\left(\mathbf{k}-\mathbf{k}'\right)C_{\mathbf{k}'}/\left(2\mathcal{V}\right)$ whose eigenvectors we are looking for is real symmetric, this eigenvector must be real within an overall $\mathbf{k}$ independent phase factor, unless the eigenvalue is degenerate. This means that all the pairs have the same phase, independently of their wave vector $\mathbf{k}$. This is what we mean by phase coherence.

Remark 347 *There is one obvious degeneracy, that associated with time-reversal symmetry. When that symmetry is broken, the order parameter is complex. This gives a non-trivial result only for values of the orbital angular momentum different from zero.*

70.4 Eliashberg equation

The idea is in a way similar to DMFT. Instead of looking for the best trial Hamiltonian, we look for the best trial Green function, taking for $V_{\mathbf{k}-\mathbf{k}'}$ the effective interaction with the phonons that is frequency dependent. We also assume that the wave vector dependence only comes from the angle between $\mathbf{k}$ and $\mathbf{k}'$, the magnitude of $\mathbf{k}$ being taken at the Fermi surface. Then, the frequency dependence survives. For an $s-$wave superconductor, the trial Green function is

$$\mathbf{G}\left(\mathbf{k},ik_n\right)=\frac{ik_nI+\left(\widetilde{\varepsilon}_{\mathbf{k}}-\mu\right)\tau^3+\Delta^1\left(ik_n\right)\tau^1}{\left(ik_n\right)^2-E_{\mathbf{k}}^2} \tag{70.15}$$

and again we ask that in the Hartree-Fock approximation, the self-energy vanishes. We will thus obtain a frequency dependent gap with a real and an imaginary part. It is customary to define the odd part of the self-energy in Matsubara frequency by

$$ik_n\left(1-Z\left(\mathbf{k},ik_n\right)\right)=\frac{1}{2}\left[\Sigma\left(\mathbf{k},ik_n\right)-\Sigma\left(\mathbf{k},-ik_n\right)\right] \tag{70.16}$$

and the even part by

$$\chi\left(\mathbf{k},ik_n\right)=\frac{1}{2}\left[\Sigma\left(\mathbf{k},ik_n\right)+\Sigma\left(\mathbf{k},-ik_n\right)\right]. \tag{70.17}$$

In the presence of spin rotational invariance, the self-consistency equations give three integral equations to solve for the above quantities, Z,χ and Δ (the equations for the two off-diagonal components of the Green's functions are equivalent).

The electron-electron interaction in the energy window ω_D that we are interested in is smaller than the bare interaction. That can be seen by integrating out scattering processes that are outside the low-energy window. The electron repulsion is taken into account by a term called μ^*. Since the interaction is mediated by phonons, the phonon spectrum leaves some structures in the frequency dependence of $\Delta^1\left(ik_n\right)$. In addition to the isotope effect, this is what convinced people that the electron-phonon mechanism was the correct explanation. As a mean-field theory, BCS by itself does not give many hints as to the origin of the superconductivity.

The reason the Eliashberg approach works so well is that Migdal's theorem tells us that the vertex corrections coming from terms other than the Fock contribution are small by a factor $\sqrt{m/M}$ that involves the ratio of the electron mass m to the ionic mass M.

Remark 348 *The DMFT equations can be obtained in a similar spirit. We look for a one-particle Green function* $\mathcal{G}^{-1}(k) = (\varepsilon_{\mathbf{k}} - \mu - \Sigma(k))$ *which is such that the self-energy computed with it, the self-energy of the effective medium, vanishes. However, instead of taking only the Fock term for the self-energy, we take the self-energy to all orders but local, i.e. computed with* $\mathcal{G}(k)$ *integrated over all wave vectors (so that it is local).*

70.5 Hamiltonien BCS réduit

Avec le changement de base

$$\psi_{\sigma}^{\dagger}(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k},\boldsymbol{\sigma}}^{\dagger} \langle \mathbf{k} | \mathbf{r} \rangle = \sum_{\mathbf{k}} c_{\mathbf{k},\boldsymbol{\sigma}}^{\dagger} \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\mathcal{V}}} \tag{70.18}$$

$$c_{\mathbf{k},\sigma}^{\dagger} = \int \psi_{\sigma}^{\dagger}(\mathbf{r}) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\mathcal{V}}} d^3\mathbf{r} \tag{70.19}$$

$$\int e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r} = \mathcal{V}\delta_{\mathbf{q},\mathbf{0}} \tag{70.20}$$

on a que

$$\begin{aligned} \rho(\mathbf{q}) &= \int e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}) d^3\mathbf{r} = \sum_{\sigma} \int e^{-i\mathbf{q}\cdot\mathbf{r}} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) d^3\mathbf{r} \\ &= \sum_{\sigma} \int e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}'} c_{\mathbf{k}',\sigma} \frac{e^{i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{\mathcal{V}}} \\ &= \sum_{\sigma} \sum_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q},\sigma} \end{aligned} \tag{70.21}$$

et la partie hamiltonien à deux corps s'écrit

$$H_I = \frac{1}{2\mathcal{V}} \sum_{\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U(\mathbf{q}) c_{\mathbf{k},\boldsymbol{\sigma}}^{\dagger} c_{\mathbf{k}',\boldsymbol{\sigma}'}^{\dagger} c_{\mathbf{k}'-\mathbf{q},\boldsymbol{\sigma}'} c_{\mathbf{k}+\mathbf{q},\boldsymbol{\sigma}} \tag{70.22}$$

où par définition,

$$U(\mathbf{q}) = \int d^3\mathbf{r} \mathbf{U}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \tag{70.23}$$

$$U(\mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} \mathbf{U}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{70.24}$$

Dans leur article de 1957, Bardeen-Cooper et Schrieffer partent d'un hamiltonien réduit très simplifié, ayant en tête que pour des énergies plus petites que l'énergie de Debye $\hbar\omega_D$, le potentiel effectif entre deux électrons peut devenir attractif. Retournons à notre Hamiltonien d'interaction général Éq.(70.22). Partant de l'idée de Cooper, on veut savoir comment traiter en champ moyen l'effet de l'attraction sur les paires d'électron de centre de masse nulle.

L'idée générale est que $c_{\mathbf{p}\uparrow}^{\dagger} c_{-\mathbf{p}\downarrow}^{\dagger}$ joue presque le rôle d'un boson $b_{\mathbf{p}}^{\dagger}$. Les relations de commutation de sont pas exactement les mêmes, mais nous voulons utiliser l'idée générale que la superfluidité pourra être décrite par une valeur moyenne non nulle de $b_{\mathbf{p}}^{\dagger}$ dans l'état supraconducteur. Cette valeur moyenne, $\left\langle c_{\mathbf{p}\uparrow}^{\dagger} c_{-\mathbf{p}\downarrow}^{\dagger} \right\rangle$

se retrouve dans l'équation de Ginzburg-Landau dans le rôle de fonction d'onde de paire. De la même façon que la suprafluidité pouvait être décrite par un ordre à longue portée hors-diagonal dans la matrice densité à une particule, ici ce phénomène apparaîtra dans la matrice densité à deux particules puisque chaque boson sera formé de deux fermions. L'état champ moyen que nous trouverons sera décrit par un état cohérent, comme vous le calculerez dans le devoir.

Dans l'esprit de la théorie de Weiss, nous supposerons que $\left\langle c^\dagger_{\mathbf{k},\boldsymbol{\sigma}} c^\dagger_{\mathbf{k}',\boldsymbol{\sigma}'} \right\rangle$ est non nul. Comme l'état fondamental conserve la quantité de mouvement et le spin, il faut que $\left\langle c^\dagger_{\mathbf{k},\boldsymbol{\sigma}} c^\dagger_{\mathbf{k}',\boldsymbol{\sigma}'} \right\rangle = \left\langle c^\dagger_{\mathbf{k},\boldsymbol{\sigma}} c^\dagger_{-\mathbf{k},-\boldsymbol{\sigma}} \right\rangle \delta_{\mathbf{k},-\mathbf{k}'} \delta_{\sigma,-\sigma'}$. En tenant compte de l'invariance sous rotation pour les spins, l'hamiltonien d'essai que nous utiliserons pour la théorie champ moyen s'écrit à partir de l'expression générale Éq.(70.22) et de quelques changement de variables comme $\mathbf{k} \to \mathbf{p}$ et $\mathbf{k}+\mathbf{q} \to \mathbf{p}'$

$$\begin{aligned} H_E - \mu N &= H_0 - \mu N + \frac{1}{\mathcal{V}} \sum_{\mathbf{p},\mathbf{p}'} U(\mathbf{p}-\mathbf{p}') \left\langle c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow} \right\rangle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \\ &\quad + \frac{1}{\mathcal{V}} \sum_{\mathbf{p},\mathbf{p}'} U(\mathbf{p}-\mathbf{p}') c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow} \left\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \right\rangle \\ &= H_0 - \mu N + \sum_{\mathbf{p}} \left(\Delta^*_{\mathbf{p}} c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} + c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow} \Delta_{\mathbf{p}} \right) \end{aligned} \tag{70.25}$$

où on a défini

$$\Delta_{\mathbf{p}} = \frac{1}{\mathcal{V}} \sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}') \left\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \right\rangle . \tag{70.26}$$

La forme de $U(\mathbf{p}-\mathbf{p}')$ sera discutée plus tard, mais ici nous gardons à l'esprit que ce potentiel est attractif pour des états qui sont à l'intérieur d'une coque d'énergie de taille $\hbar\omega_D$ autour du niveau de Fermi.

Pour la partie cinétique de l'hamiltonien on écrit

$$H_0 - \mu N = \sum_{\mathbf{p},\boldsymbol{\sigma}} (\varepsilon_{\mathbf{p}} - \mu) c^\dagger_{\mathbf{p},\boldsymbol{\sigma}} c_{\mathbf{p},\boldsymbol{\sigma}} \tag{70.27}$$

$$\equiv \sum_{\mathbf{p},\boldsymbol{\sigma}} \zeta_{\mathbf{p}} c^\dagger_{\mathbf{p},\boldsymbol{\sigma}} c_{\mathbf{p},\boldsymbol{\sigma}} . \tag{70.28}$$

Dans le modèle du jellium, $\varepsilon_{\mathbf{p}} = \hbar^2\mathbf{p}^2/2m_e$ mais on peut prendre une relation de dispersion plus générale. Sous forme matricielle, la combinaison de tous ces termes nous donne, à une constante près

$$H_E - \mu N = \sum_{\mathbf{p}} \begin{pmatrix} c^\dagger_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{-\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} . \tag{70.29}$$

Comme dans le cas de l'antiferroaimant, on veut trouver une transformation canonique qui diagonalise la matrice. Lorsque ce sera fait, les $c^{(\dagger)}_{-\mathbf{p}\downarrow}$ seront des combinaisons linéaires des opérateurs propres qui diagonalisent l'hamiltonien. Ces combinaisons linéaires feront intervenir $\Delta_{\mathbf{p}}$. Pour déterminer la valeur de $\Delta_{\mathbf{p}}$, il suffira donc de substituer pour les $c_{\mathbf{p}\boldsymbol{\sigma}}$ de l'équation définissant $\Delta_{\mathbf{p}}$, Éq.(E.2), les combinaisons linéaires d'opérateurs propres et nous obtiendrons alors une équation auto-cohérente pour $\Delta_{\mathbf{p}}$.C'est la même procédure que celle que nous avons employée dans la théorie de Weiss du modèle d'Ising.

Cette fois-ci, dans la diagonalisation ce sont les relations d'anticommutation qu'on veut préserver. Soit le spineur de Nambu, qu'on définit par

$$\Psi_{\mathbf{p}} = \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \tag{70.30}$$

on a alors que l'anticommutateur est donné par

$$\left\{\Psi_{\mathbf{p},i},\Psi^{\dagger}_{\mathbf{p}',j}\right\}=\delta_{\mathbf{p},\mathbf{p}'}\delta_{i,j} \tag{70.31}$$

où i et j identifent les composantes du spineur de Nambu. Dans le cas des bosons de Holstein-Primakov nous avions une matrice de Pauli à droite. Cette fois-ci nous avons l'identité, donc n'importe quelle transformation unitaire des spineurs de Nambu satisfera les relations d'anticommutation. On peut donc procéder par des moyens standards puisque la matrice à diagonaliser est hermitienne et donc diagonalisable par une transformation unitaire. Nous allons donner deux façons de trouver la matrice de transformation unitaire.

70.6 Méthode de diagonalisation utilisant l'algèbre des spineurs

On peut écrire la matrice hamiltonienne Éq.(70.29) sous la forme

$$H_E-\mu N=\zeta_{\mathbf{p}}\tau_3+\Delta_1\tau_1-\Delta_2\tau_2 \tag{70.32}$$

où les τ_i sont les matrices de Pauli définies dans l'espace de Nambu de la même façon que les matrices de Pauli habituelles:

$$\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}:\tau_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix};\tau_1=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{70.33}$$

Les quantités Δ_1 et Δ_2 sont, respectivement, les parties réelles et imaginaires du gap $\Delta_{\mathbf{p}}$. On peut aussi écrire

$$H_E-\mu N=|\mathbf{n}|\ \widehat{\mathbf{n}}\cdot\boldsymbol{\tau} \tag{70.34}$$

où le vecteur $\mathbf{n}$ est de norme $|\mathbf{n}|=\sqrt{\zeta_{\mathbf{p}}^2+|\Delta_{\mathbf{p}}|^2}$ et dirigé dans la direction du vecteur unité $\widehat{\mathbf{n}}$ de composantes $n_1=\zeta_{\mathbf{p}}/|\mathbf{n}|$, $n_2=\Delta_1/|\mathbf{n}|$ et $n_3=-\Delta_2/|\mathbf{n}|$. Pour diagonaliser, il suffira de faire des combinaisons linéaires qui correpondent à se placer dans la base où $\widehat{\mathbf{n}}$ pointe dans la direction 3. À ce moment, la mtrice sera diagonale et les valeurs porpres seront Les valeurs propres sont $\pm|\mathbf{n}|=\pm\sqrt{\zeta_{\mathbf{p}}^2+|\Delta_{\mathbf{p}}|^2}=\pm E_{\mathbf{p}}$.

La dépendance en $\mathbf{p}$ de $\mathbf{n}$ de Δ_1,Δ_2 et des angles θ et ϕ que nous introduisons à l'instant sont sous-entendues. En coordonnées polaires, le vecteur $\widehat{\mathbf{n}}$ est à un angle θ de l'axe 3 dont le cosinus est $\cos\theta=\zeta_{\mathbf{p}}/\sqrt{\zeta_{\mathbf{p}}^2+|\Delta_{\mathbf{p}}|^2}=\zeta_{\mathbf{p}}/E_{\mathbf{p}}$. L'angle ϕ dans le plan est obtenu de $\tan\phi=-\Delta_2/\Delta_1$, i.e. $\Delta=\Delta_1+i\Delta_2=|\Delta|\,e^{-i\phi}$. Les vecteurs propres dans le cas où $\widehat{\mathbf{n}}$ est dans la direction de l'axe 3 sont $\begin{pmatrix}1\\0\end{pmatrix}$ et $\begin{pmatrix}0\\1\end{pmatrix}$. Les vecteurs propres correspondant à $\widehat{\mathbf{n}}\cdot\boldsymbol{\tau}$ sont donc obtenus en tournant $\begin{pmatrix}1\\0\end{pmatrix}$ et $\begin{pmatrix}0\\1\end{pmatrix}$ d'un angle θ autour de l'axe 2 puis ϕ autour de l'axe 3 pour ramener l'axe de quantification dans la direction de $\widehat{\mathbf{n}}$. Ceci se fait avec la transformation unitaire $U=e^{-i\tau_3\frac{\phi}{2}}e^{-i\tau_2\frac{\theta}{2}}$ comme pour un spin 1/2. On a

$$e^{-i\tau_3\frac{\phi}{2}}=\begin{pmatrix}e^{-i\phi/2}&0\\0&e^{i\phi/2}\end{pmatrix} \tag{70.35}$$

et

$$e^{-i\tau_2\frac{\theta}{2}} = \cos\frac{\theta}{2} - i\tau_2 \sin\frac{\theta}{2}. \tag{70.36}$$

Il suffit d'utiliser des identités trigonométriques et la valeur de $\cos\theta = \zeta_{\mathbf{p}}/E_{\mathbf{p}}$ pour obtenir

$$\cos\frac{\theta}{2} = \sqrt{\frac{\cos\theta+1}{2}} = \frac{1}{\sqrt{2}}\left(1+\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} \tag{70.37}$$

$$\sin\frac{\theta}{2} = \frac{1}{\sqrt{2}}\left(1-\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} \tag{70.38}$$

ce qui donne la matrice des vecteurs propres, i.e. la transformation unitaire requise

$$\begin{aligned} U &= e^{-i\tau_3\frac{\phi}{2}}e^{-i\tau_2\frac{\theta}{2}} = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}}\left(1+\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} & -\frac{1}{\sqrt{2}}\left(1-\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} \\ \frac{1}{\sqrt{2}}\left(1-\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} & \frac{1}{\sqrt{2}}\left(1+\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}}\left(1+\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{-i\phi_{\mathbf{p}}/2} & -\frac{1}{\sqrt{2}}\left(1-\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{-i\phi_{\mathbf{p}}/2} \\ \frac{1}{\sqrt{2}}\left(1-\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{i\phi_{\mathbf{p}}/2} & \frac{1}{\sqrt{2}}\left(1+\frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{i\phi_{\mathbf{p}}/2} \end{pmatrix}. \end{aligned} \tag{70.39}$$

Nous avons réinséré la dépendance en $\mathbf{p}$ de la phase et introduit, dans la dernière ligne, les définitions conventionnelles pour $u_{\mathbf{p}}$ et $v_{\mathbf{p}}$.

Transformation de Boboliubov

La matrice U permet de diagonaliser l'hamiltonien d'essai

$$\begin{pmatrix} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{pmatrix} = U^\dagger \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{\mathbf{p}} \end{pmatrix} U.$$

donc

$$\begin{aligned} H_E - \mu N &= \sum_{\mathbf{p}} \begin{pmatrix} c^\dagger_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{pmatrix} UU^\dagger \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{\mathbf{p}} \end{pmatrix} UU^\dagger \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \\ &= \sum_{\mathbf{p}} \begin{pmatrix} \alpha^\dagger_{\mathbf{p}\uparrow} & \alpha_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \qquad (70.40) \\ &= \sum_{\mathbf{p},\boldsymbol{\sigma}} E_{\mathbf{p}} \alpha^\dagger_{\mathbf{p},\sigma}\alpha_{\mathbf{p},\boldsymbol{\sigma}} + cte. \qquad (70.41) \end{aligned}$$

où les nouveaux opérateurs sont reliés aux anciens par la transformation de Bogoliubov-Valentin (1958)

$$\begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} = U^\dagger \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} = \begin{pmatrix} u^*_{\mathbf{p}} & v_{\mathbf{p}} \\ -v^*_{\mathbf{p}} & u_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix}. \tag{70.42}$$

avec $|u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2 = 1$. Le fondamental est l'état qui est détruit par ces nouveaux opérateurs d'annihilation

$$\alpha_{\mathbf{p}\boldsymbol{\sigma}} |BCS\rangle = 0.$$

Les nouveaux opérateurs sont des combinaisons linéaires d'opérateurs de création et d'annihilation puisque l'état propre est une combinaison linéaire d'états ayant des nombres de particules différents.

État fondamental BCS

L'état fondamental s'obtient de façon systématique comme suit. Tout d'abord, on remarque que le vide de l'opérateur de destruction de Nambu Éq.(70.30) est donné par $|\Omega\rangle = \prod_{\mathbf{p}} c^\dagger_{-\mathbf{p}\downarrow} |0\rangle$, où le produit est sur toutes les valeurs de $\mathbf{p}$ dans la zone de Brillouin. Si on appelle $\boldsymbol{\gamma}_\mathbf{p}$ l'opérateur de destruction de Nambu dans la base propre, alors cet opérateur de destruction est relié aux opérateurs trouvés ci-dessus par

$$\boldsymbol{\gamma}_\mathbf{p} \equiv \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \equiv \begin{pmatrix} \gamma_{1,\mathbf{p}} \\ \gamma_{2,\mathbf{p}} \end{pmatrix}. \tag{70.43}$$

L'hamiltonien diagonalisé Éq.(70.40) s'écrit alors

$$H_E - \mu N_E = \sum_{\mathbf{p}} \begin{pmatrix} \gamma^\dagger_{1,\mathbf{p}} & \gamma^\dagger_{2,\mathbf{p}} \end{pmatrix} \begin{pmatrix} E_\mathbf{p} & 0 \\ 0 & -E_\mathbf{p} \end{pmatrix} \begin{pmatrix} \gamma_{1,\mathbf{p}} \\ \gamma_{2,\mathbf{p}} \end{pmatrix}. \tag{70.44}$$

Le fondamental s'obtient en remplissant tous les états d'énergie négative, donc

$$\begin{aligned} |BCS\rangle &= \prod_{\mathbf{p}'} \gamma^\dagger_{2,\mathbf{p}'} |\Omega\rangle = \prod_{\mathbf{p}'} \gamma^\dagger_{2,\mathbf{p}'} \prod_{\mathbf{p}} c^\dagger_{-\mathbf{p}\downarrow} |0\rangle \\ &= \prod_{\mathbf{p}'} \alpha_{-\mathbf{p}'\downarrow} \prod_{\mathbf{p}} c^\dagger_{-\mathbf{p}\downarrow} |0\rangle \\ &= \prod_{\mathbf{p}'} \left(-v_{\mathbf{p}'} c^\dagger_{\mathbf{p}'\uparrow} + u^*_{\mathbf{p}'} c_{-\mathbf{p}'\downarrow} \right) \prod_{\mathbf{p}} c^\dagger_{-\mathbf{p}\downarrow} |0\rangle \\ &= \prod_{\mathbf{p}} \left(-v_\mathbf{p} c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow} + u^*_\mathbf{p} \right) |0\rangle \end{aligned} \tag{70.45}$$

ce qui correspond bien, à un facteur de normalisation près, à la fonction d'onde de BCS mentionnée plus loin Éq.(70.68).

Équation du gap

Comme dans le cas de la théorie de Weiss pour le modèle d'Ising au chapitre 4, l'Hamiltonien dépend d'un paramètre d'ordre $\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle$ ($\langle S_z \rangle$ dans le cas d'Ising) dont la valeur peut être calculée une fois l'Hamiltonien diagonalisé. Cela donne une équation d'auto-cohérence.

Ici donc, la valeur du gap $\Delta_\mathbf{p}$ s'obtient de l'équation autocohérente Éq.(E.2). Il suffit de réécrire les opérateurs $c_{\mathbf{p}\uparrow}$ en fonction des opérateurs diagonaux $\alpha_{\mathbf{p}\boldsymbol{\sigma}}$. Inversons la transformation de Bogoliubov Éq.(E.18)

$$\begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} = \begin{pmatrix} u_\mathbf{p} & -v_\mathbf{p} \\ v^*_\mathbf{p} & u^*_\mathbf{p} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \tag{70.46}$$

dont l'adjoint donne

$$\begin{pmatrix} c^\dagger_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{pmatrix} = \begin{pmatrix} \alpha^\dagger_{\mathbf{p}\uparrow} & \alpha_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} u^*_\mathbf{p} & v_\mathbf{p} \\ -v^*_\mathbf{p} & u_\mathbf{p} \end{pmatrix} \tag{70.47}$$

On note aussi que

$$n(E_\mathbf{p}) \equiv \left\langle \alpha^\dagger_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow} \right\rangle = \frac{1}{e^{\beta E_\mathbf{p}} + 1}. \tag{70.48}$$

La distribution de Fermi Dirac vient du fait que l'hamiltonien est quadratique lorsqu'exprimé en fonction des opérateurs fermioniques $\alpha^{(\dagger)}_\mathbf{p}$. Ces quasiparticules n'ont pas de potentiel chimique qui leur est associé. Ce dernier demeure associé au nombre de particules total.

Preuve Chaque état $\mathbf{p}$ est indépendant. En d'autres mots, à une constante près, l'Hamiltonien BCS peut s'écrire

$$H_{BCS} = \sum_{\mathbf{p},\boldsymbol{\sigma}} E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\boldsymbol{\sigma}} \alpha_{\mathbf{p}\boldsymbol{\sigma}} \tag{70.49}$$

et donc, la fonction de partition factorise. Ceci veut dire que le nombre moyen $\left\langle \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow} \right\rangle$ peut s'écrire

$$\begin{aligned} \left\langle \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow} \right\rangle &= \frac{\mathrm{Tr}\left[\exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right) \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right]}{\mathrm{Tr}\left[\exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right)\right]} & (70.50) \\ &= -\frac{\partial}{\partial\left(\beta E_{\mathbf{p}}\right)} \ln \mathrm{Tr}\left[\exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right)\right] & (70.51) \end{aligned}$$

avec

$$\begin{aligned} \mathrm{Tr}\left[\exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\boldsymbol{\sigma}} \alpha_{\mathbf{p}\boldsymbol{\sigma}}\right)\right] &= \langle BCS| \exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right) |BCS\rangle & (70.52) \\ &\quad + \langle BCS| \alpha_{\mathbf{p}\uparrow} \exp\left(-\beta E_{\mathbf{p}} \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow}\right) \alpha^{\dagger}_{\mathbf{p}\uparrow} |BCS\rangle & (70.53) \\ &= 1 + \exp\left(-\beta E_{\mathbf{p}}\right). & (70.54) \end{aligned}$$

De là, on trouve

$$\begin{aligned} \left\langle \alpha^{\dagger}_{\mathbf{p}\uparrow} \alpha_{\mathbf{p}\uparrow} \right\rangle &= -\frac{\partial}{\partial\left(\beta E_{\mathbf{p}}\right)} \ln\left(1 + \exp\left(-\beta E_{\mathbf{p}}\right)\right) \\ &= \frac{\exp\left(-\beta E_{\mathbf{p}}\right)}{1 + \exp\left(-\beta E_{\mathbf{p}}\right)} = \frac{1}{e^{\beta E_{\mathbf{p}}} + 1}. \end{aligned}$$

À l'aide du résultat précédent, nous pouvons maintenant évaluer la valeur moyenne d'occupation d'une paire

$$\begin{aligned} \langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle &= \left\langle \left(v_{\mathbf{p}'} \alpha^{\dagger}_{\mathbf{p}'\uparrow} + u_{\mathbf{p}'} \alpha_{-\mathbf{p}'\downarrow}\right) \left(u_{\mathbf{p}'} \alpha_{\mathbf{p}'\uparrow} - v_{\mathbf{p}'} \alpha^{\dagger}_{-\mathbf{p}'\downarrow}\right) \right\rangle & (70.55) \\ &= v_{\mathbf{p}'} u_{\mathbf{p}'} \left\langle \alpha^{\dagger}_{\mathbf{p}'\uparrow} \alpha_{\mathbf{p}'\uparrow} - \alpha_{-\mathbf{p}'\downarrow} \alpha^{\dagger}_{-\mathbf{p}'\downarrow} \right\rangle & (70.56) \\ &= -v_{\mathbf{p}'} u_{\mathbf{p}'} \left(1 - 2f(E_{\mathbf{p}'})\right) & (70.57) \\ &= -\frac{1}{2} \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2f(E_{\mathbf{p}'})\right). & (70.58) \end{aligned}$$

Nous avons utilisé le fait que dans l'état BCS $\left\langle \alpha^{\dagger}_{\mathbf{p}'\uparrow} \alpha^{\dagger}_{-\mathbf{p}'\downarrow} \right\rangle = 0$. Dans la dernière équation, $\Delta_{\mathbf{p}'}$ est un nombre complexe. La dernière égalité est vraie, peu importe la convention qu'on prend pour les phases de $v_{\mathbf{p}'}$ et $u_{\mathbf{p}'}$. En effet, si on utilise les phases obtenues avec la méthode standard pour obtenir la transformation de Boliubov, $-v_{\mathbf{p}'} u_{\mathbf{p}'} \left(1 - 2f(E_{\mathbf{p}'})\right)$ s'écrit

$$\begin{aligned} \langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle &= -\frac{1}{2} \left(1 - \frac{\zeta^2_{\mathbf{p}'}}{E^2_{\mathbf{p}'}}\right)^{1/2} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2f(E_{\mathbf{p}'})\right) \\ &= -\frac{1}{2} \frac{|\Delta_{\mathbf{p}'}|}{E_{\mathbf{p}'}} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2f(E_{\mathbf{p}'})\right). & (70.59) \end{aligned}$$

alors qu'avec les phases de la méthode des spineurs

$$\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle = -\frac{1}{2} \frac{|\Delta_{\mathbf{p}'}|}{E_{\mathbf{p}'}} e^{-i\phi_{\mathbf{p}'}} \left(1 - 2f(E_{\mathbf{p}'})\right). \tag{70.60}$$

Dans les deux cas, les phases se combinent avec la grandeur du gap pour donner $\Delta_{\mathbf{p}'}$.

Les facteurs du type $v_{\mathbf{p}'}u_{\mathbf{p}'}$ que l'on retrouve ci-dessus s'appellent des facteurs de cohérence. En substituant l'Expression obtenue pour $\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\rangle$ dans l'équation autocohérente Éq.(E.2) on obtient

$$\Delta_{\mathbf{p}} = -\frac{1}{2\mathcal{V}}\sum_{\mathbf{p}'} U\left(\mathbf{p}-\mathbf{p}'\right)\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.61}$$

Ceci est l'équation du gap de BCS.

Remark 349 *Notons que $c_{\mathbf{p}\uparrow}$ et $c_{-\mathbf{p}\downarrow}$ créent des états qui sont reliés par la symétrie d'inversion du temps. En présence d'impuretés, il faut apparier des états propres du système qui sont aussi reliés par la symétrie d'inversion du temps. La présence d'impuretés qui ne brisent pas cette symétrie n'influence donc essentiellement pas la valeur de T_c. C'est un théorème dû à P.W. Anderson.*

Remark 350 *L'équation Éq.(70.60) révèle que le paramètre d'ordre $\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\rangle$ qui apparaît sous la forme ψ dans l'équation de Ginzburg-Landau est proportionnel au gap dans la théorie de BCS mais il n'est pas identique au gap. Il aura cependant la même symétrie.*

Remark 351 *Fonction d'onde de paire: On peut trouver l'étendue de la fonction d'onde de paire de la façon suivante.*

$$\langle c_{\mathbf{r}\downarrow}c_{\mathbf{r}'\uparrow}\rangle = \frac{1}{\mathcal{V}}\sum_{\mathbf{p}'}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{r}}e^{-i\mathbf{p}'\cdot\mathbf{r}'}\langle c_{\mathbf{p}\downarrow}c_{\mathbf{p}'\uparrow}\rangle \tag{70.62}$$

Utilisant le fait qu'il n'y a que $\mathbf{p}' = -\mathbf{p}$ qui a une valeur moyene non nulle, il reste

$$\langle c_{\mathbf{r}\downarrow}c_{\mathbf{r}'\uparrow}\rangle = \sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\langle c_{\mathbf{p}\downarrow}c_{-\mathbf{p}\uparrow}\rangle. \tag{70.63}$$

La valeur moyenne dans l'intégrand a été calculée plus haut 70.60. À $T = 0$ il reste

$$\langle c_{\mathbf{r}\downarrow}c_{\mathbf{r}'\uparrow}\rangle = -\frac{1}{2}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\left(1-\frac{\zeta_{\mathbf{p}'}^2}{E_{\mathbf{p}'}^2}\right)^{1/2} e^{-i\phi_{1\mathbf{p}}-i\phi_{2\mathbf{p}}}. \tag{70.64}$$

Nous allons voir plus loin que les phases sont indépendantes de $\mathbf{p}$. De plus, l'intégrand s'annule pour $\zeta_{\mathbf{p}}^2 >> |\Delta_{\mathbf{p}}|^2$ car dans ce cas $E_{\mathbf{p}}^2 \sim \zeta_{\mathbf{p}}^2$. Le vecteur d'onde ne peut donc varier sur des intervalles plus grand que $\zeta_{\mathbf{p}} \sim \Delta_{\mathbf{p}}$ ce qui correspond à une énergie $\hbar v_F\delta p \sim \Delta_{\mathbf{p}}$. Comme en transformée de Fourier, la largeur dans l'espace δr est reliée à la largeur en vecteur d'onde δp par $\delta x \sim 1/\delta p$, on a que $\delta x \sim \hbar v_F/\Delta_{\mathbf{p}}$.Ceci est l'ordre de grandeur de la longueur de corrélation à température nulle.

70.6.1 Approche variationnelle

Suivant l'approche générale développée antérieurement, on peut utiliser l'hamiltonien d'essai BCS Eq.(E.1) pour définir une fonctionelle à minimiser

$$\langle H-\mu N\rangle_E - TS\left(D_E\right) \tag{70.65}$$

par rapport à $\Delta_{\mathbf{p}}$. On retrouve alors les résultats précédents. C'est l'approche qui est utilisée dans l'article original de BCS. L'équation du gap est obtenu à partir de la doncition de minimisation de l'énergie libre. Pour plus de détails, voir les notes de Claude Bourbonnais.

70.6.2 Cohérence de phase, fonction d'onde

Un des résultats les plus importants du point de vue conceptuel que nous apprend BCS est que même lorsque l'interaction dépend de $\mathbf{p}-\mathbf{p}'$, la phase du gap doit nécessairement être indépendante de $\mathbf{p}$. En effet, réécrivons l'équation du gap Éq.(70.61) sous la forme

$$[C_{\mathbf{p}}\Delta_{\mathbf{p}}] = -\frac{1}{2\mathcal{V}}\sum_{\mathbf{p}'} C_{\mathbf{p}}U\left(\mathbf{p}-\mathbf{p}'\right)C_{\mathbf{p}'}\left[C_{\mathbf{p}'}\Delta_{\mathbf{p}'}\right]. \tag{70.66}$$

où

$$C_{\mathbf{p}} = \left(\frac{\left(1-2n\left(E_{\mathbf{p}}\right)\right)}{E_{\mathbf{p}}}\right)^{1/2}. \tag{70.67}$$

Tout à l'intérieur de la racine carré est positif ($E_{\mathbf{p}}$ est positif, donc $n\left(E_{\mathbf{p}}\right)$ est plus petit que $1/2$). Donc, la quantité $C_{\mathbf{p}}$ est réelle. On peut alors la réinterpréter comme une équation aux valeurs propres. Les vecteurs propres sont entre crochets et la valeur propre est l'unité. Comme la matrice $-C_{\mathbf{p}}U\left(\mathbf{p}-\mathbf{p}'\right)C_{\mathbf{p}'}/\left(2\mathcal{V}\right)$ dont on cherche le vecteur propre est réelle symétrique, ce vecteur propre est réel à une phase globale près, à moins que la valeur propre ne soit dégénérée. Il y a une dégénérescence évidente associée à la symétrie sous inversion du temps. Lorsqu'on brise cette symétrie, le paramètre d'ordre est complexe. Cela ne donne un résultat non trivial que pour les valeurs de moment cinétique orbital différents de zéro (voir plus loin).

Cela nous permet de revenir sur la notion de cohérence. Nous venons de montrer que $\Delta_{\mathbf{p}}$ est un nombre complexe dont la phase est indépendante de $\mathbf{p}$, en d'autres mots $\phi_{1\mathbf{p}}+\phi_{2\mathbf{p}}=\phi$ pour toutes les valeurs de $\mathbf{p}$. Toutes les paires sont ajoutées à la fonction d'onde avec exactement la même phase. Ceci se voit bien avec la forme de la fonction d'onde de BCS traitée en devoir:

$$\prod_{\mathbf{k}}\left(1+\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^{*}}c_{-\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}^{\dagger}\right)\left|0\right\rangle. \tag{70.68}$$

À chaque fois qu'on crée une paire, il y a un facteur de phase $e^{-i\phi_{1\mathbf{p}}-i\phi_{2\mathbf{p}}}=e^{-i\phi_{\mathbf{p}}}$ associé qui vient du $v_{\mathbf{k}}/u_{\mathbf{k}}^{*}$. Seule la phase de Δ *indépendante de* $\mathbf{p}$ est arbitraire. On brise la symétrie de jauge globale en la fixant parce que phase et nombre de particules obéissent à une relation d'incertitude. Fixer la phase correspond donc à rendre le nombre total de particules incertain. Nous reviendrons à cette discussion avec la jonction Josephson.

La structure de la fonction d'onde *BCS* est la même que dans un état cohérent. La composante à n paires de Cooper de la fonction d'onde contient un préfacteur proportionnel à $e^{-in\phi}$, analogue au z^{n} que nous avions discuté.Nous pouvons même aller plus point en réécrivant chaque facteur $\left(1+\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^{*}}c_{-\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}^{\dagger}\right)$ sous la forme exponentielle de telle sorte que la fonction d'onde s'écrit aussi

$$\prod_{\mathbf{k}} e^{\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^{*}}c_{-\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}^{\dagger}}\left|0\right\rangle. \tag{70.69}$$

Les puissances d'ordre plus élevé de l'argument de l'exponentielle s'annulent car nous avons affaire à des fermions.

Comme nous avons vu au début de cette section, ce sont les interactions qui imposent cette cohérence de phase qui est à l'origine du phénomène de supraconductivité. On peut aussi comprendre la cohérence de phase intuitivement ainsi. Considérons un des termes de l'Hamiltonien: $\sum_{\mathbf{p},\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\ c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow}\ c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow}$. On voit qu'il y a avantage à ce que les paires aient la même phase, sinon on aurait un terme $e^{i\left(\phi_{\mathbf{p}}-\phi_{\mathbf{p}'}\right)}$ qui apparaîtrait et aurait tendance à moyenner les phases à zéro. Retournant à l'expression pour l'interaction dans l'hamiltonien réduit de BCS, $\sum_{\mathbf{p}}\left(\Delta^*_{\mathbf{p}} c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} + c^\dagger_{\mathbf{p}\uparrow} c^\dagger_{-\mathbf{p}\downarrow}\Delta_{\mathbf{p}}\right)$, On voit que de défaire une paire $c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow}$ est coûteux car celle-ci est couplée à un champ moyen macroscopique $\Delta_{\mathbf{p}}$. C'est tout à fait analogues à ce que nous avons fait avec le modèle d'Ising traité dans l'approximation de Weiss où chaque spin est couplé à un champ moyen.

70.6.3 Singlet $s-wave$ superconductivity

Going to the continuum limit, the gap equation takes the form,

$$\Delta_{\mathbf{p}} = -\frac{1}{2}\int \frac{d^3p'}{(2\pi)^3} U(\mathbf{p}-\mathbf{p}')\,\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.70}$$

The wave vectors that are involved in pairing are close to the Fermi surface. I take a spherical Fermi surface to simplfy the calculations. Going to polar coordinates and using the single-spin density of states $N(\zeta)$ relating the integral over the magnitude of p to the integral over ζ

$$\int \frac{p'^2 dp'}{(2\pi)^3} = \int_{\zeta_{\min}}^{\zeta_{\max}} N\left(\zeta'\right) d\zeta' \int_{-1}^{1} \frac{d\cos\theta'}{2} \int_0^{2\pi} \frac{d\phi'}{2\pi} \tag{70.71}$$

the gap equation becomes

$$\Delta_{\mathbf{p}} = -\int_0^{\infty} N\left(\zeta'\right) d\zeta' \int_{-1}^{1} \frac{d\cos\theta'}{2} \int_0^{2\pi} \frac{d\phi'}{2\pi} U(\mathbf{p}-\mathbf{p}')\,\frac{\Delta_{\mathbf{p}'}}{2E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.72}$$

For the simplified BCS Hamiltonian, $U(\mathbf{p}-\mathbf{p}')$ is simply a negative constant, let us say U_0, that vanishes as soon as $\mathbf{p}$ or $\mathbf{p}'$ have an energy difference with the Fermi surface that is larger in absolute value than the Debye energy. In that case, the gap equation takes the simplified form

$$\Delta_{\mathbf{p}} = |U_0| \int_{-\hbar\omega_D}^{\hbar\omega_D} N\left(\zeta'\right) d\zeta' \int_{-1}^{1} \frac{d\cos\theta'}{2} \int_0^{2\pi} \frac{d\phi'}{2\pi} \frac{\Delta_{\mathbf{p}'}}{2E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.73}$$

The right-hand side of this equation is independent of $\mathbf{p}$, so we write $\Delta_{\mathbf{p}} = \Delta$ and the gap equation becomes

$$\Delta = |U_0| \int_{-\hbar\omega_D}^{\hbar\omega_D} N\left(\zeta'\right) d\zeta' \frac{\Delta}{2E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.74}$$

I will show you the solution of this equation in the following section. But first, I discuss in more details symmetry questions, and first, questions of spin symmetry of the Cooper pair wave function. The latter is related to the gap by Eq. (70.60) obtained with the Bogoliubov transformation

$$\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow}\rangle = -\frac{1}{2}\frac{\Delta}{E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right). \tag{70.75}$$

This result is invariant under symmetry operations on the lattice since Δ and $E_{\mathbf{p}} = \sqrt{\zeta_{\mathbf{p}}^2 + |\Delta|^2}$ are. But, anticommutation of destruction operators leads to

$$\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle = - \langle c_{\mathbf{p}'\uparrow} c_{-\mathbf{p}'\downarrow} \rangle . \tag{70.76}$$

Using invariance under inversion of $\mathbf{p}'$, I can change $\mathbf{p}'$ into $-\mathbf{p}'$ on the right-hand side to find,

$$\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle = - \langle c_{-\mathbf{p}'\uparrow} c_{\mathbf{p}'\downarrow} \rangle . \tag{70.77}$$

In other words, the pair wave function is odd under interchange of the spins. It is a spin singlet. Since there is no dependence on the orientation of $\mathbf{p}$, it is usually stated that the pair wave function is in an s state. In reality, we should say that it belongs to the totally symmetric irreducible representation of the symmetry group of the crystal. But that is another matter since here I am working with a continuum model.

There will be a spin singlet in all cases where $\Delta_{\mathbf{p}}$ will be even under inversion of $\mathbf{p}$,namely when the angular momentum of the pair will be even. We will end up with a spin triplet when the angular momentum is odd, following the general principle that the wave function must change sign when two particles are interchanged.

70.7 Solution de l'équation BCS, T_c et équation de Ginzburg-Landau, gap à $T = 0$

Comme seuls les états près du niveau de Fermi contribueront, supposons qu'on prenne la densité d'états comme constante. L'équation du gap BCS pour la supraconductivité de type s devient alors, avec la définition $D(E_F) = 2N(E_F)$,(on suppose la symétrie particule trou pour intégrer seulement pour ζ' positif)

$$\begin{aligned} \Delta &= |U_0| D(E_F) \int_0^{\hbar\omega_D} d\zeta' \frac{\Delta}{2E_{\mathbf{p}'}} (1 - 2f(E_{\mathbf{p}'})) \\ &= \Delta \frac{|U_0| D(E_F)}{2} \int_0^{\hbar\omega_D} \frac{\tanh\left(\frac{1}{2}\beta\sqrt{\zeta^2 + |\Delta|^2}\right)}{\sqrt{\zeta^2 + |\Delta|^2}} d\zeta. \end{aligned} \tag{70.78}$$

Nous avons utilisé $1 - 2f(E_{\mathbf{p}'}) = \tanh(\beta E_{\mathbf{p}}/2)$.

On peut retrouver la condition d'extremum d'une théorie de Landau Ginzburg en $|\Delta|^2$ simplement en notant que pour $|\Delta|^2$ petit on peut utiliser le développement de Taylor

$$\begin{aligned} \frac{\tanh\left(\sqrt{a+x}\right)}{\sqrt{a+x}} &= \frac{\tanh\sqrt{a}}{\sqrt{a}} \\ &\quad + x\left(-\frac{\tanh\sqrt{a}}{2a^{\frac{3}{2}}} + \frac{1}{2a}\frac{1}{\cosh^2\sqrt{a}}\right) + O\left(x^2\right). \end{aligned}$$

En substituant dans l'équation du gap, on obtient une équation de la forme

$$\Delta = a''\Delta + b''|\Delta|^2 \Delta \tag{70.79}$$

où les constantes a'' et b'' dépendent de la température. La valeur de T_c est celle pour laquelle $a'' = 1$. Pour $T < T_c$ on aura $a'' < 1$ de telle sorte que $|\Delta|^2$ sera positif.

Pour trouver la partie dépendante de l'espace de l'équation de Ginzburg Landau c'est plus compliqué. Il est clair cependant que le champ électromagnétique se couplera aux opérateurs de création-annihilationavec le couplage minimal de telle sorte qu'il redonnera exactement ce que nous avions dans la théorie de Ginzburg Landau.

On peut obtenir analytiquement la valeur de T_c et la valeur du gap Δ_0 à $T = 0$. Nous obtiendrons ainsi un des résultats les plus célèbres de la théorie de BCS, soit

$$\frac{2\Delta_0}{k_B T_c} = 3.53. \tag{70.80}$$

Commençons par le calcul du gap à $T = 0$. Dans ce cas, la tangente hyperbolique peut être prise égale à l'unité et l'équation du gap devient

$$\Delta_0 = \Delta_0 \frac{|U_0| D(E_F)}{2} \int_0^{\hbar\omega_D} \frac{1}{\sqrt{\zeta^2 + |\Delta_0|^2}} d\zeta. \tag{70.81}$$

La substitution $\zeta = |\Delta_0| \sinh\theta$ donne $d\zeta = d\theta\, |\Delta_0| \cosh\theta$ et

$$\begin{aligned} \int_0^{\hbar\omega_D} \frac{1}{\sqrt{\zeta^2 + |\Delta_0|^2}} d\zeta &= \int_0^{\sinh^{-1}\hbar\omega_D/|\Delta_0|} \frac{\cosh\theta\, d\theta}{\sqrt{\sinh^2\theta + 1}} \\ &= \int_0^{\sinh^{-1}\hbar\omega_D/|\Delta_0|} d\theta \\ &= \sinh^{-1}(\hbar\omega_D/|\Delta_0|) \end{aligned} \tag{70.82}$$

d'où

$$\frac{2}{|U_0| D(E_F)} = \sinh^{-1}(\hbar\omega_D/|\Delta_0|) \tag{70.83}$$

$$|\Delta_0| = \hbar\omega_D / \sinh\left(\frac{2}{|U_0| D(E_F)}\right). \tag{70.84}$$

La théorie de BCS est valide dans la limite couplage faible, c'est-à-dire $|U_0| D(E_F) \ll 1$. Cette inégalité se comprend bien intuitivement car $D(E_F)$ est inversement proportionnelle à l'énergie de Fermi alors que $|U_0|$ est une énergie beaucoup plus faible. Dans cette limite, on peut donc approximer

$$|\Delta_0| = 2\hbar\omega_D \exp\left(-\frac{2}{|U_0| D(E_F)}\right). \tag{70.85}$$

Pour calculer la valeur de T_c on évalue l'intégrale en mettant $|\Delta_0| = 0$ dans l'intégrand. On cherche donc la température telle que

$$1 = \frac{|U_0| D(E_F)}{2} \int_0^{\hbar\omega_D} \frac{\tanh(\beta_c\zeta/2)}{\zeta} d\zeta. \tag{70.86}$$

Le terme de droite est le a'' dont nous avons discuté plus haut. On intègre par parties le terme de droite pour obtenir dans la limite $\beta_c\hbar\omega_D \gg 1$

$$1 = \frac{|U_0| D(E_F)}{2} \left(\ln\left(\frac{\beta_c\hbar\omega_D}{2}\right) - \int_0^\infty \frac{\ln x}{\cosh^2 x} dx\right). \tag{70.87}$$

L'intégrale converge suffisamment rapidement que nous avons posé la borne supérieure d'intégration $\frac{\beta_c \hbar\omega_D}{2}$ égale à l'infini. Il reste

$$1 = \frac{|U_0|\, D\left(E_F\right)}{2}\left(\ln\left(\frac{\beta_c \hbar\omega_D}{2}\right) + \ln\left(\frac{4\gamma}{\pi}\right)\right) \tag{70.88}$$

où $\ln\gamma = C \approx 0.577216$ est la constante d'Euler. De là on déduit facilement

$$k_B T_c = \frac{2\gamma\hbar\omega_D}{\pi}\exp\left(-\frac{2}{|U_0|\, D\left(E_F\right)}\right) \tag{70.89}$$

$$= 1.1336\ \hbar\omega_D \exp\left(-\frac{2}{|U_0|\, D\left(E_F\right)}\right). \tag{70.90}$$

En combinant nos résultats pour $|\Delta_0|$ Éq.(70.74) et pour $k_B T_c$ ci-dessus, on trouve le fameux rapport BCS Eq.(70.80). Les résultats expérimentaux pour les éléments simples sont

Al	Cd	Hg	In	Nb	Pb	Sn	Ta
3.37 ± 0.1	$3.2 \pm .1$	4.6	$3.63 \pm .1$	$3.84 \pm .06$	$4.29 \pm .04$	$3.46 \pm .1$	$3.6 \pm .1$

Les éléments comme le plomb et le mercure sont des exemples typiques de supraconducteurs à couplage fort où la théorie d'Éliashberg est nécessaire.

Remark 352 *L'expression pour T_c explique immédiatement l'effet isotopique puisque la fréquence de Debye, comme celle pour un oscillateur harmonique, dépend de $M^{-1/2}$.*

70.7.1 $s, p, d...$ symmetries in the solution of the BCS equation

To see if it is possible to obtain angular momenta for the pair that are different from zero, we proceed as follows. Since U depends only on the magnitude of $\mathbf{p} - \mathbf{p}'$ and that $|\mathbf{p} - \mathbf{p}'| = \sqrt{p^2 + p'^2 - 2pp'\cos\Theta} \simeq \sqrt{2}p_F\sqrt{1-\cos\Theta}$ I can assume that $U\left(\mathbf{p} - \mathbf{p}'\right)$ is a function of $\cos\Theta$ only, a variable contained in the interval -1 to 1. It can thus be expanded in Legendre polynomials

$$U\left(\cos\Theta\right) = \sum_{l=0}^{\infty} U_\ell P_\ell\left(\cos\Theta\right). \tag{70.91}$$

I can then use the addition theorem for spherical harmonics that relates $P_\ell\left(\cos\Theta\right)$ to spherical harmonics defined for angles θ, ϕ and θ', ϕ' that give the orientation in polar coordinates of vectors $\mathbf{p}$ and $\mathbf{p}'$

$$P_\ell\left(\cos\Theta\right) = \frac{4\pi}{\left(2\ell+1\right)}\sum_{m=-\ell}^{\ell} Y_{\ell,m}\left(\theta,\phi\right) Y^*_{\ell,m}\left(\theta',\phi'\right). \tag{70.92}$$

Close to T_c the gap equation (E.2) can be linearized, so that for a spherical Fermi surface and the same hypothesis as before, it takes the form,

$$\Delta_{\mathbf{p}} = -2\int_0^{\hbar\omega_D} N\left(\zeta'\right)d\zeta' \int_{-1}^{1}\frac{d\cos\theta'}{2}\int_0^{2\pi}\frac{d\phi'}{2\pi} \tag{70.93}$$

$$\sum_{l=0}^{\infty} U_\ell \frac{4\pi}{\left(2\ell+1\right)}\sum_{m=-\ell}^{\ell} Y_\ell^m\left(\theta,\phi\right) Y_\ell^{m*}\left(\theta',\phi'\right)\frac{\Delta_{\mathbf{p}'}}{2\zeta'}\left(1 - 2f(\zeta')\right).$$

Using the orthogonality theorem for spherical harmonics

$$\int_{-1}^{1} d\cos\theta \int_{0}^{2\pi} d\phi Y_{\ell}^{m*}(\theta,\phi) Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell,\ell'}\delta_{m,m'} \tag{70.94}$$

and the fac that $\Delta_{\mathbf{p}}$ depends only on angle, I can define

$$\Delta_{\ell,m} = \int_{-1}^{1} d\cos\theta \int_{0}^{2\pi} d\phi Y_{\ell}^{m*}(\theta,\phi) \Delta_{\mathbf{p}}. \tag{70.95}$$

The gap equation can then be rewritten independently for each component of the spherical harmonics

$$\Delta_{\ell,m} = -2\int_{0}^{\hbar\omega_D} N(\zeta') d\zeta' U_{\ell} \frac{1}{(2\ell+1)} \frac{\Delta_{\ell,m}}{2\zeta'} \left(1-2f(\zeta')\right), \tag{70.96}$$

and the value of T_c is obtained from the temperature where the value of the right-hand side is equal to $\Delta_{\ell,m}$. This is analogous to mean-field theory for the Ising model. The value of ℓ for which U_ℓ is most negative will the that which determines the largest T_c, then determining the symmetry of the superconducting gap. If ℓ is odd, we have a triplet. This happens in superfluid ?? ^3He and in ?? UPt_3 [1]. The presence of ferromagnetic fluctuations can explain this result, especially in the case of the superfluid since in this case, triplet pairs are clearly favored. The case $\ell = 2$ is the case of high-temperature superconductors. In the above approximation, all the values of m are degenerate.

Remark 353 *In practice, the cristal field lifts that degeneracy and m combines with $-m$ so that there is no net angular momentum along an axis. A solution with a single spherical harmonic would lead to a complex order parameter that breaks time reversal symmetry.*

Note that even if the potential $U(\cos\Theta)$ is repulsive, it is possible to have pairing. Indeed, it is possible to have $U(\cos\Theta)$ positive everywhere when, for example, $U_0 > 0$ and $U_2 < 0$ if $U_0 \gg U_2$. As an example, consider the case where the boson that leads to binding is an antiferromagnetic fluctuation. On a square lattice for example, this interaction would be maximal when $\mathbf{p}-\mathbf{p}' = (\pi/a, \pi/a)$ where a is the lattice spacing. This happens when the two vectors are at $\pi/2$ one from the other. One can then write a simple model for the interaction that takes the form

$$U\left(\cos\left(\phi-\phi'\right)\right) = U_0 - V\cos^2\left(\phi-\phi'\right) \tag{70.97}$$

with the inequality $U_0 > V$ and where ϕ are azimuthal angles. In that case, we see that the repulsion is maximal, $U = U_0$, when $\phi - \phi' = \pi/2, 3\pi/2$ et and minimal, $U = U_0 - V$, when $\phi - \phi' = 0, \pi$. with the help of trigonometric identities

$$\cos^2\theta = \frac{1+\cos 2\theta}{2} \tag{70.98}$$

$$\cos(\theta_1-\theta_2) = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2 \tag{70.99}$$

one can write

$$\begin{aligned} \cos^2\left(\phi-\phi'\right) &= \frac{1+\cos 2\left(\phi-\phi'\right)}{2} = \frac{1+\cos 2\phi\cos 2\phi' + \sin 2\phi\sin 2\phi'}{2} \\ U\left(\cos\left(\phi-\phi'\right)\right) &= U_0 - V\left(\frac{1+\cos 2\phi\cos 2\phi' + \sin 2\phi\sin 2\phi'}{2}\right). \end{aligned} \tag{70.100}$$

[1] The presence of nodes in the gap was shown by C. Lupien, W.A. MacFarlane, Cyril Proust, Louis Taillefer, Z.Q. Mao and Y. Maeno
Ultrasound attenuation in Sr2RuO4: an angle-resolved study of the superconducting gap
Physical Review Letters 86 (2001) 5986.

Knowing that

$$Y_2^{\pm 2}(\theta,\phi)=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi} \tag{70.101}$$

one finds

$$\begin{aligned}
&\int\frac{d\phi}{2\pi}\int\frac{d\phi'}{2\pi}Y_2^{*\pm 2}(\pi/2,\phi)\,U\left(\cos\left(\phi-\phi'\right)\right)Y_2^{\pm 2}\left(\pi/2,\phi'\right)\\
=&\ -\frac{V}{2}\int\frac{d\phi}{2\pi}\int\frac{d\phi'}{2\pi}\frac{15}{32\pi}e^{-2i\phi}\left(\cos 2\phi\cos 2\phi'+\sin 2\phi\sin 2\phi'\right)e^{2i\phi'}\\
=&\ -\frac{V}{2}\frac{15}{32\pi}\left(\frac{1}{2}\frac{1}{2}+\frac{1}{2i}\frac{1}{(-2i)}\right)
\end{aligned} \tag{70.102}$$

that clearly shows attracition in the $\ell=2$ channel.

A simpler way to understand this last result, is to notice that the gap equation

$$\Delta_{\mathbf{p}}=-\frac{1}{2}\int\frac{d^3p'}{(2\pi)^3}U\left(\mathbf{p}-\mathbf{p}'\right)\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2f(E_{\mathbf{p}'})\right) \tag{70.103}$$

can have a solution for $U\left(\mathbf{p}-\mathbf{p}'\right)$ positive if the maximum of this function is when $\mathbf{p}$ and $\mathbf{p}'$ are separated by an angle $\pi/2$ since for a $d-$wave (i.e. $\ell=2$), $\Delta_{\mathbf{p}}$ et $\Delta_{\mathbf{p}'}$ have opposite signs in this situation. That sign will cancel the minum sign in fron of the integral, as if the potential was attractive.

Remark 354 *In the case of triplet superconductivity, there are three spin components. Take the case of ^3He where there is rotational invariance. The spatial component of the wave function can be expanded using the $\ell=1$ spherical harmonics in this tace. That allows atoms in the pair to avoid the hard-core and to take maximal advantage of the minimum of the Lennard-Jones potential. For each of the three spin components, there is a spatial part that must be described by three basis functions, p_x,p_y,p_z. There are thus 3×3 independent complex components to the order parameter, so 17 independent quantities. The global phase does not show up. One can thus play to break the symmetry in many different ways.*

One must also remark that there is nothing that forbids a superconductor that condensed in the $\ell=2$ state to make an additional phase transition to a more cmplex symmetry at lower temperature. It is also possible below T_c to have an $\ell=4$ component to the order parameter. There is only one spherical harmonic that contributes near T_c because the gap equation can be linearized. Otherwise, the equation is non-linear and it is possible to have solutions that are linear combinations of spherical harmonics.

Remark 355 *In the case of solids, it is possible in general to expand the order parameter on a basis of irreducible representations of the symmetry group of the crystal, namely*

$$\Delta_{\mathbf{p}}=\sum_{\Gamma}\eta_\Gamma f_{\mathbf{p}}^{\Gamma} \tag{70.104}$$

where Γ is the irreducible representation and $f_{\mathbf{p}}^{\Gamma}$ is a basis function that transforms like that representation. (Within each irreducible representation, one is free to expand $f_{\mathbf{p}}^{\Gamma}$ on an arbitrary basis of functions that transform according to the irreducible representation). From the linearity of the gap equation near T_c, one deduces that the order parameter must transform like one of the irreducible representations of the symmetry group of the crystal since they are orthogonal, by analoby with the spherical harmonics. There can be additional phase transitions at lower temperature, where the gap equation is non-linear. In that case, the order

parameter does not transform anymore like a single irreducible representation of the symmetry group. This has been seen for example in organic superconductors [2] *and in strontium ruthenate* Sr_2RuO_4 *??*

[2] Maxime Dion, David Fournier, Mario Poirier, Kim D. Truong, et A.-M.S., Tremblay "Mixed pairing symmetry in κ-(BEDT-TTF)$_2$X organic superconductors from ultrasonic velocity measurements"
Phys. Rev. B **80**, 220511(R) (2009) (4 pages)

71. EXERCICES FOR PART VII

71.0.2 Principe variationel et ferromagnétisme de Stoner:

Soit l'Hamiltonien de Hubbard

$$H = \sum_{\mathbf{k},\boldsymbol{\sigma}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{U}{2} \sum_{i,\sigma,\sigma'} \left(n_{i,\sigma} - \frac{1}{2} \right) \left(n_{i,\sigma'} - \frac{1}{2} \right) \tag{71.1}$$

La somme sur i s'étend sur tous les sites d'un réseau et la somme sur $\mathbf{k}$ sur la première zone de Brillouin correspondante. Comme d'habitude, $\sigma = \pm 1$ représente le spin $(\uparrow\downarrow)$ et $\sum_i n_{i,\uparrow} = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow}$.

a) Montrez qu'à une constante près le terme d'interaction peut être réécrit sous la forme habituelle

$$\frac{U}{2} \sum_{i,\sigma,\sigma'} c^{\dagger}_{i,\sigma} c^{\dagger}_{i,\sigma'} c_{i,\sigma'} c_{i,\sigma} \tag{71.2}$$

Soit l'Hamiltonien d'essai

$$\widetilde{H}_0 = \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(\epsilon_{\mathbf{k}} + \sigma \Delta + \delta \right) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{71.3}$$

Cet Hamiltonien d'essai brise la symétrie de rotation. Il correspond à un état fondamental ferromagnétique. (Δ agit comme un champ magnétique auto-cohérent).

b) Utilisez le principe variationnel dans l'ensemble grand canonique pour trouver les équations qui déterminent Δ et δ. Écrivez aussi l'équation qui détermine le potentiel chimique. Il n'est pas nécessaire de résoudre ces équations, mais exprimez δ en fonction de la densité électronique et de U. Notez que δ peut être absorbée dans la définition du potentiel chimique.

c) Redérivez ces mêmes équations à partir de l'approximation Hartree-Fock pour les fonctions de Green. Notez en passant que, *dans l'état paramagnétique* $\Delta = 0$, le terme de Hartree est ici égal à -2 fois le terme de Fock.

d) Montrez qu'il est possible d'avoir une solution avec $\Delta \neq 0$ à basse température à condition que les inégalités

$$UN(0) > 1 \quad ; \quad \left. \frac{d^2 N(E)}{dE^2} \right|_{E=0} < 0 \tag{71.4}$$

soient satisfaites. Dans ces équations, $N(0)$ est la densité d'états au niveau de Fermi pour une espèce de spins. La condition $UN(0) > 1$ s'appelle le critère de Stoner.

71.0.3 Antiferromagnétisme itinérant

La fonction de Green dans l'état Hartree-Fock d'un antiferroaimant itinérant est donnée par la matrice deux par deux suivante

$$\widetilde{\mathcal{G}}_0(\mathbf{k}, \tau) = - \left\langle T_\tau \Psi_{\mathbf{k}}(\tau) \, \Psi^{\dagger}_{\mathbf{k}}(0) \right\rangle \tag{71.5}$$

où le spineur $\Psi_{\mathbf{k}}$ est défini par

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}+\mathbf{Q}\downarrow} \end{pmatrix} \tag{71.6}$$

avec $\mathbf{Q} = (\pi, \pi)$. La forme explicite de la fonction de Green est,

$$\widetilde{\mathcal{G}}_0(\mathbf{k}, ik_n) = \frac{ik_n\tau_0 + \varepsilon_{\mathbf{k}}\tau_3 + \Delta\tau_1}{(ik_n)^2 - (\varepsilon_{\mathbf{k}}^2 + \Delta^2)} \tag{71.7}$$

où $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ alors que les τ_i sont les matrices de Pauli et la matrice identité et où Δ obéit à l'équation d'autocohérence suivante

$$\Delta = \frac{U}{N}\sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}}(1 - 2f(E_{\mathbf{k}})) \tag{71.8}$$

$$E_{\mathbf{k}}^2 \equiv \varepsilon_{\mathbf{k}}^2 + \Delta^2 \tag{71.9}$$

Exprimez

$$\mathcal{G}(\mathbf{k}, \tau) \equiv -\left\langle T_\tau c_{\mathbf{k}\uparrow}(\tau)\, c_{\mathbf{k}\uparrow}^\dagger(0)\right\rangle - \left\langle T_\tau c_{\mathbf{k}\downarrow}(\tau)\, c_{\mathbf{k}\downarrow}^\dagger(0)\right\rangle \tag{71.10}$$

en fonction de $\widetilde{\mathcal{G}}_0(\mathbf{k}, \tau)$ seulement, (*i.e.* en négligeant les termes d'interactions résiduelles) puis obtenez le poids spectral correspondant à $\mathcal{G}(\mathbf{k}, ik_n)$. Interprétez votre résultat en utilisant les idées de quasiparticules. Comment expliquez-vous le fait que les opérateurs $c_{\mathbf{k}\uparrow}(\tau)$ semblent être des combinaisons linéaires d'autres quasiparticules?

71.0.4 Supraconductivité: conductivité infinie et effet Meissner:

L'objectif de ce problème est de montrer que la théorie BCS prédit que la conductivité électrique DC transverse est infinie dans l'état supraconducteur et que l'effet Meissner existe dans cette théorie. On obtient ce résultat en calculant la réponse linéaire du courant à un potentiel vecteur transversal. Vous pouvez vous placer dans la limite de température nulle, ou très faible, et dans la limite dite de London. Ce problème est discuté dans beaucoup de volumes.

Suivez le développement du volume de votre choix en donnant toutes les étapes intermédiaires du calcul. Vous pouvez rester dans le continuum (modèle du jellium).

Partez de la formule de Kubo pour la conductivité après avoir dérivé une expression pour le courant dans la base de Nambu. Pour cette étape, notez que le courant en l'absence de potentiel vecteur s'écrit

$$\mathbf{j} = \frac{e}{2mi}\sum_{\sigma}\int d\mathbf{r}\left(\psi_\sigma^\dagger(\mathbf{r})\cdot\nabla\psi_\sigma(\mathbf{r}) - \nabla\psi_\sigma^\dagger(\mathbf{r})\cdot\psi_\sigma(\mathbf{r})\right). \tag{71.11}$$

Réexprimerez cet opérateur avec les opérateurs de Nambu et les matrices de Pauli. Passez ensuite dans l'espace des vecteurs d'onde où l'expression est plus simple. Il suffit ensuite de calculer la fonction de corrélation courant-courant avec la fonction de Green de Nambu dans l'état supraconducteur. Vous devrez faire la convolution de deux fonctions de Green, i.e. une seul boucle. C'est l'analogue de la fonction de Lindhard. Il est plus facile d'obtenir le résultat en utilisant le fait que dans

l'approximation BCS un théorème de Wick s'applique pour les fonctions de Green de Nambu. Vous pouvez utiliser pour la fonction de Green de Nambu l'expression

$$\mathbf{G}\left(\mathbf{k},ik_n\right)=\frac{ik_n+\varepsilon_{\mathbf{k}}\tau^3+\Delta\tau^1}{\left(ik_n\right)^2-\varepsilon_{\mathbf{k}}^2-\left|\Delta\right|^2}. \tag{71.12}$$

Notez que le théorème de Wick s'applique pour les fonctions de Green de Nambu dans l'approximation BCS puisque l'hamiltonien d'essai est quadratique. L'expression pour la fonction de corrélation courant-courant fera intervenir des traces sur des produits de matrice de Pauli. Les propriétés des matrices de Pauli (comme anti-commutation et trace nulle) simplifient beaucoup les calculs.

Ensuite, vous pourrez montrer qu'à température nulle tout se passe effectivement comme si seulement le terme diamagnétique contribuait à la réponse linéaire. En d'autres mots, montrez que la fonction de corrélation courant-courant retardée s'annule dans la limite $\mathbf{q}\rightarrow 0$. Pourquoi cela ne contredit-il pas la règle de somme f ? Qu'est-ce que cela implique sur la continuité de la limite $\mathbf{q}\rightarrow 0$ de la fonction de corrélation courant-courant? Discutez ensuite comment ceci est relié au fait qu'un supraconducteur est aussi caractérisé par l'existence de corrélations à longue portée de la quantité de mouvement.

71.0.5 Principe variationnel à $T=0$ pour le ferroaimant

À $T=0$, la fonction d'onde variationnelle de la Section (65.2) donne

$$\left\langle\Psi\right|H-\mu N\left|\Psi\right\rangle=\sum_{\mathbf{k},\boldsymbol{\sigma}}(\varepsilon_{\mathbf{k}}-\mu)\left\langle n_{\mathbf{k},\boldsymbol{\sigma}}\right\rangle+NU\left\langle n_{-\sigma}\right\rangle\left\langle n_{\sigma}\right\rangle. \tag{71.13}$$

Cette fonction d'onde variationnelle suppose une surface de Fermi sphérique.

a) Montrez que le côté droit de l'équation ci-dessus prend la forme

$$\int_0^{\varepsilon_{F\uparrow}}N\left(\varepsilon\right)\left(\varepsilon-\mu\right)d\varepsilon+\int_0^{\varepsilon_{F\downarrow}}N\left(\varepsilon\right)\left(\varepsilon-\mu\right)d\varepsilon+U\int_0^{\varepsilon_{F\uparrow}}N\left(\varepsilon\right)d\varepsilon\int_0^{\varepsilon_{F\downarrow}}N\left(\varepsilon\right)d\varepsilon \tag{71.14}$$

où $N\left(\varepsilon\right)$ est la densité d'états pour une espèce de spin et $\varepsilon_{F\boldsymbol{\sigma}}$ est l'énergie de Fermi correspondant à la valeur de $k_{F\boldsymbol{\sigma}}$ pour le spin σ.

b) Il est possible d'utiliser $k_{F\boldsymbol{\sigma}}$ ou $\varepsilon_{F\boldsymbol{\sigma}}$ ou $\left\langle n_{\sigma}\right\rangle$ comme paramètre variationnel puisque ces quantités sont toutes simplement reliées. En dérivant par rapport à $\varepsilon_{F\boldsymbol{\sigma}}$, trouvez les deux équations qui donnent le minimum. Le potentiel chimique détermine le remplissage, qui est fixe.

c) La différence entre les deux équations ci-dessus, donnent une équation pour le paramètre d'ordre. En supposant que $\left\langle n_{\uparrow}\right\rangle-\left\langle n_{\downarrow}\right\rangle$ est petit, montrez qu'on retrouve la condition pour l'instabilité ferromagnétique, soit $1-UN\left(\varepsilon_F\right)=0$, où ε_F est l'énergie de l'état symétrique (paramagnétique).

71.0.6 Équations de champ moyen pour le ferroaimant

Faites en détail les calculs de la section (65.4), incluant ceux dans les remarques.

71.0.7 Variational principle at $T = 0$ for the ferromagnet

At $T = 0$, the variational wave function in Section (65.2) leads to

$$\langle \Psi | H - \mu N | \Psi \rangle = \sum_{\mathbf{k},\boldsymbol{\sigma}} (\varepsilon_{\mathbf{k}} - \mu) \langle n_{\mathbf{k},\boldsymbol{\sigma}} \rangle + NU \langle n_{-\sigma} \rangle \langle n_{\sigma} \rangle . \tag{71.15}$$

This variational wave function assumes a spherical Fermi surface.

a) Show that the right-hand side of the above result can be written in the form

$$\int_0^{\varepsilon_{F\uparrow}} N(\varepsilon)(\varepsilon - \mu)\, d\varepsilon + \int_0^{\varepsilon_{F\downarrow}} N(\varepsilon)(\varepsilon - \mu)\, d\varepsilon + U \int_0^{\varepsilon_{F\uparrow}} N(\varepsilon)\, d\varepsilon \int_0^{\varepsilon_{F\downarrow}} N(\varepsilon)\, d\varepsilon \tag{71.16}$$

where $N(\varepsilon)$ is the single-spin density of states and $\varepsilon_{F\sigma}$ is the Fermi energy corresponding to the value of $k_{F\sigma}$ for spin σ.

b) It is clear that one can use either $k_{F\sigma}$ or $\varepsilon_{F\sigma}$ or $\langle n_{\sigma} \rangle$ as variational parameters since they are all simply related. Differentiating with respect to $\varepsilon_{F\sigma}$, find the two equations that give the minimum. The chemical potential determines the filling, that is fixed.

c) The difference between the above two equations gives an equation for the order parameter. Assuming that $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle$ is small, show that one recovers the condition for the ferromagnetic instability, namely $1 - UN(\varepsilon_F) = 0$, where ε_F is the Fermi energy of the symmetric (paramagnetic) state.

71.0.8 Mean-field equations for the ferromagnet

Redo in detail the calcuations of section (65.4), including those in the remarks.

Part VIII

Advanced topics: Coherent state functional integral, Luttinger Ward etc

Two useful points of view on many-body physics remain to be discussed. First the coherent-state functional integral approach. It is the many-body analog of path integrals we have discussed already in the one-body case.22 In this elegant formulation, some of the general results of many-body theory are easier to derive. Others are more complicated, but this is a very common case in physics. Feynman in his Lectures on Physics, points out that physicists work like Babylonian mathematicians. There are several ideas or starting points that are all equivalent. We should know all of them since, depending on the situation, a given formulation might be more natural. This is to be contrasted with Greek mathematicians which, after Euclid, started from a given set of axioms to do everything else. In addition to allowing simple derivations of important results in many-body theory, coherent-state functional integrals have several virtues, including the following.

- In the same way that in classical statistical physics the partition function is an integral over all configurations of the classical field (like magnetization), in the quantum case it will be an integral over all field configurations.

- Up to now, we have worked with a Hamiltonian, but we have seen that the natural object that comes everywhere is the Green function. In the coherent-state functional integral, the Green function comes out naturally right from the start as the basic object. It is very useful to have the Green function as a natural object in the context, for example, of more advanced mean-field theories, like Eliashberg theory for superconductivity and Dynamical Mean-Field theory.

- From our experience with path integrals, we expect the Lagrangian to occupy the central role, instead of the Hamiltonian. The Green function is in a way the Lagrangian equivalent of the quadratic part of the Hamiltonian. The $\partial/\partial\tau$ that comes in the Green function and not the Hamiltonian comes from the Legendre transform that takes us between the two objects.

- When we trace-out degrees of freedom, like we did in the quantum-impurity problem, for example, and in obtaining the effective interaction mediated by phonons, retardation is introduced. In other words we need time-ordered products with time differences appearing in the exponentials. This is not natural for Hamiltonians since the Hamiltonian, by construction, cannot involve more than one time: it is the generator of infinitesimal translations in time. There is no such problem in the coherent-state functional-integral representation since we have to integrate over quantum fields that are defined over all space-time.

- The coherent-state functional-integral representation allows us to formulate approximations that are less natural in the Hamiltonian formalism. For example, mean-field theories can appear as saddle-point approximations, in a spirit similar to what we saw in the infinite-range Ising model treated in Sec.60.1. Corrections can then be obtained as systematic loop expansions, Gaussian fluctuations giving the first corrections.

- The coherent-state functional integral also reveals topological properties and topological excitations that are hard to find otherwise. They are good for Feynmann diagrams, but they also allow incursions outside of the perturbative realm.

The other quantity we have not introduced yet is the Luttinger-Ward functional and the corresponding Baym-Kadanoff functional. The Luttinger Ward functional can be used in practice to obtain approximations in Many-Body theory that are

garanteed to satisfy conservation laws. In addition, it can be used to obtain other functionals to formulate naturally various approximations, such as dynamical mean-field theory.

This part then, starts with Chapters on the Luttinger-Ward functional, Kadanoff-Baym functional, the self-energy functional formulation of dynamical mean-field theory for clusters and conserving approximations. We then end with coherent states to introduce afterwards coherent-state path integrals. Coherent states are first presented for bosons, then for fermions. The functional integral is derived only in the fermion case. The boson case is an easy exercise after that. For fermions, we will need to introduce Grassman numbers and the corresponding integrals and derivatives. Some interesting results that follow simply include Wick's theorem and the expression for the partition function as a determinant, or as $\exp\left(\mathrm{Tr}\ln\right)$.

72. LUTTINGER-WARD FUNCTIONAL

There is a very elegant formulation of the Many-Body problem that focuses on a functional of the interacting Green function instead of on a functional of source fields. The two approaches are related by a Legendre transform. This is where one encounters the so-called Luttinger-Ward functional [139][197], that plays a prominent role in defining approximations that satisfy conservation laws, thermodynamic consistency and in deriving Dynamical Mean-Field Theory. But first, a short digression to argue that the self-energy can be written as a functional derivative with respect to the Green's function.

72.1 The self-energy can be expressed as a functional derivative with respect to the Green's function

In this section, I follow Baym [23] to show that the functional derivative of the self-energy obeys a curl condition that proves that the self-energy itself is a functional derivative with respect to $\mathcal{G}$ of an appropriately defined Luttinger-Ward functional that we find in the following sections.

We have seen in Eq. (35.27) that the four-point function can be written as

$$\frac{\delta \mathcal{G}}{\delta \phi} = \mathcal{G}\frac{\delta \phi}{\delta \phi}\mathcal{G} + \mathcal{G}\frac{\delta \Sigma}{\delta \phi}\mathcal{G}. \tag{72.1}$$

This suggests that the functional dependence of Σ on ϕ comes only from the dependence of $\mathcal{G}$ on ϕ. Hence, the above equation may be rewritten as follows

$$\boxed{\frac{\delta \mathcal{G}}{\delta \phi} = \mathcal{G}\frac{\delta \phi}{\delta \phi}\mathcal{G} + \mathcal{G}\left(\frac{\delta \Sigma}{\delta \mathcal{G}}\frac{\delta \mathcal{G}}{\delta \phi}\right)\mathcal{G}.} \tag{72.2}$$

Multiplying by $\mathcal{G}^{-1}$ on both sides, we are left with the following

$$\mathcal{G}^{-1}\frac{\delta \mathcal{G}}{\delta \phi}\mathcal{G}^{-1} = \frac{\delta \phi}{\delta \phi} + \left(\frac{\delta \Sigma}{\delta \mathcal{G}}\frac{\delta \mathcal{G}}{\delta \phi}\right). \tag{72.3}$$

To avoid confusion, let us rewrite all the indices. Then, the above can be rewritten as follows

$$\left[\mathcal{G}^{-1}\left(1',\overline{1}\right)\mathcal{G}^{-1}\left(\overline{2},2'\right) - \frac{\delta \Sigma\left(1',2'\right)}{\delta \mathcal{G}\left(\overline{1},\overline{2}\right)}\right]\frac{\delta \mathcal{G}\left(\overline{1},\overline{2}\right)}{\delta \phi\left(3,4\right)} = \delta\left(1'-3\right)\delta\left(2'-4\right). \tag{72.4}$$

This equation means that the quantity in brackets is the inverse of $\delta \mathcal{G}\left(1,2\right)/\delta \phi\left(3,4\right)$. But since $\mathcal{G}\left(1,2\right) = -\delta \ln Z[\phi]/\delta \phi\left(2,1\right)$, the matrix $\delta \mathcal{G}\left(1,2\right)/\delta \phi\left(3,4\right)$ is symmetric under the interchange $2,1 \to 3,4$, in other words,

$$\frac{\delta \mathcal{G}\left(1,2\right)}{\delta \phi\left(3,4\right)} = \frac{\delta \mathcal{G}\left(4,3\right)}{\delta \phi\left(2,1\right)} \tag{72.5}$$

Note that the symmetry here means interchanging indices of the numerator with those of the denominator, and then permuting the indices of the numerator and of the denominator separately. So for example, $\mathcal{G}^{-1}\left(1',\overline{1}\right)\mathcal{G}^{-1}\left(\overline{2},2'\right)$ has this symmetry taking $1'$ and $2'$ as indices in the numerator and $\overline{1},\overline{2}$ as indices of the denominator.

The inverse of as symmetric matrix is also symmetric. This will be true if and only if

$$\frac{\delta\Sigma\left(1',2'\right)}{\delta\mathcal{G}\left(1,2\right)}=\frac{\delta\Sigma\left(2,1\right)}{\delta\mathcal{G}\left(2',1'\right)}. \tag{72.6}$$

This is a curl condition that will be satisfied if and only if the self-energy is itself a functional derivative with respect to $\mathcal{G}$, in other words if

$$\frac{1}{T}\frac{\delta\Phi\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(2',1'\right)}=\Sigma\left(1',2'\right). \tag{72.7}$$

The quantity $\Phi\left[\mathcal{G}\right]$ will be the Luttinger-Ward functional. We will see that it also has a diagrammatic expansion that is related to the potential energy.

72.2 The free energy of a non-interacting but time-dependent problem is $-T\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}^{-1}}{-\mathcal{G}_{\infty}^{-1}}\right)\right]$

We know how to compute the free-energy for a non-interacting Hamiltonian. In general, we can also do it even if we know only the time-dependent Green's function. The solution of this problem will be extremely useful in what follows. The derivation will be done using a completerly different approach in Sec.(80.2) using coherent state functional integrals.

The generating function as a functional of the source field ϕ is given by

$$F\left[\phi\right]=-T\ln Z\left[\phi\right]=-T\ln\mathrm{Tr}\left[e^{-\beta K}T_{\tau}\exp\left(-\psi^{\dagger}\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\right]. \tag{72.8}$$

The derivative with respect to the source field is simply related to the Green function by

$$\frac{1}{T}\frac{\delta F\left[\phi\right]}{\delta\phi\left(1,2\right)}=\mathcal{G}\left(2,1\right)_{\phi}. \tag{72.9}$$

We know from the equations of motion Eq. (36.14) that when there are no interactions the self-energy vanishes so that

$$\mathcal{G}^{-1}\left(1,2\right)_{\phi}=\mathcal{G}_{0}^{-1}\left(1,2\right)-\phi\left(1,2\right). \tag{72.10}$$

This means that we can do a change of variables, use the chain rule and obtain

$$\frac{1}{T}\frac{\delta F\left[\phi\right]}{\delta\mathcal{G}^{-1}\left(1,2\right)}=\frac{1}{T}\frac{\delta F\left[\phi\right]}{\delta\phi\left(1,2\right)}\frac{\delta\phi\left(1,2\right)}{\delta\mathcal{G}^{-1}\left(1,2\right)}=-\mathcal{G}\left(2,1\right) \tag{72.11}$$

The solution is

$$F\left[\mathcal{G}\right]=-\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}^{-1}}{-\mathcal{G}_{\infty}^{-1}}\right)\right]. \tag{72.12}$$

For the definition of $\mathcal{G}_{\infty}$ and a thorough discussion, see Eq.(80.18). It is necessary for convergence. It plays the role of a constant of integration if we redo the proof

below with in integral instead of checking the derivative. The trace contains a factor of temperature. More specifically, when there is time and space translational invariance,

$$\mathrm{Tr}\left[\cdots\right] = T\sum_{ik_n}\sum_{\mathbf{k}}\left[\cdots\right] \tag{72.13}$$

while in general,

$$\mathrm{Tr}\left[\phi\mathcal{G}\right] = T\phi\left(\overline{1},\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{1}\right). \tag{72.14}$$

Proof: Proof of the formula for $F\left[\mathcal{G}\right]$. We show that the derivative is the correct one. $\mathcal{G}_\infty^{-1}$ is not differentiated since it is a constant. In fact in most discussions encountered in the literature, $\mathcal{G}_\infty$ is simply omitted. Let us evaluate the trace in the basis where $\mathcal{G}^{-1}$ is diagonal

$$-\mathrm{Tr}\left[\ln\left(-\mathcal{G}^{-1}\right)\right] = -T\sum_d \ln\left(-g_d^{-1}\right). \tag{72.15}$$

$\mathcal{G}^{-1}$ is related to its diagonal form by a general similarity transformation

$$g_d^{-1} = T_{d\overline{1}}^{-1}\mathcal{G}^{-1}\left(\overline{1},\overline{2}\right)T_{\overline{2}d}. \tag{72.16}$$

Then

$$\frac{1}{T}\frac{\delta F\left[\phi\right]}{\delta\mathcal{G}^{-1}\left(1,2\right)} = -\frac{1}{T}\frac{\delta\mathrm{Tr}\left[\ln\left(-\mathcal{G}^{-1}\right)\right]}{\delta\mathcal{G}^{-1}\left(1,2\right)_\phi} = -\sum_d \frac{1}{g_{-1}{}_d}\frac{\delta g_d^{-1}}{\delta\mathcal{G}^{-1}\left(1,2\right)_\phi} \tag{72.17}$$

$$= -\sum_d \frac{1}{g_d^{-1}}T_{d1}^{-1}T_{2d} = -\sum_d T_{2d}\frac{1}{g_d^{-1}}T_{d1}^{-1} = -\mathcal{G}\left(2,1\right) \tag{72.18}$$

In the last step, we used that the similarity transformation that diagonalizes a matrix also diagonalizes its inverse.

Remark 356 *Let us verify that in the non-interacting case, this leads to the correct result. Take only one energy level. Then the Matsubara basis is the diagonal basis and* $\mathcal{G}^{-1} = ik_n - \varepsilon$. *This means that*

$$F\left[\mathcal{G}\right] = -T\sum_n\left[\ln\left(\frac{ik_n-\varepsilon}{ik_n-E}\right)\right]. \tag{72.19}$$

At infinite Matsubara frequency, a Taylor expansion gives

$$-T\sum_n\left[\ln\left(\frac{1-\varepsilon/ik_n}{1-E/ik_n}\right)\right] \sim -T\sum_n\left[-\varepsilon/ik_n + E/ik_n\right] \tag{72.20}$$

which shows that the series converges if we use a convergence factor. The states involved should be those below the Fermi surface. Appeal to the complex plane methods of section (29.9) leads to

$$-T\sum_n\left[\ln\left(\frac{ik_n-\varepsilon}{ik_n-E}\right)\right] = \frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{\beta z}+1}e^{-z0^-}\left[\ln\left(\frac{z-\varepsilon}{z-E}\right)\right]. \tag{72.21}$$

This can be done most easily by integrating by parts. Note first that

$$\frac{\partial}{\partial z}\ln\left(e^{-\beta z}+1\right) = -\beta\frac{e^{-\beta z}}{e^{-\beta z}+1} = -\beta\frac{1}{e^{\beta z}+1} \tag{72.22}$$

which allows us to write

$$\frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{\beta z}+1}e^{-z0^-}\left[\ln\left(\frac{z-\varepsilon}{z-E}\right)\right] = -\frac{1}{\beta}\ln\left(e^{-\beta z}+1\right)\ln\left(\frac{z-\varepsilon}{z-E}\right)\frac{e^{-z0^-}}{2\pi i}\Bigg|_{-i\infty}^{i\infty} \quad (72.23)$$

$$+\frac{1}{2\pi i}\frac{1}{\beta}\int_{C_1}dze^{-z0^-}\ln\left(e^{-\beta z}+1\right)\left[\frac{1}{z-\varepsilon}-\frac{1}{z-E}\right] \quad (72.24)$$

$$= -\frac{1}{\beta}\left(\ln\left(e^{-\beta\varepsilon}+1\right)-\ln\left(e^{-\beta E}+1\right)\right). \quad (72.25)$$

In the first line, the second logarithm vanishes at the limits of integration because its argument becomes equal to unity. I have appealed to Cauchy's theorem in the last line. The last term can be neglected since $E\to\infty$. We thus have the expected result because the partition function in this simple case is $e^{-\beta\varepsilon}+1$.

72.3 The Luttinger-Ward functional and the Legendre transform of $-T\ln Z\left[\phi\right]$

The first two equations of the previous section can be used to define a Legendre transform of the generating function, where $\mathcal{G}$ is the natural variable:

$$\Omega[\mathcal{G}]=F\left[\phi\right]-\mathrm{Tr}\left[\phi\mathcal{G}\right]. \quad (72.26)$$

The physical free energy is $F\left[\phi=0\right]$.

Remark 357 *Legendre transforms are usually defined between convex functions. We cannot prove continuity in our case. The best we can hope is that the Legendre transform is defined locally and check that the results make sense. Recent results show that indeed there may be problems with the assumption that the Legendre transform is always well defined [124]. In the latter reference, it is shown that perturbation in the dressed $\mathcal{G}$ at large interaction can lead to an unphysical branch of the self-energy when the interaction is large. This does not happen with the expansion is in terms of $\mathcal{G}_0$.*

The functional $\Omega[\mathcal{G}]$ is the so-called Kadanoff-Baym functional. As expected for Legendre transforms

$$\frac{1}{T}\frac{\delta\Omega\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)}=-\phi\left(2,1\right). \quad (72.27)$$

Proof:

$$\frac{1}{T}\frac{\delta\Omega\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)} = \frac{1}{T}\frac{\delta F\left[\phi\right]}{\delta\phi\left(\bar{3},\bar{4}\right)}\frac{\delta\phi\left(\bar{3},\bar{4}\right)}{\delta\mathcal{G}\left(1,2\right)}-\frac{\delta}{\delta\mathcal{G}\left(1,2\right)}\left[\phi\left(\bar{3},\bar{4}\right)\mathcal{G}\left(\bar{4},\bar{3}\right)\right] \quad (72.28)$$

$$= \mathcal{G}\left(\bar{4},\bar{3}\right)\frac{\delta\phi\left(\bar{3},\bar{4}\right)}{\delta\mathcal{G}\left(1,2\right)}-\frac{\delta\phi\left(\bar{3},\bar{4}\right)}{\delta\mathcal{G}\left(1,2\right)}\mathcal{G}\left(\bar{4},\bar{3}\right)-\phi\left(2,1\right). \quad (72.29)$$

Using the equations of motion Eq. (36.14), we have that the relation between ϕ and $\mathcal{G}$ is given by

$$\mathcal{G}^{-1}\left(1,2\right)_\phi=\mathcal{G}_0^{-1}\left(1,2\right)-\phi\left(1,2\right)-\Sigma\left(1,2\right)_\phi \quad (72.30)$$

which means that

$$\frac{1}{T}\frac{\delta\Omega\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)}=-\phi\left(2,1\right)=\mathcal{G}^{-1}\left(2,1\right)_{\phi}-\mathcal{G}_{0}^{-1}\left(2,1\right)+\Sigma\left(2,1\right)_{\phi} \tag{72.31}$$

and Dyson's equation in its usual form is satisfied only for $\phi=0$ where the extremum principle

$$\frac{1}{T}\frac{\delta\Omega\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)}=0 \tag{72.32}$$

is satisfied and where the functional $\Omega[\mathcal{G}]$ is simply equal to the free energy as follows from the definition Eq.(72.26) with $\phi=0$.

We can guess an explicit expression for $\Omega\left[\mathcal{G}\right]$ by starting from its derivative Eq.(72.31). We obtain the so-called Baym-Kadanoff functional,

$$\Omega\left[\mathcal{G}\right]=\Phi\left[\mathcal{G}\right]-\mathrm{Tr}\left[\left(\mathcal{G}_{0}^{-1}-\mathcal{G}^{-1}\right)\mathcal{G}\right]+\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_{\infty}}\right)\right] \tag{72.33}$$

which gives the correct result in the non-interacting case (for the definition of $\mathcal{G}_{\infty}$ see Eq.(80.18)) and reduces to Eq.(72.31) when functionally differentiated, as long as

$$\frac{1}{T}\frac{\delta\Phi\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)}=\Sigma\left(2,1\right). \tag{72.34}$$

That this functional exists was discussed in section (72.1) above. We also need to prove that $\frac{1}{T}\frac{\delta}{\delta\mathcal{G}(1,2)}\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_{\infty}}\right)\right]=\mathcal{G}^{-1}\left(2,1\right)$. The proof follows the same steps as those in the previous section. Also, note that

$$\frac{1}{T}\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_{\infty}}\right)\right]=-\frac{1}{T}\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}^{-1}}{-\mathcal{G}_{\infty}^{-1}}\right)\right]. \tag{72.35}$$

The latter form is more common.

The functional $\Phi\left[\mathcal{G}\right]$ is the so-called Luttinger-Ward functional. We can obtain an explicit form for it by using the basic property of Legendre transforms exemplified by our example with pressure in ordinary statistical mechanics, Eq.(A.17). More specifically, multiply the potential energy term in the Hamiltonian by λ, then the physical case corresponds to $\lambda=1$ and the general properties of Legendre transforms tell us that

$$\left.\frac{\partial\Omega_{\lambda}\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}}=\left.\frac{\partial F_{\lambda}\left[\phi\right]}{\partial\lambda}\right|_{\phi}. \tag{72.36}$$

But the explicit form of the Baym-Kadanoff functional Eq.(91.10) tells us that

$$\left.\frac{\partial\Omega_{\lambda}\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}}=\left.\frac{\partial\Phi_{\lambda}\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}} \tag{72.37}$$

while the derivative of the free energy is

$$\left.\frac{\partial F_{\lambda}\left[\phi\right]}{\partial\lambda}\right|_{\phi}=\frac{1}{\lambda}\left\langle\lambda\hat{V}\right\rangle_{\lambda}. \tag{72.38}$$

The average $\langle\rangle_{\lambda}$ means that the potential energy is averaged with the Hamiltonian where the coupling constant is multiplied by λ so that $\hat{V}\rightarrow\lambda\hat{V}$. Hence, we can obtain the Luttinger-Ward functional by a coupling constant integration

$$\Phi_{\lambda=1}\left[\mathcal{G}\right]=\int_{0}^{1}d\lambda\frac{1}{\lambda}\left\langle\lambda\hat{V}\right\rangle_{\lambda}. \tag{72.39}$$

Note that since the equality of the two potentials with respect to λ, Eq.(91.12), is valid for any $\mathcal{G}$ and the corresponding ϕ, the coupling constant integration for the Luttinger-Ward functional may be evaluated for $\phi = 0$ and for $\mathcal{G}$ that satisfies the usual Dyson equation or for any $\mathcal{G}$ we wish. The average of the potential energy in the last equation is related to the density-density correlation function. The resulting integral over coupling constant gives for $\Phi_\lambda [\mathcal{G}]$ the same result that we would have obtained from the linked cluster theorem. There is a $1/n$ factor for a term of order n.

Remark 358 $\Phi [\mathcal{G}]$ *is the sum of two-particle irreducible skeleton diagrams hence* $\frac{1}{T} \frac{\delta \Phi[\mathcal{G}]}{\delta \mathcal{G}(1,2)} = \Sigma (2,1)$ *is the sum of all one-particle irreducible skeleton diagrams. This is proven in Section (76.1). A skeleton diagram is a diagram that has no self-energy insertions.*

73. * FORMAL MATTERS: RECIPES TO SATISFY CONSERVATION LAWS

Designing approximations that satisfy conservation laws and other exact results, such as the Pauli principle, is a non-trivial matter. Order by order calculations satisfy these requirements, but in general we want to sum infinite subsets of diagrams. For example, I discuss in detail in Sec. 56.5 specific approximations, such as the RPA, that fail to satisfy the Pauli principle. How to satisfy conservation laws in approximate theories is another problem. It was solved by Baym and Kadanoff [25, 23]. In practice, one starts from the Legendre transform of $\ln Z[\phi]$ that is based on the conjugate variable of ϕ, namely $\mathcal{G}$. That Legendre transform is the Kadanoff-Baym functional and approximations are based on functional derivatives of one of the components of that functional, the Luttinger-Ward functional, that I discussed in Chapter 72.

Conservation laws also imply some relations between correlation functions with n field operators ($n-$point functions) and correlation functions with $n-2$ field operators. These are also known as Ward-Takahashi identities [249]. These identities can be used to explicitly check the consistency of various approximations with conservation laws. When the the self-energy is a functional of $\mathcal{G}[\phi]$, they satisfy Ward-Takahashi identities as I will show.

In what follows, I concentrate on particle-number conservation. Other conservation laws can be derived using a similar procedure.

73.1 *Ward-Takahashi identity for charge conservation

Here I present the Ward-Takahashi identity for a $4-$ point function. This is the most useful one, but it is easy to generalize this to $6-$ point etc. Let $\widehat{\rho}(1)$ be the density operator, and $\widehat{j}(1)$ the corresponding current. Then

$$\frac{\partial \left\langle T_\tau \left[\widehat{\rho}(1)\psi(2)\psi^\dagger(3)\right]\right\rangle}{\partial \tau_1} + \nabla_1 \cdot \left\langle T_\tau \left[\widehat{j}(1)\psi(2)\psi^\dagger(3)\right]\right\rangle \tag{73.1}$$

$$= \delta(1-2)\left\langle T_\tau \left[\left[\widehat{\rho}(1),\psi(2)\right]\psi^\dagger(3)\right]\right\rangle + \delta(1-3)\left\langle T_\tau \left[\psi(2)\left[\widehat{\rho}(1),\psi^\dagger(3)\right]\right]\right\rangle \tag{73.2}$$

where the term on the right-hand side is non-zero just because of the action of the time derivative on the time-ordered product. Note that in a time-ordered product, the density operator commutes with the field operators. The commutators on the right-hand side can be evaluated because they are at equal time. The right-had side becomes

$$-\delta(1-2)\left\langle T_\tau \left[\psi(1)\psi^\dagger(3)\right]\right\rangle + \delta(1-3)\left\langle T_\tau \left[\psi(2)\psi^\dagger(1)\right]\right\rangle \tag{73.3}$$

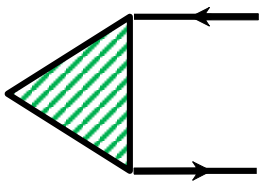

Figure 73-1 Four point function entering the Ward identity. The legs are usually "cut-off" to focus on the vertex in green.

which yields, using the definition of the Green's functions

$$\frac{\partial\left\langle T_\tau\left[\widehat{\rho}\left(1\right)\psi\left(2\right)\psi^\dagger\left(3\right)\right]\right\rangle}{\partial\tau_1}+\nabla_1\cdot\left\langle T_\tau\left[\widehat{j}\left(1\right)\psi\left(2\right)\psi^\dagger\left(3\right)\right]\right\rangle \tag{73.4}$$

$$=\quad \delta\left(1-2\right)\mathcal{G}\left(1,3\right)-\delta\left(1-3\right)\mathcal{G}\left(2,1\right)=\left(\delta\left(1-2\right)-\delta\left(1-3\right)\right)\mathcal{G}\left(2,3\right) \tag{73.5}$$

The four-point function on the left, without the derivatives, can be represented graphically as in Fig. (73-1). It is customary to cut-off the Green's functions to focus on the vertex part in green. This is done by mutiplying the above equation from the left by $\mathcal{G}^{-1}\left(4,2\right)$ and from the right by $\mathcal{G}^{-1}\left(3,5\right)$. This yields

$$\mathcal{G}^{-1}\left(4,\overline{2}\right)\left[\frac{\partial\left\langle T_\tau\left[\widehat{\rho}\left(1\right)\psi\left(\overline{2}\right)\psi^\dagger\left(\overline{3}\right)\right]\right\rangle}{\partial\tau_1}+\nabla_1\cdot\left\langle T_\tau\left[\widehat{j}\left(1\right)\psi\left(\overline{2}\right)\psi^\dagger\left(\overline{3}\right)\right]\right\rangle\right]\mathcal{G}^{-1}\left(\overline{3},5\right) \tag{73.6}$$

$$=\quad \mathcal{G}^{-1}\left(4,1\right)\delta\left(1-5\right)-\delta\left(1-4\right)\mathcal{G}^{-1}\left(1,5\right) \tag{73.7}$$

$$=\quad -\Sigma\left(4,1\right)\delta\left(1-5\right)+\delta\left(1-4\right)\Sigma\left(1,5\right). \tag{73.8}$$

Since $\mathcal{G}_0^{-1}(4,1)$ is proportional to $\delta(4-1)$ and analogously for $\mathcal{G}_0^{-1}(1,5)$ what is left on the right-hand side is the difference of the self energies. This is another way that vertices and self-energies are related.

73.2 *The Ward identity from gauge invariance

In this section, I will outline how gauge invariance and linear response theory imply the Ward-Takahashi identities of the previous section. And it will become clear that if the self-energy is a functional of $\mathcal{G}[\phi]$, in other words $\Sigma[\mathcal{G}[\phi]]$ and if the linear response is obtained from our fundtional derivative approach, namely $\delta\mathcal{G}[\phi]/\delta\phi$, that identity is satisfied.

I follow Baym [23]. I take the parabolic band model to be specific, but it works in general. The perturbation here is a pure gauge transformation, as defined in Sec. 11.1. In other words, we have, *taking the electron charge and Planck's constant equal to unity*

$$\psi^\dagger\left(\overline{3}\right)\phi\left(\overline{3},\overline{4}\right)\psi\left(\overline{4}\right) \quad=\quad -\psi^\dagger\left(\overline{3}^+\right)\left(\frac{\partial\Lambda\left(\overline{3}\right)}{\partial\tau_3}+\frac{\left(\boldsymbol{\nabla}\Lambda\left(\overline{3}\right)\right)^2}{2m}\right)\psi\left(\overline{3}\right) \tag{73.9}$$

$$-\frac{\boldsymbol{\nabla}\Lambda\left(\overline{3}\right)}{2mi}\left\{\psi^\dagger\left(\overline{3}^+\right)\boldsymbol{\nabla}\psi\left(\overline{3}\right)-\left(\boldsymbol{\nabla}\psi^\dagger\left(\overline{3}^+\right)\right)\psi\left(\overline{3}\right)\right\} \tag{73.10}$$

You recognize the coupling to the charge density and to the current. I will not do the calculation in detail. It goes as follows. Compute the linear response of say $\mathcal{G}(1,2)$ to the above pure gauge potential. Integrating by part, we obtain derivatives with respect to $\overline{3}^{+}$ and $\overline{3}$ of the four-point function

$$\left\langle T_\tau \left[\psi(1) \psi^\dagger(2) \psi^\dagger\left(\overline{3}^{+}\right) \psi\left(\overline{3}\right) \right] \right\rangle \tag{73.11}$$

times $\Lambda\left(\overline{3}\right)$. But we know from Sec. (**??**) how the Green's function transforms to linear order under a gauge transformation

$$\mathcal{G}(1,2) \to e^{i\Lambda(1)} \mathcal{G}(1,2)\, e^{-i\Lambda(2)} \to \mathcal{G}(1,2) + i\Lambda(1)\, \mathcal{G}(1,2) - \mathcal{G}(1,2)\, i\Lambda(2)\,. \tag{73.12}$$

Setting equal the two ways of computing the effect of a gauge transformation on the Green's function, we obtain the Ward-Takahashi identity Eq. (73.4).

The important point here, is that $\mathcal{G}(1,2) \to e^{i\Lambda(1)} \mathcal{G}(1,2)\, e^{-i\Lambda(2)}$ is valid only if every Green's function entering the self-energy transforms the same way. Indeed, in that case, the phase factors cancel at every interaction vertex except the one that connects to the two labels of the self-energy. Hence, the Ward-Takahashi identity is satisfied only if we do linear response theory using functional derivative and if the self-energy satisfies the above condition.

But charge conservation has consequences also on the labels $1, 2$ of the four-point function in Eq. (73.11). And to satisfy that, we will need to use the Luttinger-Ward functional, as I now explain.

73.3 *Particle-number conservation is garanteed if Σ is obtained from $\delta\Phi[\mathcal{G}]/\delta\mathcal{G}$

Particle number conservation implies that the time-derivative of the density is equal to the divergence of a current. By simple analytic continuation, this should be true also for the derivative of the density in imaginary time. But the time-derivative of the density can be obtained from the time-derivative of the Green's function, as can be seen from the following identities that follow from the definition of the Green's function:

$$\frac{\partial \left\langle \psi^\dagger(1) \psi(1) \right\rangle}{\partial \tau} = \left. \frac{\partial \left\langle \psi^\dagger(2) \psi(1) \right\rangle}{\partial \tau_1} \right|_{2\to 1} + \left. \frac{\partial \left\langle \psi^\dagger(2) \psi(1) \right\rangle}{\partial \tau_2} \right|_{2\to 1} \tag{73.13}$$

$$= \left. \frac{\partial \mathcal{G}(1,2)}{\partial \tau_1} \right|_{2\to 1^+} + \left. \frac{\partial \mathcal{G}(1,2)}{\partial \tau_2} \right|_{2\to 1^+}. \tag{73.14}$$

I have already obtained the result from the first term when I considered the equation of motion for the Green's function in Eq. (36.12). I take the physical case $\phi = 0$ so that the time derivatives can be obtained as in Eqs. (36.10) and (36.12) knowing the equations of motion for $\psi^\dagger$, the analog of that obtained for ψ in Eq. (36.7)

$$\frac{\partial \psi^\dagger(2)}{\partial \tau_2} = -\frac{\nabla_1^2}{2m} \psi^\dagger(2) - \mu \psi^\dagger(2) + \psi^\dagger(2)\, \psi^\dagger\left(\overline{1}\right)\, V\left(\overline{1} - 2\right) \psi\left(\overline{1}\right). \tag{73.15}$$

We can append $\psi(1)$ to the left and use the definition of the Green's function to obtain

$$\left[\left(\frac{\partial}{\partial\tau_2}+\frac{\nabla_2^2}{2m}+\mu\right)\right]\mathcal{G}(1,2)=\delta(1-2)-V\left(\overline{1}-2\right)\left\langle T_\tau\left[\psi(1)\psi^\dagger(2)\psi^\dagger\left(\overline{1^+}\right)\psi\left(\overline{1}\right)\right]\right\rangle. \tag{73.16}$$

which reminds us of the equation we had already found when we started from the equation of motion for $\psi(1)$, namely

$$\left[-\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\right]\mathcal{G}(1,2)=\delta(1-2)-V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi(1)\psi^\dagger(2)\right]\right\rangle \tag{73.17}$$

The difference between the next to last and the last equations and $\nabla_2^2-\nabla_1^2=(\nabla_2+\nabla_1)\cdot(\nabla_2-\nabla_1)$ lead to the usual form of current conservation, namely

$$\left.\frac{\partial\mathcal{G}(1,2)}{\partial\tau_1}\right|_{2\to1^+}+\left.\frac{\partial\mathcal{G}(1,2)}{\partial\tau_2}\right|_{2\to1^+}=-\left(\nabla_2+\nabla_1\right)\cdot\left(\nabla_2-\nabla_1\right)\mathcal{G}(1,2)|_{2\to1^+}. \tag{73.18}$$

Remark 359 *Fundamentally, potential energy has disappeared because the density commutes with itself.*

It is useful to rewrite the above equations to show that the above considerations lead to a constraint on the self-energy. Using the definition of $\mathcal{G}_0^{-1}\left(1,\overline{2}\right)$ in Eq. (36.11)

$$\mathcal{G}_0^{-1}\left(1,\overline{2}\right)\equiv-\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\delta\left(1-\overline{2}\right), \tag{73.19}$$

and

$$\mathcal{G}_0^{-1}\left(\overline{2},2\right) \equiv -\left(\frac{\partial}{\partial\tau_{\overline{2}}}-\frac{\nabla_{\overline{2}}^2}{2m}-\mu\right)\delta\left(\overline{2}-2\right) \tag{73.20}$$

$$= -\left(-\frac{\partial}{\partial\tau_2}-\frac{\nabla_{\overline{2}}^2}{2m}-\mu\right)\delta\left(\overline{2}-2\right). \tag{73.21}$$

the two equations of motion can be rewritten as follows

$$\mathcal{G}_0^{-1}\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},2\right)=\delta(1-2)-V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi(1)\psi^\dagger(2)\right]\right\rangle \tag{73.22}$$

and

$$\mathcal{G}\left(1,\overline{2}\right)\mathcal{G}_0^{-1}\left(\overline{2},2\right)=\delta(1-2)-V\left(\overline{1}-2\right)\left\langle T_\tau\left[\psi(1)\psi^\dagger(2)\psi^\dagger\left(\overline{1^+}\right)\psi\left(\overline{1}\right)\right]\right\rangle. \tag{73.23}$$

Remark 360 *The rewriting in terms of $\mathcal{G}_0^{-1}$ and $\mathcal{G}$ shows that charge conservation comes from the commutator of the density operator with the kinetic energy operator, in other words it can be written in the form $\mathcal{G}\left(1,\overline{2}\right)\mathcal{G}_0^{-1}\left(\overline{2},1^+\right)-\mathcal{G}_0^{-1}\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},1^+\right)=0$, a form that will remain true in effective models such as the Hubbard model.*

Using Dyson's equation,

$$\mathcal{G}^{-1}\left(1,\overline{2}\right)=\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right)-\Sigma\left(1-\overline{2}\right)\right). \tag{73.24}$$

the first of these equations of motion takes the form

$$\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right)-\Sigma\left(1-\overline{2}\right)\right)\mathcal{G}\left(\overline{2},2\right)=\delta\left(1-2\right) \tag{73.25}$$

as long as the self-energy is defined by

$$\Sigma\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},2\right)=-V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle \tag{73.26}$$

as in Eq. (36.13). Following a similar argument, the second form of the equation of motion, Eq. (73.17) implies

$$\mathcal{G}\left(1,\overline{2}\right)\Sigma\left(\overline{2},2\right)=-V\left(\overline{1}-2\right)\left\langle T_\tau\left[\psi\left(1\right)\psi^\dagger\left(2\right)\psi^\dagger\left(\overline{1^+}\right)\psi\left(\overline{1}\right)\right]\right\rangle_\phi \tag{73.27}$$

where $\psi\left(1\right)$ has been anticommuted twice. Since $\mathcal{G}^{-1}\mathcal{G}=1$ implies that $\mathcal{G}\mathcal{G}^{-1}=1$ this second expression for the self-energy must give the same result as the previous one. We still need to prove this. Assuming this is the case, setting $2\rightarrow 1^+$ we obtain the conservation law

$$\mathcal{G}\left(1,\overline{2}\right)\mathcal{G}_0^{-1}\left(\overline{2},1^+\right)-\mathcal{G}_0^{-1}\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},1^+\right)=0 \tag{73.28}$$

if the self-energy satisfies both equations, since we will then have

$$\Sigma\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},1^+\right)-\mathcal{G}\left(1,\overline{2}\right)\Sigma\left(\overline{2},1^+\right)=0. \tag{73.29}$$

The last step is to show that last equality. This is done using the Luttinger-Ward fuctional. First note that the relation between Luttinger-Ward functional and self-energy Eq. (72.34) gives

$$\delta\Phi[\mathcal{G}]=\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}\left(\overline{1},\overline{2}\right)}\delta\mathcal{G}\left(\overline{1},\overline{2}\right)=T\pm\left(\overline{2},\overline{1}\right)\delta\mathcal{G}\left(\overline{1},\overline{2}\right). \tag{73.30}$$

But the relation between the Luttinger Ward functional and the potential energy shows that it is gauge invariant since potential energy is an observable. Diagrammatically, for every entering Green's function at a vertex there is an outgoing one, so that under the gauge transformation,

$$\mathcal{G}\left(\overline{1},\overline{2}\right)\rightarrow e^{i\Lambda\left(\overline{1}\right)}\mathcal{G}\left(\overline{1},\overline{2}\right)e^{-i\Lambda\left(\overline{2}\right)} \tag{73.31}$$

$\Phi[\mathcal{G}]$ is invariant. Gauge transformations were discussed in Sections (11.1) and (32.3). The above gauge transformation corresponds to

$$\delta\mathcal{G}\left(\overline{1},\overline{2}\right)=\left(i\Lambda\left(\overline{1}\right)-i\Lambda\left(\overline{2}\right)\right)\mathcal{G}\left(\overline{1},\overline{2}\right) \tag{73.32}$$

which means that

$$\delta\Phi[\mathcal{G}]=T\pm\left(\overline{2},\overline{1}\right)\mathcal{G}\left(\overline{1},\overline{2}\right)\left(i\Lambda\left(\overline{1}\right)-i\Lambda\left(\overline{2}\right)\right)=0. \tag{73.33}$$

Doing a change of dummy integration variables, we have

$$\delta\Phi[\mathcal{G}]=-iT(\pm\left(\overline{2},\overline{1}\right)\mathcal{G}\left(\overline{1},\overline{2}\right)-\pm\left(\overline{1},\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{1}\right))\Lambda\left(\overline{2}\right)=0. \tag{73.34}$$

Since this must be true for any $\Lambda\left(\overline{2}\right)$, this gives the desired equation (73.29).

The conclusion is that if the self-energy is obtained from a functional derivative of any approximation for $\Phi[\mathcal{G}]$ that is a set of closed diagrams, then particle number conservation laws will be satisfied. This is true for the other conservation laws, as shown by Baym [23].

Remark 361 *Approximations obtained from the above prescription are called conserving. There is an infinite number of conserving approximations since there is an infinite number of ways of keeping diagrams to approximate the Luttinger-Ward functional.*

Remark 362 *The equivalence of these two results shows that vertex corrections to the self-energy must be included only once, either on the left or on the right of the diagram. This is more obvious in the diagrammatic language. To see this algebraically, consider the case where the self-energy is obtained from Eq. (73.26) by right multiplying by* $\mathcal{G}_{\phi}^{-1}$*, We obtain,*

$$\Sigma\left(1,3\right)_{\phi} = -V\left(1-\overline{2}\right)\left[\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(1,\overline{4}\right)_{\phi}\right]\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi} \tag{73.35}$$

$$= -V\left(1-\overline{2}\right)\left[\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi}-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\right] \tag{73.36}$$

$$= V\left(1-\overline{2}\right)\left[\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}+\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\right] \tag{73.37}$$

where the first term contains both the Fock term and the vertex corrections associated with $\frac{\delta\pm\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}$*. In the case where* Σ *is left-multiplied by* $\mathcal{G}$*, as in Eq. (73.27) above, we find*

$$\Sigma\left(3,2\right)_{\phi} = -\mathcal{G}^{-1}\left(3,\overline{4}\right)_{\phi}V\left(\overline{1}-2\right)\left[\frac{\delta\mathcal{G}\left(\overline{4},2\right)_{\phi}}{\delta\phi\left(\overline{1^{+}},\overline{1}\right)}-\mathcal{G}\left(\overline{1},\overline{1^{+}}\right)_{\phi}\mathcal{G}\left(\overline{4},2\right)_{\phi}\right] \tag{73.38}$$

$$= -V\left(\overline{1}-2\right)\left[\mathcal{G}^{-1}\left(3,\overline{4}\right)_{\phi}\frac{\delta\mathcal{G}\left(\overline{4},2\right)_{\phi}}{\delta\phi\left(\overline{1^{+}},\overline{1}\right)}-\mathcal{G}\left(\overline{1},\overline{1^{+}}\right)_{\phi}\delta\left(3-2\right)\right] \tag{73.39}$$

$$= V\left(\overline{1}-2\right)\left[\frac{\delta\mathcal{G}^{-1}\left(3,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{1^{+}},\overline{1}\right)}\mathcal{G}\left(\overline{4},2\right)_{\phi}+\mathcal{G}\left(\overline{1},\overline{1^{+}}\right)_{\phi}\delta\left(3-2\right)\right] \tag{73.40}$$

and the vertex correction comes in the other side of the self-energy diagrams.

74. *OTHER FORMAL CONSEQUENCES OF $\Phi[\mathcal{G}]$

Approximations that are obtained by starting from some $\Phi[\mathcal{G}]$ to obtain a self-energy are thermodynamically consistent. In addition, the existence of $\Phi[\mathcal{G}]$ allows us to show that Fermi liquids satisfy the so-called Luttinger's theorem. I explain these two results in this chapter.

74.1 *Thermodynamic consistency

Another advantage of approximations that are obtained from conserving approximations, as defined above, is that they satisfy thermodynamic consistency. What do I mean by that? Consider for example how we obtain particle number. Either we start from its expression in terms of the Green's function

$$N = \mathrm{Tr}\left[\mathcal{G}e^{-ik_n 0^-}\right] \tag{74.1}$$

with the definition of the trace in Eq. (72.13), or we take a derivative of the grand potential with respect to the chemical potential,

$$N = T\frac{\partial \ln Z}{\partial \mu} = -\frac{\partial F}{\partial \mu}. \tag{74.2}$$

Assume that the approximation for Z was obtained from an integration over coupling constant of some approximation for the potential energy. That approximation and the approximation for the self-energy entering the Green's function can lead to two different answers in general when we use the above two equations.

A systematic way of obtaining consistent approximations is to first approximate the Baym-Kadanoff functional Eq. (91.10), and then to obtain the number of particles from a derivative of that functional at equilibrium, where it is equal to the free energy.

So, let us start from $\Omega[\mathcal{G}]$ evaluated in equilibrium. It is a function of μ and β through its dependence on the equilibrium $\mathcal{G}$.

$$N = -\frac{\partial}{\partial \mu}\left\{\Phi[\mathcal{G}] - \mathrm{Tr}\left[\left(\mathcal{G}_0^{-1} - \mathcal{G}^{-1}\right)\mathcal{G}\right] + \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)e^{-ik_n 0^-}\right]\right\} \tag{74.3}$$

$$N = -\mathrm{Tr}\left[\Sigma\frac{\partial \mathcal{G}}{\partial \mu}\right] + \frac{\partial}{\partial \mu}\mathrm{Tr}\left[\Sigma\mathcal{G}\right] - \mathrm{Tr}\left[\mathcal{G}^{-1}\frac{\partial \mathcal{G}}{\partial \mu}e^{-ik_n 0^-}\right]. \tag{74.4}$$

As we discussed below Eq. (72.20) in the context of the free energy in the non-interacting case, the convergence factor in $\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right]$ is the same as that to compute the density. In the last term, we use $\mathcal{G}^{-1}\frac{\partial \mathcal{G}}{\partial \mu} = -\frac{\partial \mathcal{G}^{-1}}{\partial \mu}\mathcal{G}$ so that

$$N = \mathrm{Tr}\left[\frac{\partial \Sigma}{\partial \mu}\mathcal{G}\right] + \mathrm{Tr}\left[\frac{\partial \mathcal{G}^{-1}}{\partial \mu}\mathcal{G}e^{-ik_n 0^-}\right]. \tag{74.5}$$

Since

$$\frac{\partial \mathcal{G}^{-1}}{\partial \mu} = \frac{\partial \mathcal{G}_0^{-1}}{\partial \mu} - \frac{\partial \pm}{\partial \mu} \tag{74.6}$$

we are left with

$$N = \mathrm{Tr}\left[\mathcal{G} e^{-ik_n 0^-}\right], \tag{74.7}$$

which is what we wanted to prove.

74.2 * Luttinger's theorem

The theorem is that in a normal Fermi liquid, the volume of the Fermi sea in reciprocal space at zero temperature is independent of interactions. For spherical Fermi surfaces, it means that the Fermi wave vector is a constant [138][1].

The proof is as follows. At $T = 0$, we can replace the sum over Matsubara frequencies by an integral along the imaginary axis using $\Delta(i\omega_n) = 2\pi i T$ and $i\omega_n \to \omega$ with ω purely imaginary

$$T\sum_n \to \mathrm{P}\int_{-i\infty}^{i\infty} \frac{d\omega}{2\pi i} \tag{74.8}$$

where P is just to remind us that there is a cut along the real axis and that we cannot integrate across it in general. We also have that

$$\frac{\partial}{\partial \omega}\ln \mathcal{G}(\mathbf{k},\omega) = \frac{\partial}{\partial \omega}\left(\ln\left(\frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}\right)\right) \tag{74.9}$$

$$= -\frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}\left(1 - \frac{\partial \Sigma(\mathbf{k},\omega)}{\partial \omega}\right). \tag{74.10}$$

Hence, we may rewrite the expression for the density in d dimensions as follows

$$n = 2T\sum_n \int \frac{d^d k}{(2\pi)^d}\mathcal{G}(\mathbf{k},\omega)\, e^{-ik_n 0^-} \to 2\mathrm{P}\int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi i}\int \frac{d^d k}{(2\pi)^d}\mathcal{G}(\mathbf{k},\omega)\, e^{\omega 0^+} \tag{74.11}$$

$$= -2\mathrm{P}\int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi i}\int \frac{d^d k}{(2\pi)^d}\left[\frac{\partial}{\partial \omega}\ln \mathcal{G}(\mathbf{k},\omega) + \mathcal{G}(\mathbf{k},\omega)\frac{\partial \Sigma(\mathbf{k},\omega)}{\partial \omega}\right] e^{\omega 0^+} \tag{74.12}$$

The last term vanishes because integrating by parts gives

$$\int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi}\int \frac{d^d k}{(2\pi)^d}\mathcal{G}(\mathbf{k},\omega)\frac{\partial \Sigma(\mathbf{k},\omega)}{\partial \omega} \tag{74.13}$$

$$= \int \frac{d^d k}{(2\pi)^d}\,\mathcal{G}(\mathbf{k},\omega)\,\Sigma(\mathbf{k},\omega)\big|_{-i\infty}^{i\infty} - \int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi}\int \frac{d^d k}{(2\pi)^d}\frac{\partial \mathcal{G}(\mathbf{k},\omega)}{\partial \omega}\Sigma(\mathbf{k},\omega) \tag{74.14}$$

The first term vanishes because the self-energy goes to a constant at infinite frequency while $\mathcal{G}(\mathbf{k},\omega)$ decreases as $1/\omega$. The last term vanishes because it is the change in the Luttinger Ward functional when we change the origin of the frequency integral for all the Green's functions entering the diagrams, and since the integrals all go from $-i\infty$ to $i\infty$ this does not change anything.

$$\int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi}\int \frac{d^d k}{(2\pi)^d}\Sigma(\mathbf{k},\omega)\frac{\partial \mathcal{G}(\mathbf{k},\omega)}{\partial \omega} = \int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi}\int \frac{d^d k}{(2\pi)^d}\frac{1}{T}\frac{\delta \Phi[\mathcal{G}]}{\delta \mathcal{G}(\mathbf{k},\omega)}\frac{\partial \mathcal{G}(\mathbf{k},\omega)}{\partial \omega} \tag{74.15}$$

$$= 0 \tag{74.16}$$

We are thus left with

$$n = -2\mathrm{P}\int_{-i\infty}^{i\infty}\frac{d\omega}{2\pi i}\int\frac{d^dk}{(2\pi)^d}e^{\omega 0^+}\frac{\partial}{\partial\omega}\ln\mathcal{G}\left(\mathbf{k},\omega\right). \tag{74.17}$$

To evaluate the integral, form a closed contour by adding at infinity a half-circle with $\mathrm{Re}\,\omega < 0$. The convergence factor $e^{\omega 0^+}$ gives us permission to do that. There is no contribution from the half-circle, but now we can use Cauchy's theorem. There is a discontinuity along the real axis, so we are left with

$$n = -2\int_{-\infty}^{0}\frac{d\omega}{2\pi i}\int\frac{d^dk}{(2\pi)^d}e^{\omega 0^+}\frac{\partial}{\partial\omega}\ln\left(\frac{\mathcal{G}^A\left(\mathbf{k},\omega\right)}{\mathcal{G}^R\left(\mathbf{k},\omega\right)}\right) \tag{74.18}$$

where $\mathcal{G}^A\left(\mathbf{k},\omega\right)$ is the Green's function when ω is infinitesimally below the real axis and $\mathcal{G}^R\left(\mathbf{k},\omega\right)$ when ω is infinitesimally above the real axis. In general

$$\mathcal{G}^{R/A}\left(\mathbf{k},\omega\right) = \mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right) \mp \frac{1}{2}iA\left(\mathbf{k},\omega\right) \tag{74.19}$$

where $A\left(\mathbf{k},\omega\right)$ is the spectral weight, which is positive. The integral over frequency can thus be written in the form

$$\begin{aligned} n &= -\frac{1}{\iota\pi}\int\frac{d^dk}{(2\pi)^d}\ln\left(\frac{\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right)+\frac{1}{2}iA\left(\mathbf{k},\omega\right)}{\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right)-\frac{1}{2}iA\left(\mathbf{k},\omega\right)}\right)\Bigg|_{-\infty}^{0} &(74.20)\\ &= -\frac{1}{\iota\pi}\int\frac{d^dk}{(2\pi)^d}\,2i\tan^{-1}\left(\frac{1}{2}\frac{A\left(\mathbf{k},\omega\right)}{\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right)}\right)\Bigg|_{-\infty}^{0} &(74.21)\end{aligned}$$

The argument of the arctangent is the phase of the complex valuee of the Green's function. We have that $A\left(\mathbf{k},\omega\right)$ falls much faster than $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right)$, which vanishes like $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega\right)\sim 1/\omega < 0$ at $\omega = -\infty$. This means that

$$\tan^{-1}\left(\frac{1}{2}\frac{A\left(\mathbf{k},\omega=-\infty\right)}{\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=-\infty\right)}\right) = \tan^{-1}\left(-0\right) = \pi. \tag{74.22}$$

So far, everything is very general. For a Fermi liquid, there is a further simplification. Indeed, the self-energy satisfies $\Sigma''\left(\mathbf{k},\omega=0\right)=0$ *for all wave vectors* so the spectral weight also vanishes, namely $A\left(\mathbf{k},\omega=0\right)=+0$. So in the domain of $\mathbf{k}$ where $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=0\right)<0$, the arctangent at $\omega=0$ will also be π and the integrand vanishes. But when $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=0\right)>0$

$$\tan^{-1}\left(\frac{1}{2}\frac{A\left(\mathbf{k},\omega=-\infty\right)}{\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=-\infty\right)}\right) = \tan^{-1}\left(+0\right) = 0 \tag{74.23}$$

and we are left with

$$n = 2\int_{\mathrm{Re}\,\mathcal{G}(\mathbf{k},\omega=0)>0}\frac{d^dk}{(2\pi)^d}. \tag{74.24}$$

Since $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=0\right)$ changes sign when this equation is satisfied $\varepsilon_{\mathbf{k}_F}-\mu+\Sigma\left(\mathbf{k}_F,\omega=0\right)=0$, this gives the value of the wave vectors where the Fermi surface is located. The expression for n then is exactly the same as that for a non-interacting Fermi gas. Otherwise, interactions do not modify the volume of the Fermi surface but its shape can change. The chemical potential μ is simply renormalized for parabolic bands in arbitrary dimensions, but the Fermi wave vector is unmodified.

Remark 363 *The sign of* $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=0\right)$ *can change not only because it goes through infinity, as above, but also because it goes to zero. So, we also have the possibility to have a gap at* $\omega=0$*, so that the spectral weight vanishes there, and* $\mathrm{Re}\,\mathcal{G}\left(\mathbf{k},\omega=0\right)$ *that changes sign because it goes through zero.*

Remark 364 *Various elegant derivations and generalizations of Luttinger's theorem are in the litterature. For example, Masaki Oshikawa [181] has given a non-perturbative proof based on topological arguments. This proof has been generalized to Z_2 fractionalized phases of matter for example [184].*

75. CONSERVING APPROXIMATIONS ARE NOT A PANACEA

Conserving approximations are based from an approximation for the Baym-Kadanoff functional. Such approximations satisfy conservation laws and are thermodynamically consistent as we saw above. But they also have limitations that I discuss here following Ref. [255].

In the conserving approximation schemes [23], one takes any physically motivated subset of skeleton diagrams to define a Luttinger-Ward functional Φ. Skeleton diagrams contain fully dressed Green's functions and no self-energy insertions. This functional is functionally differentiated to generate a self-energy that is then calculated self-consistently since it appears implicitly in the Green's functions used in the original set of diagrams. A further functional differentiation allows one to calculate the irreducible vertices necessary to obtain the collective modes in a way that preserves Ward identities. If one uses for the free energy the formula

$$\ln Z = \mathrm{Tr}\left[\ln\left(-G\right)\right] + \mathrm{Tr}\left(\Sigma G\right) - \Phi \tag{75.1}$$

then one obtains thermodynamic consistency in the sense that thermodynamic quantities obtained by derivatives of the free energy are identical to quantities computed directly from the single-particle Green's function, as we just saw in Sec. 74.1. For example, particle number can be obtained either from a trace of the Green's function or from a chemical potential derivative of the free energy. In this scheme, Luttinger's theorem is satisfied as long as perturbation theory converges since then any initial guess for the Luttinger-Ward functional will satisfy Luttinger's theorem, again as we saw above in Sec. 74.2.

Requiring that an approximation be conserving does not constrains the approximation very much in the sense that there is an infinite number of Luttinger-Ward functionals that one can write by summing subserts of diagrams. The Fluctuation exachange approximation (FLEX) is a broadly used conserving approximation that refers to a particular physically motivated choice of diagrams for Φ. This choice leads to the following self-consistent expression for the self-energy

$$\Sigma_\sigma^{BS}\left(k\right) = Un_{-\sigma} + \frac{U}{4}\frac{T}{N}\sum_q \left[\left(3U\tilde{\chi}_{sp}^{RPA}(q) - 2U\tilde{\chi}_0(q)\right) + U\tilde{\chi}_{ch}^{RPA}(q)\right] G_\sigma(k+q). \tag{75.2}$$

This expression for the self-energy does not contain vertex corrections, despite the fact that, contrary to the electron-phonon case, Migdal's theorem does not apply here. This may lead to qualitatively wrong results, such as the absence of precursors of antiferromagnetic bands and of the pseudogap in $A(\vec{k}_F, \omega)$ in two dimensions.

Another drawback of this approach is that it does not satisfy the Pauli principle in any form, either local or through crossing symmetry [188]. Indeed, one would need to include all exchange diagrams to satisfy it. In practice this is never done. In the same way that there is nothing to constrain the value of $\langle n_\uparrow n_\uparrow \rangle$ obtained by the fluctuation-dissipation theorem to be equal to $\langle n_\uparrow \rangle$, there is nothing to explicitly constrain the value of $\langle n_\uparrow n_\downarrow \rangle$. Nevertheless, the Mermin-Wagner theorem is believed to be satisfied in FLEX because the feedback through the self-energy tends to prevent the divergence of fluctuations in low dimension [1],[64]. Physi-

[1] N.E. Bickers, private communication

cally however, this seems to be an artificial way of satisfying the Mermin-Wagner theorem since this theorem should be valid even in localized spin systems where single-particle properties are negligibly influenced by thermal fluctuations. Note that the proof of the Mermin-Wagner theorem in $n \to \infty$ models implies that a finite temperature phase transition in two dimensions is not simply removed by thermal fluctuations, it is replaced by a crossover to the renormalized classical regime with exponentially growing susceptibility. The fact that the conserving susceptibility in FLEX does not show such behavior [64] means that FLEX is actually inconsistent with the generic phase space arguments responsible for the absence of finite-temperature phase transition in two dimensions. The case of one dimension also suggests that collective modes by themselves should suffice to guarantee the Mermin-Wagner theorem without feedback on single-particle properties. Indeed, in one dimension one shows by diagrammatic methods (parquet summation or renormalization) that the zero-temperature phase transition is prohibited at the two-particle level even *without* self-energy effects [41].

Although, the second-order diagram is included correctly in FLEX, it does not have the correct coefficient in the $1/ik_n$ expansion of the self-energy. More importantly, the high-frequency behavior sets-in too late to give the Hubbard bands. We have also seen a case where FLEX, as judged from comparisons with Monte Carlo simulations (Fig.(1a) of Ref. [247] and Fig. 5 of [168]), does not reproduce the results of second-order perturbation theory even when it is a good low-energy approximation.

One of the inconsistencies of conserving approximations that is seldom realized, is that the self-energy is inconsistent with the collective modes. In other words the explicit calculation of ΣG leads to an estimate of $U \langle n_\uparrow n_\downarrow \rangle$ that differs from the one obtained by applying the fluctuation-dissipation theorem to the *conserving* spin and charge susceptibilities, namely those obtained with the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$.

76. THE CONSTRAINING FIELD METHOD

I first derive the Baym-Kadanoff functional more rigorously using the co-called constraining-field method [120], and then I extend this methodology for perturbative calculations.

76.1 Another derivation of the Baym-Kadanoff functional

Instead of "guessing" the correct form of the Baym-Kadanoff functional Eq. (91.10), as we did above, we can start from the differential equation (91.12) for the coupling-constant dependence of the Baym-Kadanoff functional $\Omega_\lambda[\mathcal{G}]$. We find that

$$\Omega_{\lambda=1}[\mathcal{G}] = \Omega_{\lambda=0}[\mathcal{G}] + \int_0^1 d\lambda \frac{1}{\lambda}\left\langle \lambda \hat{V}\right\rangle_\lambda \tag{76.1}$$

$$= \Omega_{\lambda=0}[\mathcal{G}] + \Phi_{\lambda=1}[\mathcal{G}] \tag{76.2}$$

But we know $\Omega_{\lambda=0}[\mathcal{G}]$ since $\mathcal{G}$ is given and $\lambda = 0$ means that we are considering a case when there is no interaction but where $\mathcal{G}$ takes the value it should have for the full problem. So, using the Legendre transform formula Eq.(72.26), we have

$$\Omega_{\lambda=0}[\mathcal{G}] = F_{\lambda=0}[\phi_0] - \mathrm{Tr}[\phi_0 \mathcal{G}] \tag{76.3}$$

where the "constraining field" ϕ_0 is the value of the source field that is necessary for $\mathcal{G}$ to take the correct value for the Green's function. When $\lambda = 0$ we know that

$$F_{\lambda=0}[\phi_0] = \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] \tag{76.4}$$

because (see Secs. (72.2) and (80.2)) this is the result for the non-interacting case when we know $\mathcal{G}$, the actual value of $\mathcal{G}$ as enforced by our choice of ϕ_0. Substituting the equation for $F_{\lambda=0}[\phi_0]$ in our expression for $\Omega_{\lambda=0}[\mathcal{G}]$ and then in our expression for $\Omega_\lambda[\mathcal{G}]$ in Eq.(76.2), we are left with

$$\Omega_{\lambda=1}[\mathcal{G}] = \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] - \mathrm{Tr}[\phi_0\mathcal{G}] + \Phi_{\lambda=1}[\mathcal{G}] \tag{76.5}$$

All that we need to know is $\phi_0(1,2)$.But by definition of $\phi_0(1,2)$ as the source field that allows the non-interacting problem to have the same Green's function as the interacting one, we have that

$$\mathcal{G}^{-1}(1,2)_\phi = \mathcal{G}_0^{-1}(1,2) - \phi_0(1,2). \tag{76.6}$$

This gives us the expression for $\phi_0(1,2)$ (basically the self-energy when $\phi = 0$) so that, finally, $\Omega_{\lambda=1}[\mathcal{G}]$ in the next to last equation takes the form

$$\Omega_{\lambda=1}[\mathcal{G}] = \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] - \mathrm{Tr}\left[(\mathcal{G}_0^{-1} - \mathcal{G}^{-1})\mathcal{G}\right] + \Phi_{\lambda=1}[\mathcal{G}], \tag{76.7}$$

which is what we were looking for.

76.2 The Luttinger-Ward functional can be written in terms of two-particle irreducible skeleton diagrams

I follow Ref. [120], To prove that the lines in the diagrams that give the Luttinger-Ward functional do not have self-energy insertions, in other words that they are skeleton diagrams, start from the expression in the previous section for the Luttinger Ward functional

$$\Phi_{\lambda=1}\left[\mathcal{G}\right]=\int_0^1 d\lambda\frac{1}{\lambda}\left\langle\lambda\hat{V}\right\rangle_{\lambda,\phi[\lambda,\mathcal{G}]}. \tag{76.8}$$

For each value of λ, we need a ϕ that leads to the final self-consistent Green's function. And the Green's function that is used to do the expansion is $\mathcal{G}^{-1}\left(1,2\right)=\mathcal{G}_0^{-1}\left(1,2\right)-\phi_0\left(1,2\right)$. This means that in addition to the usual interaction, there is an additional iteraction that is of the form $-\psi^{\dagger}\left(\overline{1}\right)\left(\phi\left(\overline{1},\overline{2}\right)-\phi_0\left(\overline{1},\overline{2}\right)\right)\psi\left(\overline{2}\right)$ that goes in the perturbation series for the potential energy because $\phi_0\left(1,2\right)$ is just helping us to work with the self-consistent Green's function even at $\lambda=0$. But, given that

$$\mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\phi_0=\mathcal{G}_0^{-1}-\phi_\lambda-\Sigma_\lambda \tag{76.9}$$

we have that

$$\phi_\lambda-\phi_0=-\Sigma_\lambda \tag{76.10}$$

so that every self-energy insertion is cancelled by $\phi_\lambda-\phi_0$. So the diagrams for the Luttinger-Ward functional do not have self-energy insertions and they are fully connected since they do not depend on external variables. The self-energy, which is $\frac{1}{T}\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1,2)}$, can then be written in terms of skeleton diagrams. Since it is one-particle irreducible, it means that $\Phi\left[\mathcal{G}\right]$ is two-particle irreducible. If it was one-particle irreducible, it would be a self-energy.

76.3 A non-perturbative approach based on the constraining field vs the skeleton expansion

The above results are exact. But we can use this procedure to derive a non-perturbative approach where, instead of expanding about $\mathcal{G}_0$, we expand around $\mathcal{G}$ [120]. Instead of doing the replacement $\hat{V}\rightarrow\lambda\hat{V}$, assume this time that λ is the actual value of the coupling constant, for example e^2 in the case of electron-electron interactions. We start from

$$\Omega_{\lambda=e^2}\left[\mathcal{G}\right]=F_{\lambda=0}\left[\phi_0\right]-\mathrm{Tr}\left[\phi_0\mathcal{G}\right]+\Phi_{\lambda=e^2}\left[\mathcal{G}\right]. \tag{76.11}$$

We expand the source field ϕ in powers of the coupling constant:

$$\phi=\phi_0+e^2\phi_1+\left(e^2\right)^2\phi_2+\ldots \tag{76.12}$$

Similarly, we assume that the Luttinger Ward functional can be expanded. Recalling that $\Phi_{\lambda=0}\left[\mathcal{G}\right]=0$,we have that

$$\Phi_{\lambda=e^2}\left[\mathcal{G}\right]=0+e^2\Phi_1+\left(e^2\right)^2\Phi_2+\ldots \tag{76.13}$$

By construction, $\Omega_{\lambda=e^2}[\mathcal{G}]$ is stationnary with respect to ϕ_0 since ϕ_0 simply gives the appropriate $\mathcal{G}$**:**

$$\frac{\delta F_{\lambda=0}[\phi_0]}{\delta \phi_0} = \mathcal{G}. \tag{76.14}$$

The stationnarity condition on $\Omega_{\lambda=e^2}[\mathcal{G}]$ with respect to $\mathcal{G}$ then becomes, for the physical solution at $\phi = 0$,

$$\begin{aligned} \frac{\delta \Omega_{\lambda=e^2}[\mathcal{G}]}{\delta \mathcal{G}} &= -\phi = 0 = -\phi_0 - e^2\phi_1 - \left(e^2\right)^2 \phi_2 + \dots \\ \frac{\delta \Omega_{\lambda=e^2}[\mathcal{G}]}{\delta \mathcal{G}} &= 0 = -\phi_0 + e^2 \frac{\delta \Phi_1}{\delta \mathcal{G}} + \left(e^2\right)^2 \frac{\delta \Phi_2}{\delta \mathcal{G}} + \dots \end{aligned} \tag{76.15}$$

and this last equation with the definition of ϕ_0 may be written as

$$\phi_0 = e^2 \frac{\delta \Phi_1}{\delta \mathcal{G}} + \left(e^2\right)^2 \frac{\delta \Phi_2}{\delta \mathcal{G}} + \dots = \mathcal{G}_0^{-1} - \mathcal{G}^{-1} \tag{76.16}$$

where the last equality give an implicit equation for $\mathcal{G}$. This is just like saying that the self-energy is expanded in powers of e^2, but with dressed $\mathcal{G}$ instead of $\mathcal{G}_0$. The expansion is not with respect to $\mathcal{G}_0$, it is instead with respect to the full Green's function $\mathcal{G}$. So the self-consistent solution of the above equation differs from a straightforward perturbation expansion.

Remark 365 *This approach can be used to derive ordinary mean-field theory for the Ising model for example, or for the Thouless-Anderson-Palmer solution of the spin glass.*

Remark 366 *In the many-body context, this gives the skeleton expansion for the Green's function. Unfortunately, the vertex and the Green's function in this approach are not expanded with respect to $\mathcal{G}_0$ to the same order in coupling constant and this may lead to problems.*

Remark 367 ** Formal matters: conservation laws are satisfied*

77. THE SELF-ENERGY FUNCTIONAL APPROACH AND DMFT

It is possible to formulate dynamical mean-field theory either by restricting all the diagrams in $\Omega[\mathcal{G}]$ to local diagrams, but the self-consistency relations comes out more naturally in the so-called self-energy functional approach. After introducing this functional, introduced by Potthoff, we show its relation to DMFT and its cluster generalizations.

77.1 The self-energy functional

There are various ways to use the stationarity property Eq.(72.32) that we described above. The most common one, is to approximate $\Phi[G]$ by a finite set of diagrams. This is how one obtains the Hartree-Fock, the FLEX approximation[30] or other so-called thermodynamically consistent theories. This is what Potthoff calls a type II approximation strategy.[193] A type I approximation simplifies the Euler equation itself. In a type III approximation, one uses the exact form of $\Phi[G]$ but only on a limited domain of trial Green functions.

Following Potthoff, I consider here type III approximation on a functional of the self-energy instead of on a functional of the Green function. This will lead to the dynamical mean-field equations. Suppose we can locally invert Eq. (72.34) for the self-energy to write $\mathcal{G}$ as a functional of Σ. We can use this result to write,

$$\Omega_{\mathbf{t}}[\Sigma] = P[\Sigma] - \mathrm{Tr}\ln(-\mathcal{G}_{0\mathbf{t}}^{-1} + \Sigma). \tag{77.1}$$

where we defined

$$P[\Sigma] = \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma\mathcal{G}). \tag{77.2}$$

and where it is implicit that $\mathcal{G} = \mathcal{G}[\Sigma]$ is now a functional of Σ. I have added a subscript $\mathbf{t}$ to the non-interacting Green function $\mathcal{G}_{0\mathbf{t}}^{-1}$ to suggest which Hamiltonian we refer to. This will become necessary shortly. The quantity $P[\Sigma]$ along with the expression (72.34) for the derivative of the Luttinger-Ward functional, define the Legendre transform of the Luttinger-Ward functional. It is easy to verify that, as expected

$$\frac{\delta P[\Sigma]}{\delta\Sigma} = \frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}}\frac{\delta\mathcal{G}[\Sigma]}{\delta\Sigma} - \Sigma\frac{\delta\mathcal{G}[\Sigma]}{\delta\Sigma} - \mathcal{G} = -\mathcal{G} \tag{77.3}$$

hence, $\Omega_{\mathbf{t}}[\Sigma]$ is stationary with respect to Σ when Dyson's equation is satisfied

$$\frac{\delta\Omega_{\mathbf{t}}[\Sigma]}{\delta\Sigma} = -\mathcal{G} + (\mathcal{G}_{0\mathbf{t}}^{-1} - \Sigma)^{-1} = 0. \tag{77.4}$$

To perform a type III approximation on $P[\Sigma]$, we must take advantage of the fact that it is universal, i.e., that it depends only on the interaction part of the Hamiltonian and not on the one-body part. This follows from the analogous universal character of its Legendre transform $\Phi[G]$. To be convinced of this universal character, it suffices to think of its two-particle irreducible skeleton diagrams that is a functional of whatever Green functions we decide to use.

The strategy then consists in evaluating $P[\Sigma]$ exactly for a Hamiltonian H' that shares the same interaction part as the Hubbard Hamiltonian, but that is exactly solvable. This Hamiltonian H' is taken as a cluster decomposition of the original problem, i.e., we tile the infinite lattice into identical, disconnected clusters that can be solved exactly. Denoting the corresponding quantities with a prime, we obtain,

$$\Omega_{\mathbf{t}'}[\Sigma'] = P[\Sigma'] - \mathrm{Tr}\ln(-G_{0\mathbf{t}'}^{-1} + \Sigma'). \tag{77.5}$$

from which we can extract $P[\Sigma']$. It follows that

$$\Omega_{\mathbf{t}}[\Sigma'] = \Omega_{\mathbf{t}'}[\Sigma'] + \mathrm{Tr}\ln(-G_{0\mathbf{t}'}^{-1} + \Sigma') - \mathrm{Tr}\ln(-G_{0\mathbf{t}}^{-1} + \Sigma'). \tag{77.6}$$

The type III approximation comes from the fact that the self-energy Σ' is restricted to the exact self-energy of the cluster problem H', so that variational parameters appear in the definition of the one-body part of H'.

In practice, we look for values of the cluster one-body parameters $\mathbf{t}'$ such that $\delta\Omega_{\mathbf{t}}[\Sigma']/\delta\mathbf{t}' = 0$. It is useful for what follows to write the latter equation formally, although we do not use it in actual calculations. Given that $\Omega_{\mathbf{t}'}[\Sigma']$ is the actual grand potential evaluated for the cluster, $\partial\Omega_{\mathbf{t}'}[\Sigma']/\partial\mathbf{t}'$ is canceled by the explicit $\mathbf{t}'$ dependence of $\mathrm{Tr}\ln(-G_{0\mathbf{t}'}^{-1} + \Sigma')$ and we are left with

$$\begin{aligned} 0 &= \frac{\delta\Omega_{\mathbf{t}}[\Sigma']}{\delta\Sigma'}\frac{\delta\Sigma'}{\delta\mathbf{t}'} \\ &= -\mathrm{Tr}\left[\left(\frac{1}{G_{0\mathbf{t}'}^{-1} - \Sigma'} - \frac{1}{G_{0\mathbf{t}}^{-1} - \Sigma'}\right)\frac{\delta\Sigma'}{\delta\mathbf{t}'}\right]. \end{aligned} \tag{77.7}$$

Given that the clusters corresponding to $\mathbf{t}'$ are disconnected and that translation symmetry holds on the superlattice of clusters, each of which contains N_c sites, the last equation may be written

$$\begin{aligned} &\sum_{\omega_n}\sum_{\mu\nu}\left[\frac{N}{N_c}\left(\frac{1}{G_{0\mathbf{t}'}^{-1} - \Sigma'(ik_n)}\right)_{\mu\nu}\right. \\ &\left. - \sum_{\tilde{\mathbf{k}}}\left(\frac{1}{G_{0\mathbf{t}}^{-1}(\tilde{\mathbf{k}}) - \Sigma'(ik_n)}\right)_{\mu\nu}\right]\frac{\delta\Sigma'_{\nu\mu}(ik_n)}{\delta\mathbf{t}'} = 0. \end{aligned} \tag{77.8}$$

77.2 Variational cluster perturbation theory, or variational cluster approximation

In Variational Cluster Perturbation Theory (VCPT), more aptly named the Variational Cluster Approach (VCA), solutions to the Euler equations (77.8) are found by looking for numerical minima (or more generally, saddle-points) of the functional. Typically, the VCA cluster Hamiltonian H' will have the same form as H except that there is no hopping between clusters and that long-range order is allowed by adding some Weiss fields. The hopping terms and chemical potential within H' may also be treated like additional variational parameters. In contrast with Mean-Field theory, these Weiss fields are not mean fields, in the sense that they do not coincide with the corresponding order parameters. The interaction part of H (or H') is not factorized in any way and short-range correlations are treated exactly. In fact, the Hamiltonian H is not altered in any way; the Weiss fields are introduced to let the variational principle act on a space of self-energies

that includes the possibility of specific long-range orders, without imposing those orders. Indeed, the more naturally an order arises in the system, the smaller the Weiss field needs to be, and one observes that the strength of the Weiss field at the stationary point of the self-energy functional generally decreases with increasing cluster size, as it should since in the thermodynamic limit no Weiss field should be necessary to establish order.

77.3 Cellular dynamical mean-field theory

The Cellular dynamical mean-field theory (CDMFT) is obtained by including in the cluster Hamiltonian H' a bath of uncorrelated electrons that somehow must mimic the effect on the cluster of the rest of the lattice. Explicitly, H' takes the form

$$H' = -\sum_{\mu,\nu,\sigma} t'_{\mu\nu} c^\dagger_{\mu\sigma} c_{\nu\sigma} + U \sum_{\mu} n_{\mu\uparrow} n_{\mu\downarrow} + \sum_{\mu,\alpha,\sigma} V_{\mu\alpha} (c^\dagger_{\mu\sigma} a_{\alpha\sigma} + \text{H.c.}) + \sum_{\alpha} \epsilon_\alpha a^\dagger_{\alpha\sigma} a_{\alpha\sigma} \tag{77.9}$$

where $a_{\alpha\sigma}$ annihilates an electron of spin σ on a bath orbital labelled α. The bath is characterized by the energy of each orbital (ϵ_α) and the bath-cluster hybridization matrix $V_{\mu\alpha}$. This representation of the environment through an Anderson impurity model was introduced in Ref. [46] in the context of DMFT (i.e., a single site). The effect of the bath on the electron Green function is encapsulated in the so-called hybridization function

$$\Gamma_{\mu\nu}(\omega) = \sum_{\alpha} \frac{V_{\mu\alpha} V^*_{\nu\alpha}}{\omega - \epsilon_\alpha} \tag{77.10}$$

that enters the Green function as

$$[\mathcal{G}'^{-1}]_{\mu\nu} = \omega + \mu - t'_{\mu\nu} - \Gamma_{\mu\nu}(\omega) - \Sigma_{\mu\nu}(\omega). \tag{77.11}$$

Moreover, the CDMFT does not look for a strict solution of the Euler equation (77.8), but tries instead to set each of the terms between brackets to zero separately. Since the Euler equation (77.8) can be seen as a scalar product, CDMFT requires that the modulus of one of the vectors vanish to make the scalar product vanish. From a heuristic point of view, it is as if each component of the Green function in the cluster were equal to the corresponding component deduced from the lattice Green function. This clearly reduces to single site DMFT when there is only one lattice site.

When the bath is discretized, i.e., is made of a finite number of bath "orbitals", the left-hand side of Eq. (77.8) cannot vanish separately for each frequency, since the number of degrees of freedom in the bath is insufficient. Instead, one adopts the following self-consistent scheme: (1) one starts with a guess value of the bath parameters $(V_{\mu\alpha}, \epsilon_\alpha)$ and solves the cluster Hamiltonian H' numerically. (2) One then calculates the combination

$$\hat{\mathcal{G}}_0^{-1}(ik_n) = \left[\sum_{\tilde{\mathbf{k}}} \frac{1}{\hat{G}^{-1}_{0\mathbf{t}}(\tilde{\mathbf{k}}) - \hat{\Sigma}'(ik_n)} \right]^{-1} + \hat{\Sigma}'(ik_n) \tag{77.12}$$

and (3) minimizes the following canonically invariant distance function:

$$d = \sum_{n,\mu,\nu} \left| \left(ik_n + \mu - \hat{t}' - \hat{\Gamma}(ik_n) - \hat{\mathcal{G}}_0^{-1} \right)_{\mu\nu} \right|^2 \tag{77.13}$$

over the set of bath parameters (changing the bath parameters at this step does not require a new solution of the Hamiltonian H', but merely a recalculation of the hybridization function $\hat{\Gamma}$). The bath parameters obtained from this minimization are then put back into step (1) and the procedure is iterated until convergence.

In practice, the distance function (77.13) can take various forms, for instance by adding a frequency-dependent weight in order to emphasize low-frequency properties[**?**, 37, 224] or by using a sharp frequency cutoff.[**?**] These weighting factors can be considered as rough approximations for the missing factor $\delta\Sigma'_{\nu\mu}(ik_n)/\delta\mathbf{t}'$ in the Euler equation (77.8). The frequencies are summed over on a discrete, regular grid along the imaginary axis, defined by some fictitious inverse temperature β, typically of the order of 20 or 40 (in units of t^{-1}). Even when the total number of cluster plus bath sites in CDMFT equals the number of sites in a VCA calculation, CDMFT is much faster than the VCA since the minimization of a grand potential functional requires many exact diagonalizations of the cluster Hamiltonian H'.

The final lattice Green function from which one computes observable quantities may be obtained by periodizing the self-energy, as in Ref. [121] or in the as in cluter perturbation theory. I prefer the last approach because it corresponds to the Green function needed to obtain the density from $\partial\Omega/\partial\mu = -\mathrm{Tr}(\mathcal{G})$ and also because periodization of the self-energy gives additional unphysical states in the Mott gap[212] (see also Ref. [225]).

77.4 The Dynamical cluster approximation

The DCA[93] cannot be formulated within the self-energy functional approach.[1] It is based on the idea of discretizing irreducible quantities, such as the self-energy, in reciprocal space. It is believed to converge faster for $\mathbf{q} = \mathbf{0}$ quantities whereas CDMFT converges exponentially fast for local quantities.[35, 19, 34]

[1] Th. Maier, M. Potthoff and D. Sénéchal, unpublished.

78. COHERENT-STATES FOR BOSONS

In the many-body context, the amplitudes that are interesting are of the form

$$\mathrm{Tr}\left[\rho c_f\left(t\right)c_i^\dagger\right]. \tag{78.1}$$

In the special case where only the ground state contibutes and that state is the vacuum state (i.e. no particle present), the above reduces precisely to the definition for the one-body Schrödinger equation since $c_i^\dagger\left|0\right\rangle = \left|x_i\right\rangle$ and $\left\langle 0\right| e^{-\beta H}c_f\left(t\right) = \left\langle 0\right| e^{-\beta H}e^{iHt}c_f e^{-iHt} = \left\langle 0\right| c_f e^{-iHt} = \left\langle x_f\right| e^{-iHt}$.

To derive a path integral formulation for that type of amplitude, we note that destruction operators in H always appear first on the right. Hence, if we replace the position eigenstates in the one-particle case by eigenstates of the destruction operator, we will be able to derive a path integral formulation in the many-body case by following a route analogous to that followed for the one-body cases.22 States that are eigenstates of the destruction operator are so-called coherent states. We introduce them for bosons first, that are simpler.

Let $\left[a,a^\dagger\right]=1$, then define the coherent state $\left|z\right\rangle$ by

$$\left|z\right\rangle = e^{-\left|z\right|^2/2}e^{za^\dagger}\left|0\right\rangle. \tag{78.2}$$

To show that this is an eigenstate of the destruction operator a, note first that one can easily show by induction that

$$\left[a,\left(a^\dagger\right)^n\right] = n\left(a^\dagger\right)^{n-1} \tag{78.3}$$

which formally looks like

$$\left[a,\left(a^\dagger\right)^n\right] = \frac{\partial\left(a^\dagger\right)^n}{\partial a^\dagger} \tag{78.4}$$

and since the exponential is defined in terms of its power series

$$\left[a,e^{za^\dagger}\right] = \frac{\partial e^{za^\dagger}}{\partial a^\dagger} = ze^{za^\dagger} \tag{78.5}$$

Using our little theorem on commutators of ladder operators (B.2), we have that since $a\left|0\right\rangle = 0$ then

$$a\left(e^{za^\dagger}\left|0\right\rangle\right) = z\left(e^{za^\dagger}\left|0\right\rangle\right)$$

and $\left|z\right\rangle$ is an eigenstate of a.

To show that $\left|z\right\rangle$ is normalized, consider

$$\begin{aligned}\left\langle z\right.\left|z\right\rangle &= e^{-\left|z\right|^2}\left\langle 0\right| e^{z^*a}e^{za^\dagger}\left|0\right\rangle = e^{-\left|z\right|^2}e^{\left|z\right|^2}\left\langle 0\right| e^{za^\dagger}\left|0\right\rangle \\ &= 1\end{aligned} \tag{78.6}$$

In the last step, one has simply expanded the exponential in a power series and used the normalization of the vacuum.

Finally we give the closure relation

$$I = \frac{1}{\pi}\int dzdz^*\left|z\right\rangle\left\langle z\right| \tag{78.7}$$

that can be proven by taking matrix elements with states with arbitrary number of bosons $|n\rangle = \left(a^\dagger\right)^n |0\rangle / \sqrt{n!}$ and doing the integral in polar coordinates. More specifically, we prove that

$$\langle n \, | m \rangle = \frac{1}{\pi} \int dz dz^* \, \langle n \, | z \rangle \, \langle z | \, m \rangle = \delta_{n,m} \tag{78.8}$$

Proof: First, note that

$$\langle n \, | z \rangle = \frac{1}{\sqrt{n!}} \, \langle 0 | \, (a)^n \, | z \rangle = \frac{z^n}{\sqrt{n!}} \, \langle 0 \, | z \rangle = \frac{z^n}{\sqrt{n!}} e^{-|z|^2/2}. \tag{78.9}$$

Hence, going to polar coordinates

$$\begin{aligned} \frac{1}{\pi} \int dz dz^* \, \langle n \, | z \rangle \, \langle z | \, m \rangle &= \frac{1}{\pi} \int dz dz^* \frac{z^n}{\sqrt{n!}} \frac{z^{*m}}{\sqrt{m!}} e^{-|z|^2} \\ &= \frac{1}{\pi} \int d\phi \int_0^\infty r dr e^{-r^2} \frac{r^{(n+m)}}{\sqrt{n!}\sqrt{m!}} e^{i(n-m)\phi} \\ &= \int_0^\infty dr^2 e^{-r^2} \frac{r^{2n}}{n!} \delta_{n,m} = \delta_{n,m}. \end{aligned}$$

The derivation of the coherent state path integral for bosons is left as an exerice that should not be too difficult after we see the procedure for fermions in the following sections.

79. COHERENT STATES FOR FERMIONS

Let us go back momentarily to first quantization: the Feynman path integral is an integral over all coordinates. The coordinates are operators in the Hamiltonian formalism. In the path integral case, the argument of the exponential is the action in units of $\hbar$.

By analogy, in second quantization, we want a path integral where the argument of the exponential is the action and the integrals are over fields. For bosons, it suffices to work in the coherent state basis. Coherent states for bosons are the analogs of classical fields. What are coherent states for fermions? This is what we set to do first. Then the functional integral follows naturally. An excellent reference is J.W. Negele and H. Orland, "Quantum Many-Particle Systems" (Addison-Wesley, Redwood city, 1988).

79.1 Grassmann variables for fermions

We wish to compute the partition function for time-ordered products with imaginary-time dependent Hamiltonians. This situation occurs for example when one does perturbation theory, obtains an effective Hamiltonian, or with source fields. Fermion coherent states are defined by analogy with the bosonic case. For simplicity, we work with spinless fermions. It is easy to introduce spins afterwards.

Let c be a fermion destruction operator, then $c\,|0\rangle = 0$ while the fermion coherent state $|\eta\rangle$ is an eigenstate of the destruction operator, by analogy with bosons.

$$c\,|\eta\rangle = \eta\,|\eta\rangle\,. \tag{79.1}$$

Since $c_1c_2\,|\eta_1,\eta_2\rangle = -c_2c_1\,|\eta_1,\eta_2\rangle$ the eigenvalues η must be numbers that anti-commute. Namely,

$$\{\eta_1,\eta_2\} = 0. \tag{79.2}$$

Since Grassmann numbers occur only inside time-ordered products, it turns out that it suffices to define the adjoint in such a way that it also anticommutes, there is no delta function:

$$\left\{\eta,\eta^\dagger\right\} = 0. \tag{79.3}$$

Given the definition of Grassmann numbers, one can write an explicit definition of fermion coherent states in the Fock basis if we add the definition that Grassmann numbers and fermion operators also anticommute:

$$|\eta\rangle = \left(1-\eta c^\dagger\right)|0\rangle \tag{79.4}$$

Given that $\eta^2 = 0$, one can verify the defining property $c\,|\eta\rangle = \eta\,|\eta\rangle$ Eq.(79.1):

$$c\,|\eta\rangle = c\,|0\rangle + \eta cc^\dagger\,|0\rangle = \eta\,|0\rangle = \eta\left(1-\eta c^\dagger\right)|0\rangle = \eta\,|\eta\rangle\,. \tag{79.5}$$

Also, again since $\eta^2 = 0$, we can use the definition

$$|\eta\rangle = e^{-\eta c^\dagger}\,|0\rangle \tag{79.6}$$

that has the same structure as a boson coherent state.

Note that while η and $\eta^\dagger$ must be considered independent, the same way that z and z^* must be considered independent, they are nevertheless adjoint from each other. Namely, we have that

$$\langle \eta | = \langle 0 | \left(1 - c\eta^\dagger \right). \tag{79.7}$$

79.2 Grassmann integrals

In the case of bosons, the amplitude of a coherent state is arbitrary. For fermions, we imagine something analog. We must define then Grassmann integrals. To have meaning as integrals, these must satisfy properties such as

$$\int d\eta f\left(\eta + \xi\right) = \int d\eta f\left(\eta\right) \tag{79.8}$$

where ξ is another Grassmann number. The most general function of a Grassmann variable is $f\left(\eta\right) = a + b\eta$ since $\eta^2 = 0$. Hence, the above property is satisfied if $\int d\eta b\xi = 0$, which implies

$$\boxed{\int d\eta = 0.} \tag{79.9}$$

For derivatives and integrals to be consistent, the formula for integration by parts is also satisfied with the above definition (as if f vanished at infinity) because $\frac{df}{d\eta}$ can only be an ordinary number ($f\left(\eta\right)$ can only be linear in η).

$$\int d\eta \frac{df}{d\eta} = 0. \tag{79.10}$$

This definition is thus consistent with the natural definition of a derivative

$$\boxed{\frac{df}{d\eta} = \frac{d(a+b\eta)}{d\eta} = b} \tag{79.11}$$

with a and b ordinary C numbers.

Linearity

$$\int d\eta \left(af\left(\eta\right) + bg\left(\eta\right)\right) = \int d\eta af\left(\eta\right) + \int d\eta bg\left(\eta\right) \tag{79.12}$$

will be satisfied as long as $\int d\eta\eta$ is a number. The choice

$$\boxed{\int d\eta\eta = 1} \tag{79.13}$$

is convenient. The last property is consistent with the fact that the product of two Grassmann numbers is an ordinary number.

In the end, note that the formula for integration looks the same as the formula for differentiation. The two rules Eqs.79.9 and 79.13 are all we need to remember. Grassmann calculus is much easier than ordinary calculus. Not many things to remember!

79.3 Change of variables in Grassmann integrals

The changes of variables we will need will usually be unitary. Consider for example the following change of variable

$$\psi_i = \sum_{j=1}^{N} U_{ij}\eta_j \tag{79.14}$$

Then

$$\prod_{i=1}^{N}\int d\psi_i = \prod_{i=1}^{N}\sum_{j_i=1}^{N} U_{ij_i}\int d\eta_{j_i}. \tag{79.15}$$

All the j_i indices need to be different because of the properties of the Grassmann numbers. In addition, if you rearrange all the $d\eta_{j_i}$ in increasing order of index, $j_1 = 1$, $j_2 = 2$ etc, the signature of the permutation appears. This can be summarized with the help of the completely antisymmetric (Levi-Civita) tensor $\varepsilon^{j_1 j_2 \cdots j_N}$,

$$\begin{aligned}
\prod_{i=1}^{N}\sum_{j_i=1}^{N} U_{ij_i}\int d\eta_{j_i} &= \sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\cdots\sum_{j_N=1}^{N} U_{1j_1}U_{2j_2}\cdots U_{Nj_N}\int d\eta_{j_1}\int d\eta_{j_2}\cdots\int d\eta_{jN} \\
&= \sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\cdots\sum_{j_N=1}^{N} U_{1j_1}U_{2j_2}\cdots U_{Nj_N}\varepsilon^{j_1 j_2\cdots j_N}\int d\eta_1\int d\eta_2\cdots\int d\eta_N \\
&= \det[U]\prod_{k=1}^{N}\int d\eta_k
\end{aligned} \tag{79.16}$$

Note that the change of variables between imaginary time and Matsubara frequencies is almost unitary, but not quite since

$$\mathcal{G}(\tau) = T\sum_n e^{-ik_n\tau}\mathcal{G}(ik_n) \tag{79.17}$$

$$\mathcal{G}(ik_n) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}(\tau) \tag{79.18}$$

gives a transformation matrix $Te^{-ik_n\tau}$ whose inverse is $d\tau e^{ik_n\tau}$ is not just the complex conjugate of the transpose. There is a numerical factor that comes in. This will lead to subtleties in the expression for the partition function below. Contrast this with the unitary transformation $\frac{1}{\sqrt{N}}e^{i\mathbf{k}\cdot\mathbf{r}_i}$ that allows one to go from discrete momentum space to discrete lattice sites.

79.4 Grassmann Gaussian integrals

Let us practice with the integral we will meet all the time, the analog of the Gaussian integral. With the above rules for integration, and $e^{-\eta^\dagger\eta} = 1 - \eta^\dagger\eta$ that follows from $\eta^2 = 0$, we find

$$\int d\eta^\dagger\int d\eta e^{-\eta^\dagger a\eta} = \int d\eta^\dagger\int d\eta\left(1-\eta^\dagger a\eta\right) = a = \exp(\log(a)) \tag{79.19}$$

where a is an ordinary number. We used,

$$\int d\eta^\dagger \int d\eta \left(-\eta^\dagger a \eta\right) = \int d\eta^\dagger \eta^\dagger \int d\eta \eta a = a.$$

Note the order of $\int d\eta^\dagger \int d\eta$. We have to keep this order for the rest of our calculations. This is a mere convention, but since Grassmann variables anticommute, we should stick with one convention.

If we have two Grassman variables,

$$\begin{aligned}
\int d\eta_1^\dagger \int d\eta_1 e^{-\eta_1^\dagger a_1 \eta_1} \int d\eta_2^\dagger \int d\eta_2 e^{-\eta_2^\dagger a_2 \eta_2} &= \\
\int d\eta_1^\dagger \int d\eta_1 \int d\eta_2^\dagger \int d\eta_2 e^{-\eta_1^\dagger a_1 \eta_1} e^{-\eta_2^\dagger a_2 \eta_2} &= a_1 a_2 \qquad (79.20)\\
&= \exp\left[\ln a_1 + \ln a_2\right] \qquad (79.21)
\end{aligned}$$

The quantity $a_1 a_2$ is the determinant of the diagonal matrix with a_1 and a_2 on the diagonal. Since it can easily be proven by power series expansion (or from the fact that $\eta_1^\dagger \eta_1$ commutes with $\eta_2^\dagger \eta_2$) that exponentials of sums of quadratic Grassmann expressions behave as classical objects, namely

$$e^{-\eta_1^\dagger a_1 \eta_1} e^{-\eta_2^\dagger a_2 \eta_2} = e^{-\eta_1^\dagger a_1 \eta_1 - \eta_2^\dagger a_2 \eta_2}, \qquad (79.22)$$

we can write in matrix notation for a general basis

$$\boxed{\prod_i \int d\eta_i^\dagger \int d\eta_i e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta}} = \det(A) = \exp\left[\mathrm{Tr} \ln(A)\right].} \qquad (79.23)$$

The last equalities follow by using the fact that the determinant and the trace are both basis independent. We abbreviate further the notation with the definition of the integration measure

$$\boxed{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta}} \equiv \prod_i \int d\eta_i^\dagger \int d\eta_i e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta}}.} \qquad (79.24)$$

There is another gaussian integral to do that is simple and that will allow us to use source fields to our benefit. Defining the Grassman source fields J and $J^\dagger$, we can use what we know about shifting the origin of integration, Eq.(79.8), and obtain

$$\begin{aligned}
\int d\eta^\dagger \int d\eta e^{-\eta^\dagger a \eta - \eta^\dagger J - J^\dagger \eta} &= \int d\eta \int d\eta^\dagger e^{-\left(\eta^\dagger + J^\dagger a^{-1}\right) a \left(\eta + a^{-1} J\right) + J^\dagger a^{-1} J} \qquad (79.25)\\
&= a \exp\left(J^\dagger a^{-1} J\right). \qquad (79.26)
\end{aligned}$$

The generalization to integrals over many Grassmann variables gives

$$\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta} - \boldsymbol{\eta}^\dagger \mathbf{J} - \mathbf{J}^\dagger \boldsymbol{\eta}} = \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\left(\boldsymbol{\eta}^\dagger + \mathbf{J}^\dagger \mathbf{A}^{-1}\right) \mathbf{A} \left(\boldsymbol{\eta} + \mathbf{A}^{-1} \mathbf{J}\right) + \left(\mathbf{J}^\dagger \mathbf{A}^{-1} \mathbf{J}\right)}$$

$$\boxed{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta} - \boldsymbol{\eta}^\dagger \mathbf{J} - \mathbf{J}^\dagger \boldsymbol{\eta}} = \det(A) \exp\left(\mathbf{J}^\dagger \mathbf{A}^{-1} \mathbf{J}\right)} \qquad (79.27)$$

We will be able to use this result to obtain Green's functions or multipoint functions from functional derivatives with respect to J.

79.5 Closure, overcompleteness and trace formula

To find the expression for the partition function, we will need the completeness relation. From the last result of the previous section, you can verify the following closure formula by applying it successively on $|0\rangle$ and on $c^\dagger |0\rangle$:

$$\boxed{\int d\eta^\dagger \int d\eta e^{-\eta^\dagger \eta} |\eta\rangle \langle\eta| = \int d\eta^\dagger \int d\eta \left(1-\eta^\dagger\eta\right) |\eta\rangle \langle\eta| = I.} \tag{79.28}$$

Indeed, recalling that only terms of the form $\int d\eta^\dagger \int d\eta \eta^\dagger \eta = -1$ survive, we are left with

$$\begin{aligned} & \int d\eta^\dagger \int d\eta \left(1-\eta^\dagger\eta\right)\left(1-\eta c^\dagger\right)|0\rangle\langle 0|\left(1-c\eta^\dagger\right) \\ = & \int d\eta^\dagger \int d\eta \left[\left(-\eta^\dagger\eta\right)|0\rangle\langle 0| + \eta c^\dagger |0\rangle\langle 0| c\eta^\dagger\right] \\ = & |0\rangle\langle 0| + |1\rangle\langle 1| \end{aligned}$$

Take a single state that can be empty or occupied, as above. The trace of an operator O can be written as follows,

$$\boxed{\mathrm{Tr}[O] = \int d\eta^\dagger \int d\eta e^{-\eta^\dagger\eta} \langle -\eta| O |\eta\rangle.} \tag{79.29}$$

The minus sign reflects the antiperiodicity that we encounter with fermions. To prove the above formula, it suffices to use the definition of the fermionic coherent state Eq.(92.4). Indeed,

$$\begin{aligned} \int d\eta^\dagger \int d\eta e^{-\eta^\dagger\eta} \langle -\eta| O |\eta\rangle &= \int d\eta^\dagger \int d\eta e^{-\eta^\dagger\eta} \langle 0|\left(1+c\eta^\dagger\right) O \left(1-\eta c^\dagger\right)|0\rangle \\ &= \int d\eta^\dagger \int d\eta \left(1-\eta^\dagger\eta\right)\langle 0|\left(1+c\eta^\dagger\right) O \left(1-\eta c^\dagger\right)|0\rangle \\ &= \int d\eta^\dagger \int d\eta \left(1-\eta^\dagger\eta\right)\left(\langle 0| O |0\rangle - \langle 0| c\eta^\dagger O \eta c^\dagger |0\rangle\right) \\ &= \int d\eta^\dagger \int d\eta \left(1-\eta^\dagger\eta\right)\left(\langle 0| O |0\rangle - \eta^\dagger\eta \langle 0| cOc^\dagger |0\rangle\right) \\ &= \langle 0| O |0\rangle + \langle 1| O |1\rangle . \end{aligned} \tag{79.30}$$

In the next to last equation, we assumed that O contains an even number of fermion operators so that

$$\eta O = O\eta. \tag{79.31}$$

The set is overcomplete since using the definition in terms of Fock states Eq.(92.4), one finds

$$\boxed{\langle \eta_1 |\eta_2\rangle = \langle\eta|\left(1-c\eta_1^\dagger\right)\left(1-\eta_2 c^\dagger\right)|0\rangle = 1+\eta_1^\dagger\eta_2 = e^{\eta_1^\dagger\eta_2}.} \tag{79.32}$$

80. THE COHERENT STATE FUNCTIONAL INTEGRAL FOR FERMIONS

The coherent state functional integral is obtained by using the Trotter decomposition Eq.(80.3) and inserting complete sets of variables everywhere. We first perform this task with non-interacting spinless fermions, keeping the discreteness explicit. When you move to the continuum limit, everything becomes elegant looking, but there are some hidden subtelties to take care of. We apply the formalism to quantum impurities and establish Wick's theorem.

80.1 A simple example for a single fermion without interactions

For spinless fermions whose Hamiltonian is given by $H = \sum_i \varepsilon_i c_i^\dagger c_i$, the partition function is

$$Z = \mathrm{Tr}\left(\exp\left(-\beta H\right)\right) = \prod_i \left(1 + e^{-\beta\varepsilon_i}\right) = \det\left(1 + e^{-\beta\boldsymbol{\varepsilon}}\right) \tag{80.1}$$

where $\boldsymbol{\varepsilon}$ is the diagonal matrix. The expression remains valid in an arbitrary basis. What is the generalization of this result when H depends on τ and we want a time-ordered product

$$Z = \mathrm{Tr}\left(T_\tau \exp\left(-\int_0^\beta d\tau H\left(\tau\right)\right)\right)? \tag{80.2}$$

We can work this out in the usual operator formalism. With Grassmann variables, we need to suffer first, but then the calculations are easy and formally very close to those for bosons.

Let us start with a single fermion state, so that

$$H = \varepsilon c^\dagger c.$$

Then, we express the trace in the coherent fermion basis. In that basis, we do not know how to compute $e^{-\beta H}\left|\eta\right\rangle$ since the expansion of the exponential gives an infinite number of terms. We can however use the Trotter decomposition to do a Taylor expansion that will be easy to evaluate in the coherent state basis. The Trotter decomposition is given by

$$e^{-\beta H} = \lim_{N_\tau\to\infty} \prod_{i=1}^{N_\tau} e^{-\Delta\tau_i H} = \lim_{N_\tau\to\infty} \prod_{i=1}^{N_\tau} \left(1 - \Delta\tau_i H\right). \tag{80.3}$$

with $\Delta\tau = \beta/N_\tau$. The index i on $\Delta\tau$ is just to allow us to keep track of the different terms. Even if H was time dependent, we could use this approximation

in the limit $\Delta\tau \to 0$ because $[\Delta\tau H(\tau_1), \Delta\tau H(\tau_2)] = \mathcal{O}(\Delta\tau)^2$ and we will neglect terms of that order. In other words, for $\Delta\tau \to 0$ we can assume that exponentials of sums of operators can be rewritten as a product of exponentials.[1] To linear order in $\Delta\tau$ then, we have that

$$\langle\eta_2| e^{-\Delta\tau_i H\left[c^\dagger, c\right]} |\eta_1\rangle = e^{-\Delta\tau_i H\left[\eta^\dagger, \eta\right]} \langle\eta_2 |\eta_1\rangle \tag{80.4}$$

In this expression, we have assumed that all destruction operators were on the right and all creation operators on the left so that they can be replaced by the corresponding Grassmann variable when acting on coherent states.

Back to our task. Using the trace formula in the coherent state basis Eq.(79.29) and inserting the completeness relation Eq.(79.28) between each term of the product, we can evaluate the exponential in the coherent-state basis. We find, with the definitions $\eta_\beta = \eta_{N_\tau} = -\eta_0$ and

$$\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta = \int d\eta_0^\dagger \int d\eta_0 \prod_{i=1}^{N_\tau} \int d\eta_i^\dagger \int d\eta_i$$

that

$$\begin{aligned} Z &= \lim_{N_\tau\to\infty} \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\eta_\beta^\dagger \eta_\beta} \langle\eta_\beta| e^{-\Delta\tau_{N_\tau} \varepsilon \eta_\beta^\dagger \eta_{N_\tau - 1}} |\eta_{N_\tau - 1}\rangle \; e^{-\eta_{N_\tau-1}^\dagger \eta_{N_\tau-1}} \langle\eta_{N_\tau-1}| \\ &\quad \ldots |\eta_1\rangle e^{-\eta_1^\dagger \eta_1} \langle\eta_1| e^{-\Delta\tau_1 \varepsilon \eta_1^\dagger \eta_0} |\eta_0\rangle \qquad (80.5) \\ &= \lim_{N_\tau\to\infty} \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\eta_\beta^\dagger \eta_\beta} \langle\eta_\beta |\eta_{N_\tau-1}\rangle e^{-\varepsilon \eta_\beta^\dagger \eta_{N_\tau-1} \Delta\tau} \; e^{-\eta_{N_\tau-1}^\dagger \eta_{N_\tau-1}} \langle\eta_{N_\tau-1}| \\ &\quad \ldots |\eta_1\rangle \; e^{-\eta_1^\dagger \eta_1} e^{\eta_1^\dagger \eta_0} e^{-\varepsilon \eta_1^\dagger \eta_0 \Delta\tau}. \qquad (80.6) \end{aligned}$$

which is a time-ordered product. We have used, $e^{-\eta_1^\dagger \eta_1} \langle\eta_1 |\eta_0\rangle = e^{-\eta_1^\dagger \eta_1 + \eta_1^\dagger \eta_0}$. The above formula is obviously generalizable to a time-dependent Hamiltonian that appears in a time-ordered product. To evaluate this quantity on a computer, we need to first do the integrals over Grassmann variables and express the result in terms of matrices, remembering that the definition of the matrices must be read off the above formula. There is no ambiguity. The matrix A that appeared in the Gaussian Grassmann integral Eq.(79.23) can thus be written as

$$\boxed{A = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 & (1-\varepsilon\Delta\tau) \\ -(1-\varepsilon\Delta\tau) & 1 & 0 & \ldots & 0 & 0 \\ 0 & -(1-\varepsilon\Delta\tau) & 1 & \ldots & 0 & 0 \\ 0 & 0 & -(1-\varepsilon\Delta\tau) & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 1 & 0 \\ 0 & 0 & 0 & \ldots & -(1-\varepsilon\Delta\tau) & 1 \end{bmatrix} \equiv -\mathcal{G}^{-1}.} \tag{80.7}$$

The above matrix has dimension $N_\tau \times N_\tau$. Labels 0 to $N_\tau - 1$ or 1 to N_τ can be used. In other words, either time $\tau = 0$ or $\tau = \beta$ can be present as independent labels, but not both. They are related by antiperiodicity. The matrix element in the upper right corner comes from

$$\langle\eta_\beta |\eta_{N_\tau-1}\rangle e^{-\varepsilon\eta_\beta^\dagger \eta_{N_\tau-1}\Delta\tau} = \langle -\eta_0 |\eta_{N_\tau-1}\rangle e^{\varepsilon\eta_0^\dagger \eta_{N_\tau-1}\Delta\tau} = e^{(-1+\varepsilon\Delta\tau)\eta_0^\dagger \eta_{N_\tau-1}}. \tag{80.8}$$

[1] There is one subtlety. We have many time-slices. Since $N_\tau(\Delta\tau)^2 = \beta\Delta\tau$, it looks as if the error is of order $\Delta\tau$, not $(\Delta\tau)^2$. Fye has shown that the prefactor of $\beta\Delta\tau$ vanishes when one is interested in expectation values of certain kinds of operators. This is basically because the operator in front of $\Delta\tau$ is a commutator and is thus anti-Hermitian. The trace of that anti-hermitian operator vanishes.

Note that in actual computations, it is more accurate to replace $-1+\varepsilon\Delta\tau$ by $-e^{\varepsilon\Delta\tau}$. If ε is time dependent, it suffices to replace its value at the appropriate time slice. If ε is time independent, the determinant of the matrix A is equal, when N_τ tends to infinity, to $\left(1+(1-\varepsilon\Delta\tau)^{N_\tau}\right)=\left(1+e^{-\beta\varepsilon}\right)$, as we would expect from the free fermion formula Eq.(80.1) when there is a single fermion state.

80.2 Generalization to a continuum and to a time dependent one-body Hamiltonian

The continuum limit can also be taken formally. We can combine the exponentials coming from the completeness relation and from the overlap of fermion coherent states as follows

$$e^{-\eta_1^\dagger\eta_1}\left\langle\eta_1\right|\left.\eta_0\right\rangle=e^{-\eta_1^\dagger\eta_1+\eta_1^\dagger\eta_0}=e^{-\eta_1^\dagger(\eta_1-\eta_0)}=e^{-\eta_1^\dagger\frac{\partial}{\partial\tau}\eta_1\Delta\tau}. \tag{80.9}$$

Also, to leading order in $\Delta\tau$, we approximate terms such as $\eta_1^\dagger\eta_0\Delta\tau$ by $\eta_0^\dagger\eta_0\Delta\tau$. If we take the limit and impose the $\eta_\beta=-\eta_0$ on the last matrix element to the left, we can rewrite the partition function as

$$Z=\int\mathcal{D}\eta^\dagger\int\mathcal{D}\eta\exp\left(-S\right) \tag{80.10}$$

where, by analogy with the Lagrangian formalism, we define the following quantity

$$S=\int_0^\beta d\tau\left(\eta^\dagger\left(\tau\right)\frac{\partial}{\partial\tau}\eta\left(\tau\right)+\varepsilon\left(\tau\right)\eta^\dagger\left(\tau\right)\eta\left(\tau\right)\right) \tag{80.11}$$

as the action S. In writing this, the $\varepsilon\left(\tau\right)$ shows that we have generalized also to a time-dependent Hamiltonian. The integrand is like a Lagrangian when $\eta^\dagger\left(\tau\right)$ and $\eta\left(\tau\right)$ are taken as conjugate variables.

Thinking of the η at different times as different variables, we can use our formula for Gaussian integrals over Grassmann variables Eq.(79.23) the partition funciton can be written as

$$Z=\det\left(\frac{\partial}{\partial\tau}+\varepsilon\left(\tau\right)\right)=\exp\left[\operatorname{Tr}\log\left(\frac{\partial}{\partial\tau}+\varepsilon\left(\tau\right)\right)\right]. \tag{80.12}$$

The matrix entering determinant and trace above is defined by returning to the discrete representation.

In the case of a time-independent Hamiltonian, the determinant can be formally evaluated as follows. Go to the basis where the time derivative is diagonal, namely the Matsubara-frequency basis. Then, we obtain

$$\begin{aligned} Z &= \exp\left[\operatorname{Tr}\log\left(-ik_n+\varepsilon\right)\right]=\exp\left[\sum_n\log\left(-ik_n+\varepsilon\right)e^{-ik_n0^-}\right] && (80.13)\\ &= \exp\left[\sum_n\log\left(-\mathcal{G}^{-1}\left(ik_n\right)\right)e^{-ik_n0^-}\right]. && (80.14)\end{aligned}$$

The factor $e^{-ik_n0^-}$ is made necessary to have a unique result. Read the important remark below to understand the difficulties of interpretation of the above formula.

Remark 368 *You will see this formula very often in the literature, but it is in fact not quite correct because the sum over Matsubara frequencies does not converge. Proofs that use integrals in the complex plane neglect a contribution from a contour at infinity that itself gives an infinite contribution. The derivatives of this formula, nevertheless, give correct results if we proceed without asking questions. To verify this, look at the expression for the occupation number*

$$\begin{aligned} n &= \frac{\mathrm{Tr}\left(\exp\left(-\beta H\right)c^{\dagger}c\right)}{\mathrm{Tr}\left(\exp\left(-\beta H\right)\right)} = -\frac{\partial \ln Z}{\partial\left(\beta\varepsilon\right)} \\ &= -\frac{\partial \sum_{n} \log\left(-ik_n+\varepsilon\right)e^{-ik_n 0^-}}{\partial\left(\beta\varepsilon\right)} = T\sum_{n}\frac{e^{-ik_n 0^-}}{\left(ik_n-\varepsilon\right)} = \frac{1}{1+e^{\beta\epsilon}}. \end{aligned} \tag{80.15}$$

In this expression, we have assumed that the sum converged to invert the sum and the derivative. This is not quite legal but it works. To understand how to obtain expressions that are more meaningful and recover the formula obtained in the canonical formalism Eq.(80.1) consider the following integral

$$\begin{aligned} \int_{\infty}^{\varepsilon} d\varepsilon' \frac{\partial \ln Z}{\partial \varepsilon'} &= \ln Z\left(\varepsilon\right) - \ln Z\left(\varepsilon=\infty\right) = -\beta\int_{\infty}^{\varepsilon} d\varepsilon' \frac{1}{1+e^{\beta\epsilon'}} \\ &= -\beta\int_{\infty}^{\varepsilon} d\varepsilon' \frac{e^{-\beta\epsilon'}}{e^{-\beta\epsilon'}+1} = \ln\left(1+e^{-\beta\epsilon'}\right)\Big|_{\infty}^{\varepsilon}, \end{aligned} \tag{80.16}$$

Hence, if you notice that $\ln Z\left(\varepsilon=\infty\right) = \ln(1) = 0$ *we can make sense of the trace-log formula Eq.(80.14) by rewriting it in the form*

$$\boxed{-T\ln Z = \ln\left(1+e^{-\beta\epsilon'}\right)\Big|_{\infty}^{\varepsilon} = -\left[T\sum_{n}\log\left(\frac{-\mathcal{G}^{-1}(ik_n)}{-\mathcal{G}_{\infty}^{-1}(ik_n)}\right)e^{-ik_n 0^-}\right]} \tag{80.17}$$

where

$$\mathcal{G}_{\infty}^{-1}\left(ik_n\right) = \lim_{E\to\infty}\left(ik_n - E\right). \tag{80.18}$$

For a numerical calculation the choice of E *is important (see more below). The difficulties outlined here seem to originate from the fact that the transformation between imaginary time and Matsubara frequency is not unitary. It involves constant factors, as discussed in Sec.79.3. Note that it is also possible to use the following formula*

$$-T\ln Z + T\ln 2 = \ln\left(1+e^{-\beta\epsilon'}\right)\Big|_{0}^{\varepsilon} = -\left[T\sum_{n}\log\left(\frac{-\mathcal{G}^{-1}\left(ik_n\right)}{-\mathcal{G}_{\varepsilon=0}^{-1}\left(ik_n\right)}\right)e^{-ik_n 0^-}\right]$$

where

$$\mathcal{G}_{\varepsilon=0}^{-1}\left(ik_n\right) = ik_n. \tag{80.19}$$

With either formula, the sum can be computed by a contour integral that does not neglect an infinite contribution. However, in the general case where $\mathcal{G}^{-1}\left(ik_n\right)$ *contains a self-energy, in which case* $T\sum_{n}\log\left(\frac{-\mathcal{G}^{-1}(ik_n)}{-\mathcal{G}_{\varepsilon=0}^{-1}(ik_n)}\right)e^{-ik_n 0^-}$ *is just one of the contributions to* Z*, the quantity* $\log\left(\frac{-\mathcal{G}^{-1}(ik_n)}{-\mathcal{G}_{\varepsilon=0}^{-1}(ik_n)}\right)e^{-ik_n 0^-}$ *behaves at infinity like* $Ae^{-ik_n 0^-}/ik_n$*, where* A *is a constant. This series is not so well behaved numerically. So, ideally one must be careful to choose the denominator in such as way that the coefficient* A *in the asymptotic behavior vanishes. .*

80.3 Wick's theorem

To find the Green function, we can first assume again that we work in the diagonal basis. Then, in this diagonal basis, we expand the exponential to find

$$\begin{aligned}\frac{-\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}}\eta_1\eta_1^\dagger}{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}}} &= \frac{-\int d\eta_1^\dagger \int d\eta_1 \left(1+\mathcal{G}_{11}^{-1}\eta_1^\dagger\eta_1\right)\eta_1\eta_1^\dagger}{\int d\eta_1^\dagger \int d\eta_1 \left(1+\mathcal{G}_{11}^{-1}\eta_1^\dagger\eta_1\right)} \\ &= -\frac{\int d\eta_1^\dagger \int d\eta_1 \eta_1\eta_1^\dagger}{\int d\eta_1^\dagger \int d\eta_1 \left(1+\mathcal{G}_{11}^{-1}\eta_1^\dagger\eta_1\right)} \\ &= \mathcal{G}_{11} \end{aligned} \tag{80.20}$$

To compute higher order correlation functions, notice that

$$\begin{aligned}\frac{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}}\eta_1\eta_1^\dagger\eta_2\eta_2^\dagger}{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}}} &= \frac{-\int d\eta_1^\dagger \int d\eta_1 e^{-\eta_1^\dagger(-\mathcal{G}_{11}^{-1})\eta_1}\eta_1\eta_1^\dagger \int d\eta_2^\dagger \int d\eta_2 e^{-\eta_2^\dagger(-\mathcal{G}_{22}^{-1})\eta_2}\eta_2\eta_2^\dagger}{\int d\eta_1^\dagger \int d\eta_1 e^{-\eta_1^\dagger(-\mathcal{G}_{11}^{-1})\eta_1}\int d\eta_2^\dagger \int d\eta_2 e^{-\eta_2^\dagger(-\mathcal{G}_{22}^{-1})\eta_2}} \\ &= -\frac{1}{\int d\eta_1^\dagger \int d\eta_1 e^{-\eta_1^\dagger(-\mathcal{G}_{11}^{-1})\eta_1}\int d\eta_2^\dagger \int d\eta_2 e^{-\eta_2^\dagger(-\mathcal{G}_{22}^{-1})\eta_2}} \\ &= \mathcal{G}_{11}\mathcal{G}_{22}. \end{aligned} \tag{80.21}$$

In this diagonal basis, this is the determinant of the $\mathcal{G}$ matrix. This result thus clearly generalizes, for imaginary time labels, to

$$\begin{aligned} & (-1)^n \left\langle T_\tau c\left(\tau_n\right) c^\dagger\left(\tau_n'\right) \cdots c\left(\tau_2\right) c^\dagger\left(\tau_2'\right) c\left(\tau_1\right) c^\dagger\left(\tau_1'\right)\right\rangle \qquad (80.22) \\ = \; & (-1)^n \frac{1}{Z}\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}}\eta\left(\tau_n\right)\eta^\dagger\left(\tau_n'\right)\cdots\eta\left(\tau_2\right)\eta^\dagger\left(\tau_2'\right)\eta\left(\tau_1\right)\eta^\dagger\left(\tau_1'\right) \\ = \; & \det\begin{bmatrix} \mathcal{G}\left(\tau_1,\tau_1'\right) & \mathcal{G}\left(\tau_1,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_1,\tau_n'\right) \\ \mathcal{G}\left(\tau_2,\tau_1'\right) & \mathcal{G}\left(\tau_2,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_2,\tau_n'\right) \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{G}\left(\tau_n,\tau_1'\right) & \mathcal{G}\left(\tau_n,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_n,\tau_n'\right) \end{bmatrix}. \qquad (80.23) \end{aligned}$$

This is Wick's theorem. We have the product of all contractions with appropriate sign for the permutations.

80.4 *Source fields and Wick's theorem

We can also find this result the hard way by adding source fields and using derivatives. The following lemma will be useful:

Lemma: Grassmann derivatives of $e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}-\boldsymbol{\eta}^\dagger\mathbf{J}-\mathbf{J}^\dagger\boldsymbol{\eta}}$ behave as derivatives of ordinary exponentials. Indeed, consider

$$\frac{\partial}{\partial J_i}\left(e^{-\boldsymbol{\eta}^\dagger(-\mathcal{G}^{-1})\boldsymbol{\eta}-\boldsymbol{\eta}^\dagger\mathbf{J}-\mathbf{J}^\dagger\boldsymbol{\eta}}\right) = \frac{\partial}{\partial J_i}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\boldsymbol{\eta}^\dagger\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^\dagger\mathbf{J}-\mathbf{J}^\dagger\boldsymbol{\eta}\right)^n. \tag{80.24}$$

When we differentiate the term of order n, we use the rules fo differentiating a product. So each of the n factors must be differentiated. But the derivative

commutes with each of the factors separately since they each have an even number of Grassmann variables. This means for example that

$$\frac{\partial}{\partial J_i}\left[\frac{1}{n!}\left(-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}\right)^{n}\right] = \frac{1}{(n-1)!}\left(-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}\right)^{n-1} \times\frac{\partial}{\partial J_i}\left(-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}\right) \quad (80.25)$$

In the end, the derivative of $\frac{\partial}{\partial J_i}\left(-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}\right)$ can be to the left or the right of the exponential.

To see how derivatives with respect to Grassmann source fields work, let us first look at the level of the Green function by starting from our previous result for Gaussian Grassmann integrals with sources, Eq.(79.27). We just rename the matrix $\mathbf{A}$ as $-\mathcal{G}^{-1}$ and check that this is consistent with the definition of the Green function

$$\begin{aligned} Z &= \int\mathcal{D}\eta^{\dagger}\int\mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}} \\ \mathcal{G}\left(ik_n\right) &= -\frac{1}{Z}\int\mathcal{D}\eta^{\dagger}\int\mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}}\eta_{ik_n}\eta_{ik_n}^{\dagger} \\ &= \frac{1}{\det\left[-\mathcal{G}^{-1}\right]}\left.\frac{\partial^2\left[\det\left(-\mathcal{G}^{-1}\right)\exp\left(\mathbf{J}^{\dagger}\left(-\mathcal{G}^{-1}\right)^{-1}\mathbf{J}\right)\right]}{\partial J^{\dagger}\left(ik_n\right)\partial J\left(ik_n\right)}\right|_{J,J^{\dagger}=0} \end{aligned}$$

The $\det\left[-\mathcal{G}^{-1}\right]$ simplifies and I have used the fact that an odd number of interchanges is needed when differentiating with respect to J (not $J^{\dagger}$). Also, η, $\eta^{\dagger}$, J and $J^{\dagger}$ commute with terms in the exponential since there are an even number of them. Expanding the exponential to linear order, we find

$$\begin{aligned} \mathcal{G}\left(ik_n\right) &= \left.\frac{\partial^2\left(\mathbf{J}^{\dagger}\left(-\mathcal{G}^{-1}\right)^{-1}\mathbf{J}\right)}{\partial J^{\dagger}\left(ik_n\right)\partial J\left(ik_n\right)}\right|_{J,J^{\dagger}=0} = -\left.\frac{\partial^2\left(\sum_{n'}J^{\dagger}\left(ik_n\right)\mathcal{G}\left(ik_n\right)J\left(ik_n\right)\right)}{\partial J^{\dagger}\left(ik_n\right)\partial J\left(ik_n\right)}\right|_{J,J^{\dagger}=0} \\ &= \left.\frac{\partial\left(J^{\dagger}\left(ik_n\right)\mathcal{G}\left(ik_n\right)\right)}{\partial J^{\dagger}\left(ik_n\right)}\right|_{J,J^{\dagger}=0}. \end{aligned}$$

Remark 369 *This works in imaginary-time as well if we interpret the derivatives with respect to J as functional derivatives. Just to change the perspective, we evaluate $\mathcal{G}(\tau)$ as a cumulant, i.e. as a derivative of $\ln Z$. This does not change anything for that correlation function since the cumulant in that case is the same as the moment.*

$$\mathcal{G}(\tau) = -\frac{1}{Z}\int\mathcal{D}\eta^{\dagger}\int\mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}}\eta(\tau)\eta^{\dagger}(0) \quad (80.26)$$

$$= \left.\frac{\delta^2\ln Z}{\delta J^{\dagger}(\tau)\delta J(0)}\right|_{J,J^{\dagger}=0} = \left.\frac{\delta^2\ln\left[\det\left(-\mathcal{G}^{-1}\right)\exp\left(\mathbf{J}^{\dagger}\left(-\mathcal{G}^{-1}\right)^{-1}\mathbf{J}\right)\right]}{\delta J^{\dagger}(\tau)\delta J(0)}\right|_{J,J^{\dagger}=0} \quad (80.27)$$

$$= \left.\frac{\delta^2\left(\int d\tau\int d\tau' J^{\dagger}(\tau)\left(-\mathcal{G}^{-1}\right)^{-1}(\tau,\tau')J(\tau')\right)}{\delta J^{\dagger}(\tau)\delta J(0)}\right|_{J,J^{\dagger}=0} = \left.\frac{\delta\left(\int d\tau'\delta J^{\dagger}(\tau)\mathcal{G}(\tau,\tau')\right)}{\delta J^{\dagger}(\tau)}\right|_{J,J^{\dagger}=0}$$

Note that, given the way we have derived the functional integral, expectation values of observables means time ordered quantities. It is trivial to include spatial indices in the above result.

To derive Wick's theorem, we follow Negele and Orland[2] and notice that, returning to our convention that overbar means integration

$$\frac{1}{Z}\int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}}\eta\left(\tau_1\right)\eta\left(\tau_2\right)\cdots\eta\left(\tau_n\right)\eta^{\dagger}\left(\tau_n'\right)\cdots\eta^{\dagger}\left(\tau_2'\right)\eta^{\dagger}\left(\tau_1'\right) \tag{80.28}$$

$$= (-1)^n\frac{1}{Z}\left.\frac{\delta^{2n}\int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta\exp\left[\eta^{\dagger}\left(\bar{\tau}\right)\mathcal{G}^{-1}\left(\bar{\tau},\bar{\tau}'\right)\eta\left(\bar{\tau}'\right)-\eta^{\dagger}\left(\bar{\tau}\right)J\left(\bar{\tau}\right)-J^{\dagger}\left(\bar{\tau}\right)\eta\left(\bar{\tau}\right)\right]}{\delta J^{\dagger}\left(\tau_1\right)\delta J^{\dagger}\left(\tau_2\right)\cdots\delta J^{\dagger}\left(\tau_n\right)\delta J\left(\tau_n'\right)\cdots\delta J\left(\tau_2'\right)\delta J\left(\tau_1'\right)}\right|_{J,J^{\dagger}=0}$$

$$= (-1)^n\left.\frac{\delta^{2n}\exp\left[J^{\dagger}\left(\bar{\tau}\right)\left(-\mathcal{G}\left(\bar{\tau},\bar{\tau}'\right)\right)J\left(\bar{\tau}'\right)\right]}{\delta J^{\dagger}\left(\tau_1\right)\delta J^{\dagger}\left(\tau_2\right)\cdots\delta J^{\dagger}\left(\tau_n\right)\delta J\left(\tau_n'\right)\cdots\delta J\left(\tau_2'\right)\delta J\left(\tau_1'\right)}\right|_{J,J^{\dagger}=0}. \tag{80.29}$$

The $(-1)^n$ above is generated by the derivatives with respect to J and $J^{\dagger}$ since a derivative with respect to J has to pass one more $\eta^{\dagger}$ than a derivative with respect to $J^{\dagger}$. The determinant obtained from Z cancels in the numerator and the denominator, as in the first example of this section. To evaluate the last line above, we use the lemma to find

$$(-1)^n\left.\frac{\delta^{2n}\exp\left[J^{\dagger}\left(\bar{\tau}\right)\left(-\mathcal{G}\left(\bar{\tau},\bar{\tau}'\right)\right)J\left(\bar{\tau}'\right)\right]}{\delta J^{\dagger}\left(\tau_1\right)\delta J^{\dagger}\left(\tau_2\right)\cdots\delta J^{\dagger}\left(\tau_n\right)\delta J\left(\tau_n'\right)\cdots\delta J\left(\tau_2'\right)\delta J\left(\tau_1'\right)}\right|_{J,J^{\dagger}=0}$$

$$= (-1)^{3n}\frac{\delta^n}{\delta J^{\dagger}\left(\tau_1\right)\cdots\delta J^{\dagger}\left(\tau_n\right)}\left[J^{\dagger}\left(\bar{\tau}_n\right)\mathcal{G}\left(\bar{\tau}_n,\tau_n'\right)\right]\cdots\left[J^{\dagger}\left(\bar{\tau}\right)\mathcal{G}\left(\bar{\tau},\tau_1'\right)\right]\exp\left[\left(J^{\dagger}\left(\bar{\tau}\right)\mathcal{G}\left(\bar{\tau},\bar{\tau}'\right)J\left(\bar{\tau}'\right)\right)\right]\Big|_{J,J^{\dagger}=}$$

where again an additional factor $(-1)^n$ comes from the fact that each time we differentiate with respect to J, there is one $J^{\dagger}$ we must go through that is not multiplied by another Grassmann variable. There is another $(-1)^n$ that comes from all the (-1) multiplying each of the $\mathcal{G}$. The above expression can be evaluated at $J=0$ so that we are left with

$$\begin{aligned}
&(-1)^n\frac{\delta^n}{\delta J^{\dagger}\left(\tau_1\right)\cdots\delta J^{\dagger}\left(\tau_n\right)}\left[J^{\dagger}\left(\bar{\tau}_n\right)\mathcal{G}\left(\bar{\tau}_n,\tau_n'\right)\right]\cdots\left[J^{\dagger}\left(\bar{\tau}\right)\mathcal{G}\left(\bar{\tau},\tau_1'\right)\right]\\
= \;&(-1)^n\left[\mathcal{G}\left(\tau_n,\tau_n'\right)\cdots\mathcal{G}\left(\tau_2,\tau_2'\right)\mathcal{G}\left(\tau_1,\tau_1'\right)\right. && (80.30)\\
&-\mathcal{G}\left(\tau_n,\tau_n'\right)\cdots\mathcal{G}\left(\tau_1,\tau_2'\right)\mathcal{G}\left(\tau_2,\tau_1'\right)\\
&\left.+\cdots\right] && (80.31)
\end{aligned}$$

In the second term there is a sign because $\delta/\delta J^{\dagger}\left(\tau_1\right)$ has to pass a $\delta J^{\dagger}\left(\tau_2\right)$. The order of the τ_i' indices of all the $\mathcal{G}$ above is fixed. The τ_n by contrast will be found in any order and the overall sign will be determined by the spign of the permutation. Recalling the definition of the determinant, the final result may be written as

$$\begin{aligned}
&\frac{1}{Z}\int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}}\eta\left(\tau_1\right)\eta\left(\tau_2\right)\cdots\eta\left(\tau_n\right)\eta^{\dagger}\left(\tau_n'\right)\cdots\eta^{\dagger}\left(\tau_2'\right)\eta^{\dagger}\left(\tau_1'\right)\\
= \;&(-1)^n\det\begin{bmatrix}
\mathcal{G}\left(\tau_1,\tau_1'\right) & \mathcal{G}\left(\tau_1,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_1,\tau_n'\right)\\
\mathcal{G}\left(\tau_2,\tau_1'\right) & \mathcal{G}\left(\tau_2,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_2,\tau_n'\right)\\
\cdots & \cdots & \cdots & \cdots\\
\mathcal{G}\left(\tau_n,\tau_1'\right) & \mathcal{G}\left(\tau_n,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_n,\tau_n'\right)
\end{bmatrix}. && (80.32)
\end{aligned}$$

Again, it is easy to add spatial indices.

This result is equivalent to the statement that one must pair all destruction operator with each of the creation operators, associating a $\mathcal{G}\left(\tau_i,\tau_j'\right)$ with each of the pairings. This is called a contraction. The overall sign of the product of contractions follows from the signature of the permutation. This is the usual statement of Wick's theorem.

[2] Note the sign difference in the definition of the Green function in that reference.

80.5 Interactions and quantum impurities as an example

Assume I have a single level with some Hubbad interaction and hybridization to a bath of non-interacting electrons. This time we restore spins. Let ψ_σ be the Grassman variables associated with the impurity, and $\eta_\sigma(\mathbf{k})$ those associated with the bath. The levels in the bath are labeled by $\mathbf{k}$. You have considered such a problem in exercise 62.0.3.

The interaction is easy to add to the action. It suffices to return to the derivation above to realize that all exponentials can be evaluated to leading order in $\Delta\tau$ so that a term

$$\left\langle \psi_\uparrow(\tau)\psi_\downarrow(\tau)\right| Uc_\uparrow^\dagger(\tau)c_\downarrow^\dagger(\tau)c_\downarrow(\tau)c_\uparrow(\tau)\Delta\tau\left|\psi_\uparrow(\tau)\psi_\downarrow(\tau)\right\rangle$$

in the Trotter-decomposed partition function simply becomes

$$U\psi_\uparrow^\dagger(\tau)\psi_\downarrow^\dagger(\tau)\psi_\downarrow(\tau)\psi_\uparrow(\tau)\Delta\tau.$$

The partition function then is

$$Z=\int\mathcal{D}\psi^\dagger\int\mathcal{D}\psi\int\mathcal{D}\eta^\dagger\int\mathcal{D}\eta\exp\left[-S\right] \tag{80.33}$$

with

$$S=S_I+S_{Ib}+S_b \tag{80.34}$$

where the impurity action is

$$\begin{aligned} S_I &= \int_0^\beta d\tau\left[\sum_\sigma\left(\psi_\sigma^\dagger(\tau)\frac{\partial}{\partial\tau}\psi_\sigma(\tau)+(\varepsilon-\mu)\psi_\sigma^\dagger(\tau)\psi_\sigma(\tau)\right)+U\psi_\uparrow^\dagger(\tau)\psi_\downarrow^\dagger(\tau)\psi_\downarrow(\tau)\psi_\uparrow(\tau)\right] \\ &= \int_0^\beta d\tau\left[\sum_\sigma\left(\psi_\sigma^\dagger(\tau)\left(-\mathcal{G}_0^{-1}\right)\psi_\sigma(\tau)\right)+U\psi_\uparrow^\dagger(\tau)\psi_\downarrow^\dagger(\tau)\psi_\downarrow(\tau)\psi_\uparrow(\tau)\right] \end{aligned} \tag{80.35}$$

with the bath

$$\begin{aligned} S_b &= \int_0^\beta d\tau\sum_{\mathbf{k}}\sum_\sigma\left[\eta_\sigma^\dagger(\mathbf{k},\tau)\frac{\partial}{\partial\tau}\eta_\sigma(\mathbf{k},\tau)+(\varepsilon_{\mathbf{k}}-\mu)\eta_\sigma^\dagger(\mathbf{k},\tau)\eta_\sigma(\mathbf{k},\tau)\right] \\ &= \int_0^\beta d\tau\sum_{\mathbf{k}}\sum_\sigma\eta_\sigma^\dagger(\mathbf{k},\tau)\left(-\mathcal{G}_b^{-1}(\mathbf{k},\tau)\right)\eta_\sigma(\mathbf{k},\tau) \end{aligned} \tag{80.36}$$

$$= \tag{80.37}$$

and the hybridization between impurity and bath

$$S_{Ib}=\int_0^\beta d\tau\sum_{\mathbf{k}}\sum_\sigma\left[V_{i\mathbf{k}}^*\psi_\sigma^\dagger(\tau)\eta_\sigma(\mathbf{k},\tau)+\eta_\sigma^\dagger(\mathbf{k},\tau)V_{\mathbf{k}i}\psi_\sigma(\tau)\right]. \tag{80.38}$$

Remark 370 *In general, we change from the Hamiltonian to the above action formalism, simply by using the recipe*

$$S_I=\int_0^\beta d\tau\left[\left(\sum_\sigma\psi_\sigma^\dagger(\tau)\frac{\partial}{\partial\tau}\psi_\sigma(\tau)\right)+H\left(\psi_\sigma^\dagger(\tau),\psi_\sigma(\tau)\right)\right] \tag{80.39}$$

where we simply replace the creation operators in the original H by $\psi_\sigma^\dagger(\tau)$ and the destruction operators by $\psi_\sigma(\tau)$. In the classical formalism, $L=p\dot{q}-H$ with

$$p=\frac{\partial L}{\partial\dot{q}}. \tag{80.40}$$

For the corresponding quantum fields then, $\psi_\sigma^\dagger(\tau)$ is the conjugate field and

$$\psi_\sigma^\dagger(\tau) = \frac{\partial L}{\partial \dot{\psi}_\sigma(\tau)}. \tag{80.41}$$

Since ψ and $\psi^\dagger$ obey $\left\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}')$ it is natural to expect that they are conjugate variables and that they should appear in the combination $\psi_\sigma^\dagger(\tau)\frac{\partial}{\partial\tau}\psi_\sigma(\tau)$ when changing from Hamiltonian to Lagrangian.

Remark 371 *It is now clear that $-\mathcal{G}_0^{-1}$ instead of H_0 is now the basic object since it appears in the quadratic term of the action. In addition to $\partial/\partial\tau$, other imaginary-time dependent single-particle quantities can appear in $\mathcal{G}_0^{-1}$.*

The functional integral over the bath degrees of freedom $\eta_\sigma^\dagger(\mathbf{k},\tau), \eta_\sigma(\mathbf{k},\tau)$ can be done easily if we identify the source fields in the Gaussian Grassmann integral Eq.(79.27) as

$$J_\sigma(\mathbf{k},\tau) = V_{\mathbf{k}i}\psi_\sigma(\tau). \tag{80.42}$$

The integral over the bath degrees of freedom leaves us with

$$Z = \exp\left[\mathrm{Tr}\ln\left(-\mathcal{G}_b^{-1}\right)\right]\int\mathcal{D}\psi^\dagger\int\mathcal{D}\psi\exp\left[-S_I + \mathbf{J}^\dagger\left(-\mathcal{G}_b^{-1}\right)^{-1}\mathbf{J}\right]. \tag{80.43}$$

The prefator is the determinant associated with the bath. It will drop out from observables associated only with the impurity. In Matsubara frequencies the bath Green's function is diagonal so it is easy to rewrite the term involving the source as

$$\mathbf{J}^\dagger\left(-\mathcal{G}_b\right)\mathbf{J} = \sum_n\sum_\sigma\psi_\sigma^\dagger(ik_n)\left(\sum_{\mathbf{k}}V_{i\mathbf{k}}^*\frac{-1}{ik_n-\varepsilon(\mathbf{k})}V_{\mathbf{k}i}\right)\psi_\sigma(ik_n). \tag{80.44}$$

This term thus just modifies $\mathcal{G}_0^{-1}$ in the impurity action. We define the hybridization function by

$$\Delta(ik_n) \equiv \sum_{\mathbf{k}}V_{i\mathbf{k}}^*\frac{1}{ik_n-\varepsilon(\mathbf{k})}V_{\mathbf{k}i}. \tag{80.45}$$

Part IX

Many-body in a nutshell

These are some of the most widely used results in many-body theory. This is an extremely succinct presentation, not to say just a cookbook, that refers to the main text if you really want to learn the subject. Much of the text here repeats word for word what is in the main text, but keeping only the main points.

81. HANDELING MANY-INTERACTING PARTICLES: SECOND QUANTIZATION

A detailed explanation of the concepts of this Chapter can be found in Chapter 24.

When there is more than one particle and they are identical, the wave function say $\psi(x_1, x_2, x_3)$ is not arbitrary. If we want particles to be indistinguishable, all coordinates should be equivalent. This means in particular that if x_1 takes any particular value, say a and x_2 takes another value, say b, then we expect that $\psi(a, b, x_3) = \psi(b, a, x_3)$. But that is not the only possibility since the only thing we know for sure is that if we exchange twice the coordinates of two particles then we should return to the same wave function. This means that under one permutation of two coordinates (exchange), the wave function can not only stay invariant, or have an eigenvalue of $+1$ as in the example we just gave, it can also have an eigenvalue of -1. These two cases are clearly the only possibilities and they correspond respectively to bosons and fermions. There are more possibilities in two dimensions, but that is beyond the scope of this chapter.

Second quantization allows us to take into account these symmetry or antisymmetry properties in a straightforward fashion. To take matrix elements directly between wave functions would be very cumbersome. In second quantization, both states and operators are written in terms of the same set of creation-annihilation operators that obey simple commutation or anticommutation relations for bosons and fermions respectively. We will focus on fermions.

Remark 372 *Second quantization for us is just a trick to work with many particles. Formally, it is called second quantization because in first quantization we start with particles, set up commutation relations between position and momentum, and end up with a wave function. Second quantization can be seen as starting from a wave function, or field, ψ, setting up commutation relations with the conjugate field and ending up with particles, or excitations of that field. With the electromagnetic field in a sense we do not have the choice to do this.*

81.1 Fock space, creation and annihilation operators

Here we are interested most of the time in Hamiltonians that conserve the number of particles. Nevertheless, it is easier to work in a space that contains an arbitrary number of particles. That is Fock space. Annihilation and creation operators allow us to change the number of particles while preserving indistinguishability and antisymmetry. In this representation, a three-electron state comes out as three excitations of the same vacuum state $|0\rangle$, a rather satisfactory state of affairs.

It will be very helpful if you review creation-annihilation operators, also called ladder operators, in the context of the harmonic oscillator.

For the time being our fermions are spinless, it will be easy to add spin later on. We assume that the one-particle states $|\alpha_i\rangle$ form an orthonormal basis for one particle, namely $\langle\alpha_i|\ \alpha_j\rangle = \delta_{i,j}$. The state $|\alpha_1\alpha_2\rangle$ is antisymmetrized, namely

$$|\alpha_1\alpha_2\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle\right).$$

The first Hilbert space on the right of the above expression can be either in state α_1 or α_2. Antisymmetry means that $|\alpha_1\alpha_2\rangle = -|\alpha_2\alpha_1\rangle$.

We define a vaccum $|0\rangle$ that contains no particle. Then, we define $a^\dagger_{\alpha_1}$ that creates a particle from the vacuum to put it in state $|\alpha_1\rangle$ and for fermions it antisymmetrizes that state will all others. In other words, $a^\dagger_{\alpha_1}|0\rangle = |\alpha_1\rangle$. Up to now, there is nothing to antisymmetrize with, but if we add another particle,

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}|0\rangle = |\alpha_1\alpha_2\rangle$$

then that state has to be antisymmetric. In other words, we need to have $|\alpha_2\alpha_1\rangle = -|\alpha_1\alpha_2\rangle$, or

$$|\alpha_2\alpha_1\rangle = a^\dagger_{\alpha_2} a^\dagger_{\alpha_1}|0\rangle = -|\alpha_1\alpha_2\rangle = -a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}|0\rangle.$$

Clearly this will automatically be the case if we impose that the creation operators anticommute, i.e. $a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} = -a^\dagger_{\alpha_j} a^\dagger_{\alpha_i}$ or

$$\left\{a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \equiv a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j} a^\dagger_{\alpha_i} = 0. \tag{81.1}$$

This property is a property of the operators, independently of the specific state they act on. The anticommutation property garantees the Pauli principle as we know it, since if $i = j$ then the above leads to

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_i} = -a^\dagger_{\alpha_i} a^\dagger_{\alpha_i}. \tag{81.2}$$

The only operator that is equal to minus itself is zero. Hence we cannot create two particles in the same state.

If we want the whole formalism to make sense, we want to have a change sign to occur whenever we interchange two fermions, wherever they are in the list.You can check that his works with our formalism.

Note that with fermions we need to determine an initial order of operators for the states. That is totally arbitrary because of the phase arbitrariness of quantum mechanics. But then, during the calculations we need to keep track of the minus signs.

Now that we know how to create, let us move to destruction. The destruction operators are the adjoints of $a^\dagger_{\alpha_i}$. Their anticommutation property will follows by taking the adjoint of $\left\{a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right\} = 0$:

$$\left\{a_{\alpha_i}, a_{\alpha_j}\right\} \equiv a_{\alpha_i} a_{\alpha_j} + a_{\alpha_j} a_{\alpha_i} = 0. \tag{81.3}$$

These adjoint operators are defined as follows

$$\langle\alpha_1| = \langle 0|\, a_{\alpha_1}. \tag{81.4}$$

They create and antisymmetrize in bras instead of kets. When they act on kets instead of bras, they remove a particle instead of adding it. In particular,

$$a_{\alpha_1}|0\rangle = 0. \tag{81.5}$$

This is consistent with $\langle\alpha_1|\ 0\rangle = 0 = \langle 0|\, a_{\alpha_1}|0\rangle$.

Since we also want states to be normalized, we need

$$\langle \alpha_i |\ \alpha_j \rangle = \langle 0 |\, a_{\alpha_i} a^\dagger_{\alpha_j} \,| 0 \rangle = \delta_{i,j}. \tag{81.6}$$

Since we already know that $a_{\alpha_1} |0\rangle = 0$, that will automatically be satisfied if we write the following anticommutation realtion between creation and annihilation operators

$$\left\{ a_{\alpha_i}, a^\dagger_{\alpha_j} \right\} \equiv a_{\alpha_i} a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j} a_{\alpha_i} = \delta_{i,j} \tag{81.7}$$

because then $\langle 0 |\, a_{\alpha_i} a^\dagger_{\alpha_j} \,| 0 \rangle = - \langle 0 |\, a^\dagger_{\alpha_j} a_{\alpha_i} \,| 0 \rangle + \langle 0 |\, \delta_{i,j} \,| 0 \rangle = 0 + \delta_{i,j}$. The above three sets of anticommutation relations are called canonical.

At this point one may ask why anticommutation instead of commutation, which would also have satisfied $\langle 0 |\, a_{\alpha_i} a^\dagger_{\alpha_j} \,| 0 \rangle = \delta_{i,j}$. Well, two reasons. The first one is that given the previous anticommutation rules, this one seems elegant. The second one is that with this rule, we can define the very useful operator, the number operator

$$\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{81.8}$$

That operator just counts the number of particles in state α_i. To see that this is so and that anticommutation is needed for this to work, we look at a few simple cases. First note that if $\widehat{n}_{\alpha_i}$ acts on a state where α_i is not occupied, then

$$\widehat{n}_{\alpha_i} |\alpha_j\rangle = \widehat{n}_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = -a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_i} |0\rangle = 0. \tag{81.9}$$

If I build an arbitrary many-particle state $|\alpha_j, \alpha_k, \ldots\rangle$, if the state α_i does not appear in the list, then when I compute $\widehat{n}_{\alpha_i} |\alpha_j, \alpha_k, \ldots\rangle$, I will be able to anticommute the destruction operator all the way to the vacuum and obtain zero. On the other hand, if α_i appears in the list then

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots \widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \,. \tag{81.10}$$

I have been able to move the operator all the way to the indicated position without any additional minus sign because both the destruction and the annihilation operators anticommute with the creation operators that do not have the same labels. The minus signs from the creation and from the annihilation operators in $a^\dagger_{\alpha_i} a_{\alpha_i}$ cancel each other. This would not have occured if a_{α_i} and $a^\dagger_{\alpha_j}$ had commuted instead of anticommuted. Now, let us focus on $\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i}$ in the last equation. Using our anticommutation properties, one can check that

$$\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} \left(1 - a^\dagger_{\alpha_i} a_{\alpha_i} \right). \tag{81.11}$$

Since there are never two fermions in the same state, now the destruction operator in the above equation is free to move and annihilate the vacuum state, and

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right). \tag{81.12}$$

This means that $\widehat{n}_{\alpha_i}$ does simply count the number of particles. It gives one or zero depending on whether the state is occupied or not.

81.2 Change of basis

Creation-annihilation operators change basis in a way that is completely determined by the way one changes basis in single-particle states. Suppose one wants

to change from the α basis to the μ basis, namely

$$|\mu_m\rangle = \sum_i |\alpha_i\rangle \langle\alpha_i| \mu_m\rangle \tag{81.13}$$

which is found by inserting the completeness relation. Let creation operator $a^\dagger_{\alpha_i}$ create single particle state $|\alpha_i\rangle$ and antisymmetrize while creation operator $c^\dagger_{\mu_m}$ creates single particle state $|\mu_m\rangle$ and antisymmetrize. Then the correspondance between both sets of operators is clearly

$$c^\dagger_{\mu_m} = \sum_i a^\dagger_{\alpha_i} \langle\alpha_i| \mu_m\rangle \tag{81.14}$$

with the adjoint

$$c_{\mu_m} = \sum_i \langle\mu_m| \alpha_i\rangle a_{\alpha_i} \tag{81.15}$$

given as usual that $\langle\alpha_i| \mu_m\rangle = \langle\mu_m| \alpha_i\rangle^*$. Physically then, creating a particle in a state $|\mu_m\rangle$ is like creating it in a linear combination of states $|\alpha_i\rangle$. We can do the change of basis in the other direction as well.

If the transformation between basis is unitary, the new operators, obey canonical anticommutation relations, namely

$$\left\{c_{\mu_m}, c^\dagger_{\mu_n}\right\} = \delta_{m,n}. \tag{81.16}$$

When the change of basis is unitary, we say that we have made a canonical transformation. The same steps show that a unitary basis change also preserves the canonical commutation relations for bosons.

81.2.1 The position and momentum space basis

On can use a basis where we take continuum notation for space and discrete notation for momentum. This is described in more details in Sec.18.2.1. In this basis,

$$\boxed{\left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = \delta_{\mathbf{k},\mathbf{k}'} \quad ; \quad \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = \left\{c^\dagger_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = 0} \tag{81.17}$$

while the position space creation-annihilation operators obey

$$\boxed{\{\psi(\mathbf{r}), \psi(\mathbf{r}')\} = \left\{\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = 0} \tag{81.18a}$$

$$\boxed{\left\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle\mathbf{r}|\mathbf{k}\rangle \left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} \langle\mathbf{k}'|\mathbf{r}'\rangle = \sum_{\mathbf{k}} \langle\mathbf{r}|\mathbf{k}\rangle \langle\mathbf{k}|\mathbf{r}'\rangle = \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')} \tag{81.19}$$

which is precisely what we expect from the continuum normalization of the one-body states, namely

$$\langle 0| \left\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} |0\rangle = \langle 0| \psi(\mathbf{r}) \psi^\dagger(\mathbf{r}') |0\rangle = \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \tag{81.20}$$

Remark 373 *We define the bra* $\langle\alpha_1\alpha_2|$ *by*

$$\langle\alpha_1\alpha_2| = (|\alpha_1\alpha_2\rangle)^\dagger = \left(a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle\right)^\dagger = \langle 0| a_{\alpha_2} a_{\alpha_1}. \tag{81.21}$$

Notice the change in the order of labels between $\langle\alpha_1\alpha_2|$ *and* $\langle 0| a_{\alpha_2} a_{\alpha_1}$.

With N-particles, the wave function is obtained by projection on a position basis. If we have a single many-body state, $a_{\alpha_1}^{\dagger}a_{\alpha_2}^{\dagger}\ldots a_{\alpha_i}^{\dagger}\ldots a_{\alpha_N}^{\dagger}\left|0\right\rangle$ then the corrresponding wave function

$$\left\langle \mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N\right| \alpha_1\alpha_2...\alpha_N\rangle = \left\langle 0\right| \psi\left(\mathbf{r}_N\right)\ldots\psi\left(\mathbf{r}_2\right)\psi\left(\mathbf{r}_1\right)a_{\alpha_1}^{\dagger}a_{\alpha_2}^{\dagger}\ldots a_{\alpha_i}^{\dagger}\ldots a_{\alpha_N}^{\dagger}\left|0\right\rangle$$

is proportional to a so-called Slater determinant if we have fermions. Indeed, using our change of basis formula,

$$\psi\left(\mathbf{r}\right) = \sum_i \left\langle \mathbf{r}\right.\left|\alpha_i\right\rangle a_{\alpha_i} = \sum_i \phi_{\alpha_i}\left(\mathbf{r}\right)a_{\alpha_i} \tag{81.22}$$

any of the positions $\mathbf{r}$ can be in a state α_i, or vice versa the position $\mathbf{r}$ has amplitudes on all states, so you can check that the wave function is equal to

$$\sum_p \varepsilon_p \phi_{\alpha_{p(1)}}\left(\mathbf{r}_1\right)\phi_{\alpha_{p(2)}}\left(\mathbf{r}_2\right)...\phi_{\alpha_{p(N)}}\left(\mathbf{r}_N\right) = \mathrm{Det}\begin{bmatrix} \phi_{\alpha_1}\left(\mathbf{r}_1\right) & \phi_{\alpha_1}\left(\mathbf{r}_2\right) & ... & \phi_{\alpha_1}\left(\mathbf{r}_N\right) \\ \phi_{\alpha_2}\left(\mathbf{r}_1\right) & \phi_{\alpha_2}\left(\mathbf{r}_2\right) & ... & \phi_{\alpha_2}\left(\mathbf{r}_N\right) \\ ... & ... & ... & \\ \phi_{\alpha_N}\left(\mathbf{r}_1\right) & \phi_{\alpha_N}\left(\mathbf{r}_2\right) & & \phi_{\alpha_N}\left(\mathbf{r}_N\right) \end{bmatrix} \tag{81.23}$$

where the sum is over all permutations $p\left(i\right)$ of the set i and ε_p is the signature of the permutation, given by $+1$ if the number of transpositions (interchanges) of pairs of creation operators to get back to the original order is even and -1 if the number of transpositions is odd.

81.3 One-body operators

The matrix elements of an arbitrary one-body operator $\widehat{U}$ (in the $N-$particle case) may be computed in the many-body basis made of one-body states where $\widehat{U}$ is diagonal. As an example of one-body operator, the operator $\widehat{U}$ could be an external potential so that the diagonal basis is position space. In the diagonal basis,

$$\widehat{U}\left|\alpha_i\right\rangle = U_{\alpha_i}\left|\alpha_i\right\rangle = \left\langle\alpha_i\right|\widehat{U}\left|\alpha_i\right\rangle\left|\alpha_i\right\rangle \tag{81.24}$$

where U_{α_i} is the eigenvalue. In this basis, one sees that the effect of the one-body operator is to produce the same eigenvalue, whatever the particular order of the states on which the first-quantized operator acts. For example, suppose we have three particles in an external potential, then the potential-energy operator is

$$V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right) \tag{81.25}$$

where $\mathbf{R}_i$ acts on the i^{th} position of the many body state. If we act on a symmetrized or antisymmetrized version of that state, then

$$\left(V\left(\mathbf{R}_1\right) + V\left(\mathbf{R}_2\right) + V\left(\mathbf{R}_3\right)\right)\left|\mathbf{r}',\mathbf{r},\mathbf{r}''\right\rangle = \left(V\left(\mathbf{r}'\right) + V\left(\mathbf{r}\right) + V\left(\mathbf{r}''\right)\right)\left|\mathbf{r}',\mathbf{r},\mathbf{r}''\right\rangle \tag{81.26}$$

since the eigenvalue is $V\left(\mathbf{r}'\right)+V\left(\mathbf{r}\right)+V\left(\mathbf{r}''\right)$, whatever the order in which $\mathbf{r}',\mathbf{r},\mathbf{r}''$ appear. In general then when we have N particles in a many-body state, the action of the one-body operator is

$$\sum_{\mu=1}^{N}\widehat{U}_\mu\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle = \left(U_{\alpha_i}+U_{\alpha_j}+U_{\alpha_k}+\ldots\right)\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle \tag{81.27}$$

Knowing the action of the number operator, we can write the same result differently

$$\sum_{\mu=1}^{N}\widehat{U}_{\mu}\left|\alpha_{i},\alpha_{j},\alpha_{k}\ldots\right\rangle=\sum_{m}U_{\alpha_{m}}\widehat{n}_{\alpha_{m}}\left|\alpha_{i},\alpha_{j},\alpha_{k}\ldots\right\rangle \tag{81.28}$$

in other words, there will be a contribution as long as α_i appears in the state. And if α_i occurs more than once, the corresponding eigenvalue U_{α_i} will appear more than once.

We hold a very elegant result. The one-body operator $\sum_m U_{\alpha_m}\widehat{n}_{\alpha_m}$ in second quantized notation makes no reference to the total number of particles nor to whether we are dealing with bosons of fermions. Note that in first quantization the sum extends over all particle coordinates whereas in second quantization the sum over m extends over all *states*.

Using the change of basis formula explained above, we have that

$$\sum_{i}\left\langle\alpha_{i}\right|\widehat{U}\left|\alpha_{i}\right\rangle a_{\alpha_{i}}^{\dagger}a_{\alpha_{i}}=\sum_{i}\sum_{m}\sum_{n}c_{\mu_{m}}^{\dagger}\left\langle\mu_{m}\right.\left|\alpha_{i}\right\rangle\left\langle\alpha_{i}\right|\widehat{U}\left|\alpha_{i}\right\rangle\left\langle\alpha_{i}\right.\left|\mu_{n}\right\rangle c_{\mu_{n}}. \tag{81.29}$$

Since U is diagonal, we can add a sum over α_j and use the closure relation to arrive at the final result

$$\boxed{\textstyle\sum_{i}U_{\alpha_{i}}\widehat{n}_{\alpha_{i}}=\sum_{m}\sum_{n}c_{\mu_{m}}^{\dagger}\left\langle\mu_{m}\right|\widehat{U}\left|\mu_{n}\right\rangle c_{\mu_{n}}.} \tag{81.30}$$

Let us give examples in the position and momentum representation. A one-body scattering potential in the continuum would be represented in second quantized version[1] by

$$\boxed{\widehat{U}=\int d\mathbf{r}U\left(\mathbf{r}\right)\psi^{\dagger}\left(\mathbf{r}\right)\psi\left(\mathbf{r}\right)} \tag{81.31}$$

which looks similar to the usual Schrödinger average. Similarly, the kinetic energy operator in the momentum representation is diagonal and it can be rewritten in the position basis using the change of variables of the previous section.

$$\widehat{T}=\sum_{\mathbf{k}}\left\langle\mathbf{k}\right|\frac{\hbar^{2}k^{2}}{2m}\left|\mathbf{k}\right\rangle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}=\sum_{\mathbf{k}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)\left\langle\mathbf{r}\right.\left|\mathbf{k}\right\rangle\left\langle\mathbf{k}\right|\frac{\hbar^{2}k^{2}}{2m}\left|\mathbf{k}\right\rangle\left\langle\mathbf{k}\right.\left|\mathbf{r}'\right\rangle\psi\left(\mathbf{r}'\right) \tag{81.32}$$

$$=\frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)e^{i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\frac{\hbar^{2}k^{2}}{2m}\psi\left(\mathbf{r}'\right) \tag{81.33}$$

$$=\int\frac{d^{3}\mathbf{k}}{\left(2\pi\right)^{3}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)\left(-\frac{\hbar^{2}}{2m}\nabla_{\mathbf{r}'}^{2}e^{i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\right)\psi\left(\mathbf{r}'\right) \tag{81.34}$$

$$=\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)\left(-\frac{\hbar^{2}}{2m}\nabla_{\mathbf{r}'}^{2}\delta\left(\mathbf{r}-\mathbf{r}'\right)\right)\psi\left(\mathbf{r}'\right) \tag{81.35}$$

Using partial integration and assuming that everything vanishes at infinity or is periodic, we obtain,

$$\boxed{\widehat{T}=\left(-\tfrac{\hbar^{2}}{2m}\right)\int d\mathbf{r}\psi^{\dagger}\left(\mathbf{r}\right)\left(\nabla^{2}\psi\left(\mathbf{r}\right)\right)=\tfrac{\hbar^{2}}{2m}\int d\mathbf{r}\boldsymbol{\nabla}\psi^{\dagger}\left(\mathbf{r}\right)\cdot\nabla\psi\left(\mathbf{r}\right)}. \tag{81.36}$$

Again notice that second-quantized operators look like simple Schrödinger averages over wave functions.

[1] We have denoted by $\widehat{U}$ the operator in both first and second quantization. Strictly speaking the operators are different. One needs to specify which representation one is working in.

81.4 Two-body operators.

A two-body operator involves the coordinates of two particles. An example is the Coulomb potential with position basis where $\widehat{V}_{1,2} = \widehat{V}(\mathbf{R}_1, \mathbf{R}_2)$ which is diagonal in position space, namely $\widehat{V}(\mathbf{R}_1, \mathbf{R}_2)|\mathbf{r}'\rangle \otimes |\mathbf{r}\rangle = V(\mathbf{r}', \mathbf{r})|\mathbf{r}'\rangle \otimes |\mathbf{r}\rangle$.

Let us return to the general discussion. If we let the indices in $\widehat{V}_{1,2}$ refer to the potential energy between the first and second particles in the direct product, and if we are in the diagonal basis, we have in first quantization that

$$\widehat{V}_{1,2}|\alpha_i\rangle \otimes |\alpha_j\rangle = V_{\alpha_i\alpha_j}|\alpha_i\rangle \otimes |\alpha_j\rangle \tag{81.37}$$

$$\widehat{V}_{1,3}|\alpha_i\rangle \otimes |\alpha_j\rangle \otimes |\alpha_k\rangle = V_{\alpha_i\alpha_k}|\alpha_i\rangle \otimes |\alpha_j\rangle \otimes |\alpha_k\rangle \tag{81.38}$$

In this basis, one sees that again the eigenvalue does not depend on the order in which the states are when the first-quantized operator acts. This means that

$$\frac{1}{2}\sum_{\mu=1}^{N}\sum_{\substack{\nu=1\\ \nu\neq\mu}}^{N}\widehat{V}_{\mu,\nu}|\alpha_i, \alpha_j, \alpha_k \ldots\rangle = \left(V_{\alpha_i\alpha_j} + V_{\alpha_i\alpha_k} + V_{\alpha_j\alpha_k} + \ldots\right)|\alpha_i, \alpha_j, \alpha_k \ldots\rangle \tag{81.39}$$

where now on the right-hand side every interaction is counted only once. As above, $\widehat{V}_{\mu,\nu}$ refers to the potential energy between the μ and ν particles. If $|\alpha_i\rangle \neq |\alpha_j\rangle$, then the number of times that $V_{\alpha_i\alpha_j}$ occurs in the double sum is equal to $n_{\alpha_i}n_{\alpha_j}$. However, when $|\alpha_i\rangle = |\alpha_j\rangle$, then the number of times that $V_{\alpha_i\alpha_j}$ occurs is equal to $n_{\alpha_i}(n_{\alpha_i} - 1)$ because we are not counting the interaction of the particle with itself, as specified by $\nu \neq \mu$ in the sum. In general then,

$$\frac{1}{2}\sum_{\mu=1}^{N}\sum_{\substack{\nu=1\\ \nu\neq\mu}}^{N}\widehat{V}_{\mu,\nu}|\alpha_i, \alpha_j, \alpha_k \ldots\rangle = \frac{1}{2}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}V_{\alpha_m\alpha_n}\left(\widehat{n}_{\alpha_m}\widehat{n}_{\alpha_n} - \delta_{m,n}\widehat{n}_{\alpha_n}\right)|\alpha_i, \alpha_j, \alpha_k \ldots\rangle\,. \tag{81.40}$$

Again the expression for the operator to the right is independent of the state it acts on. It is valid in general. I assumed that the basis α has an infinite number of states.

We can simplify the expression further. Defining

$$\boxed{\zeta = -1 \quad \text{for} \quad \text{fermions}} \tag{81.41}$$

$$\boxed{\zeta = 1 \quad \text{for} \quad \text{bosons}} \tag{81.42}$$

we can rewrite $\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j} - \delta_{i,j}\widehat{n}_{\alpha_i}$ in terms of creation and annihilation operators in such a way that the form is valid for both fermions and bosons

$$\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j} - \delta_{i,j}\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i}a_{\alpha_i}a^\dagger_{\alpha_j}a_{\alpha_j} - \delta_{i,j}a^\dagger_{\alpha_i}a_{\alpha_i} = a^\dagger_{\alpha_i}\zeta a^\dagger_{\alpha_j}a_{\alpha_i}a_{\alpha_j} = a^\dagger_{\alpha_i}a^\dagger_{\alpha_j}a_{\alpha_j}a_{\alpha_i}. \tag{81.43}$$

Second quantized operators are thus written in the simple form

$$\boxed{\tfrac{1}{2}\textstyle\sum_i\sum_j V_{\alpha_i\alpha_j}\left(\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j} - \delta_{i,j}\widehat{n}_{\alpha_i}\right) \equiv \tfrac{1}{2}\sum_i\sum_j(\alpha_i\alpha_j|\,V\,|\alpha_i\alpha_j)\,a^\dagger_{\alpha_i}a^\dagger_{\alpha_j}a_{\alpha_j}a_{\alpha_i}} \tag{81.44}$$

where

$$|\alpha_i\alpha_j) \equiv |\alpha_i\rangle \otimes |\alpha_j\rangle\,. \tag{81.45}$$

Under unitary transformation to an arbitrary basis we have

$$\boxed{\widehat{V} = \tfrac{1}{2}\textstyle\sum_m\sum_n\sum_p\sum_q(\mu_m\mu_n|\,V\,|\mu_p\mu_q)\,c^\dagger_{\mu_m}c^\dagger_{\mu_n}c_{\mu_q}c_{\mu_p}}. \tag{81.46}$$

Definition 36 *When a series of creation and annihilation operators are placed in such an order where all destruction operators are to the right, one calls this "normal order".*

Remark 374 *Note the inversion in the order of μ_p and μ_q in the annihilation operators compared with the order in the matrix elements (This could have been for the creation operator instead).*

Remark 375 *The notation $(\mu_m \mu_n | V | \mu_p \mu_q)$ for the two-body matrix element means, in the coordinate representation for example,*

$$\int d\mathbf{r}_1 d\mathbf{r}_2 \phi^*_{\mu_m}(\mathbf{r}_1) \phi^*_{\mu_n}(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \phi_{\mu_p}(\mathbf{r}_1) \phi_{\mu_q}(\mathbf{r}_2). \tag{81.47}$$

Example 37 *In the case of a potential, such as the Coulomb potential, which acts on the densities, we have*

$$\boxed{\widehat{V} = \frac{1}{2} \int d\mathbf{x} \int d\mathbf{y} v(\mathbf{x} - \mathbf{y}) \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{y}) \psi(\mathbf{y}) \psi(\mathbf{x})}. \tag{81.48}$$

82. THE HUBBARD MODEL TO ILLUSTRATE SOME OF THE CONCEPTS

A general Hamiltonian of the form described above can be solved in the Hartree-Fock approximation. This approximation, discussed in Appendix C, consists in using the variational principle for the most general wave function that can be written as a single Slater determinant, i.e. as $|\psi_{HF}\rangle = c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\dots c^\dagger_{N/2\uparrow}c^\dagger_{N/2\downarrow}|0\rangle$ where indices such as 1 etc can denote momentum eigenstates or other types of one-body states. This is very important for density-functional based approaches that are discussed in Chapter 53. We consider here a simplification of the full many-body problem to illustrate the most general form that the many-body wavefunction can take.

Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. Nevertheless, it does not diagonalize the Hamiltonian. If the problem has been solved for a translationally invariant lattice, the one-particle states will be Bloch states indexed by crystal momentum $\mathbf{k}$ and band index n. If we expand the creation-annihilation operators in that basis using the general formulas for one-particle Eq.(B.16) and two-particle Eq.(B.24) parts of the Hamiltonian, clearly it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

Model Hamiltonians can now explicitly be constructed using cold atoms in optical traps. A laser interference pattern can be used to create an optical lattice potential using the AC Stark effect. One can control tunneling between potential minima as well as the interaction of atoms between them.

82.1 The Hubbard model

Restricting ourselves to a single band and expanding the $\psi^\dagger(\mathbf{y})$ and $\psi(\mathbf{y})$ in the Wannier basis associated with the Bloch states, our change of basis formula leads to the Hamiltonian

$$H = \sum_\sigma \sum_{i,j} c^\dagger_{i\sigma} \langle i|\hat{T}'|j\rangle c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\langle i|\langle j|\hat{V}_c|k\rangle|l\rangle c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{l\sigma'}c_{k\sigma}. \qquad (82.1)$$

where $\hat{T}' = \hat{T} + \hat{V}$ contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. The operator $c^{(\dagger)}_{i\sigma}$ annihilate (create) a particle in a Wannier state centered at lattice site i and with spin σ. The one-body

part by itself is essentially the DFT band structure. In 1964, Hubbard, Kanamori and Gutzwiller did the most dramatic of approximations, hoping to have a model simple enough to solve. They assumed that $\langle i|\langle j|\hat{V}_c|k\rangle|l\rangle$ would be much larger than all other interaction matrix elements when all lattice sites are equal. Defining $t_{ij} \equiv \langle i|\hat{K}|j\rangle$ and $U \equiv \langle i|\langle i|\hat{V}_c|i\rangle|i\rangle$, and using $c_{i\sigma}c_{i\sigma} = 0$ they were left with

$$\begin{aligned} H &= \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_i U c^\dagger_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'} c_{i\sigma} \\ &= \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \qquad (82.2) \\ &= \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\downarrow} n_{i\uparrow}. \qquad (82.3) \end{aligned}$$

Most of the time, one considers hopping only to nearest neighbors. The model can be solved exactly only in one dimension using the Bethe ansatz, and in infinite dimension. The latter solution is the basis for Dynamical Mean Field Theory (DMFT) that is discussed in these notes. Despite the fact that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve. The size of the Hilbert space is huge. There are four states per lattice site (up, down, empty and doubly occupied), so in the grand canonical ensemble, the size of the Hilbert space is 4^N, i.e. exponentially large with the number of lattice sites N.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable. The laser intensity of the trapping potential and the magnetic field are the control parameters. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of cold atoms, one can find conditions where the Hubbard model description is very accurate. By the way, interesting physics occurs only in the nano Kelvin range. Discussing how such low temperatures are achieved would distract us to much.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. More specifically, if $U = 0$, then the ground state can be written as in elementary statistical mechanics, by filling a Fermi sea, namely

$$|\psi\rangle_{U=0} = c^\dagger_{\mathbf{k}_0\uparrow} c^\dagger_{\mathbf{k}_0\downarrow} c^\dagger_{\mathbf{k}_1\uparrow} c^\dagger_{\mathbf{k}_1\downarrow} \dots c^\dagger_{\mathbf{k}_{N/2}\uparrow} c^\dagger_{\mathbf{k}_{N/2}\downarrow} |0\rangle . \qquad (82.4)$$

However, if we have only the interaction U, namely $t_{ij} = 0$, the ground state can simply be written in the Wannier basis (think of states localized around each atom if you are not familiar with this notion). For example, at half-filling the ground state consists of a single electron per site:

$$|\psi\rangle_{t_{ij}=0} = c^\dagger_{\mathbf{R}_o\uparrow} c^\dagger_{\mathbf{R}_1\downarrow} c^\dagger_{\mathbf{R}_2\downarrow} \dots c^\dagger_{\mathbf{R}_N\uparrow} |0\rangle . \qquad (82.5)$$

The spin at each site is arbitrary, so there is a massive degeneracy of 2^N.

What happens in the general case, where U and t_{ij} are both non-zero? Applying H on the last wave function above, $|\psi\rangle_{t_{ij}=0}$, we see that t_{ij} will move electrons around. This means that the true eigenstate can only be a linear combination of states that involve electrons on different sites. In other words, the full many-body wave function is a linear combination of Slater derterminants. This is a very important lesson that is also reached if we apply H on $|\psi\rangle_{U=0}$ where the kinetic energy term is diagonal since the interaction U written in momentum space removes particles from two momentum states and puts them in momentum states that are in general different from the original ones. Clearly then, when

both kinetic and potential energy are equally important, neither the momentum nor the position state basis suffice to build a many-body eigenstate with a single Slater determinant. Instead, we need a large fraction of the full, exponentially large Hilbert space to faithfully represent the many-body wave function. That is what we mean by correlations. Note that the coefficients of the linear combination that is the true eigenstate will in general be complex, unless the Hamiltonian is real.

A bit of jargon: When a single Slater determinant dominates in the wave function, we call the other components of the wave function quantum fluctuations.

Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a Mott insulator and the extended one a metal.

The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe high-temperature superconductivity, depending on lattice and range of interaction parameters.

83. PERTURBATION THEORY AND TIME-ORDERED PRODUCTS

In the grand canonical ensemble, we want to evaluate

$$e^{-\beta\left(\widehat{H}-\mu\widehat{N}\right)} \tag{83.1}$$

where H is the Hamiltonian, N the number of particles and μ the chemical potential. For convenience, define

$$\widehat{K} = \widehat{H} - \mu\widehat{N}. \tag{83.2}$$

In general you will be facing a situation where

$$\widehat{K} = \widehat{H}_0 + \widehat{H}_1 - \mu\widehat{N} \equiv \widehat{K}_0 + \widehat{K}_1 \tag{83.3}$$

where $\widehat{K}_0 = H_0 - \mu N$ can easily be diagonalized but not $\widehat{K}$ because $\widehat{K}_0$ and $\widehat{K}_1$ do not commute. In that case, perturbation theory can help. We now prove

$$\boxed{e^{-\beta\widehat{K}} = e^{-\beta\widehat{K}_0}\widehat{U}(\beta)} \tag{83.4}$$

$$\boxed{\widehat{U}(\beta) \equiv T_\tau \left[e^{-\int_0^\beta \widehat{K}_1(\tau)d\tau}\right]} \tag{83.5}$$

$$\boxed{\widehat{K}_1(\tau) \equiv e^{\widehat{K}_0\tau}\widehat{K}_1 e^{-\widehat{K}_0\tau}}. \tag{83.6}$$

In the above expression, T_τ is the so-called time-ordering operator. It orders operators from left to right in increasing order of τ. Note that if $\widehat{K}_0$ and $\widehat{K}_1$ commute, then $\widehat{K}_1$ is independent of τ, $\widehat{U}(\beta) = e^{-\beta\widehat{K}_1}$ and $e^{-\beta\widehat{K}} = e^{-\beta\widehat{K}_0}e^{-\beta\widehat{K}_1}$ as expected.

Remark 376 *Imaginary time: The quantity, τ, is called imaginary time because the ordinary time evolution operator is e^{-iHt} and in the Heisenberg representation, operators evolve as follows: $\widehat{K}_1(t) = e^{i\widehat{K}_0 t/\hbar}\widehat{K}_1 e^{-i\widehat{K}_0 t/\hbar}$.*

To prove the above very important result is not difficult. It suffices to find a differential equation for $\widehat{U}$. Start from

$$\begin{aligned}
\frac{\partial}{\partial\tau}e^{-\widehat{K}\tau} &= \left(-\widehat{K}_0 - \widehat{K}_1\right)e^{-\widehat{K}\tau} \\
\frac{\partial}{\partial\tau}\left(\widehat{U}(\tau)\right) &= \frac{\partial}{\partial\tau}\left(e^{\widehat{K}_0\tau}e^{-\widehat{K}\tau}\right) && (83.7)\\
&= e^{\widehat{K}_0\tau}\left(\widehat{K}_0 - (\widehat{K}_0 + K_1)\right)e^{-\widehat{K}\tau} && (83.8)
\end{aligned}$$

where in the second equation, we have used the definition of $\widehat{U}$, Eq.(83.4) and the chain rule. We are left with

$$\begin{aligned}
\frac{\partial}{\partial\tau}\widehat{U}(\tau) &= -\left(e^{\widehat{K}_0\tau}\widehat{K}_1 e^{-\widehat{K}_0\tau}\right)\widehat{U}(\tau) && (83.9)\\
&= -\widehat{K}_1(\tau)\,\widehat{U}(\tau) && (83.10)
\end{aligned}$$

where $\widehat{K}_1(\tau)$ takes the form advertized in Eq.(83.6).

To find $\widehat{U}(\beta)$, integrate both sides of the equation, remembering that $\widehat{U}(0) = 1$. Then

$$\widehat{U}(\beta) = 1 - \int_0^\beta \widehat{K}_1(\tau)\,\widehat{U}(\tau)\,d\tau. \tag{83.11}$$

To solve in powers of $\widehat{K}_1$, which is the whole idea behind perturbation theory after all, we just iterate the above equation

$$\begin{aligned}\widehat{U}(\beta) &= 1 - \int_0^\beta d\tau \widehat{K}_1(\tau) + (-1)^2 \int_0^\beta d\tau \widehat{K}_1(\tau) \int_0^\tau d\tau' \widehat{K}_1(\tau') \\ &\quad + (-1)^3 \int_0^\beta d\tau \widehat{K}_1(\tau) \int_0^\tau d\tau' \widehat{K}_1(\tau') \int_0^{\tau'} d\tau'' \widehat{K}_1(\tau'') + \cdots \end{aligned} \tag{83.12}$$

Note that the operators are always ordered from right to left in increasing order of τ. This means that with the help of the time-ordering operator T_τ, the above equation can be rearranged in the form

$$\begin{aligned}\widehat{U}(\beta) &= 1 - \int_0^\beta d\tau \widehat{K}_1(\tau) + \frac{(-1)^2}{2!} T_\tau \left[\int_0^\beta d\tau \widehat{K}_1(\tau) \int_0^\beta d\tau' \widehat{K}_1(\tau') \right] \\ &\quad + \frac{(-1)^3}{3!} T_\tau \left[\int_0^\beta d\tau \widehat{K}_1(\tau) \int_0^\beta d\tau' \widehat{K}_1(\tau') \int_0^\beta d\tau'' \widehat{K}_1(\tau'') \right] + \cdots \end{aligned} \tag{83.13}$$

where the factorial takes care of the fact that by completing all the integrals so that the upper bound is β for all of them, operators will come in all possible orders in τ so they will need to be rearranged in the proper order $\widehat{K}!$ times for the term of order $\widehat{K}$. The series can now be resummed in an exponential, as written in Eq.(83.5).

84. GREEN FUNCTIONS CONTAIN USEFUL INFORMATION

In many-body theory, it is often very convenient to focus on correlation functions instead of the full wave function because correlation functions are directly related to experiments. I begin with using the Golden rule to interpret angle-resolved photoemission experiment and then define a funny looking correlation function, the imaginary-time Green function, and show that if we can calculate it, then we have a calculation for the photoemission experiment. After you have seen the Green function for a few simple Hamiltonian, you will appreciate the notions of self-energy, spectral weight, Wick's theorem. We will be ready to set up (not to solve) the quantum impurity problem, which is fundamental to an important approach to the Many-body problem, Dynamical Mean-Field Theory.

We drop the spin index for many parts of the following discussion to unclutter the notation. In general, $c_{\mathbf{p}}$ for example should be written $c_{\mathbf{p}\sigma}$ since the spin is necessary to characterize the state. I hope this will not lead to confusion.

84.1 Photoemission experiments and fermion correlation functions

Photoemission experiments can be represented schematically as in Fig.26-1. Given the fom of the interaction beween matter and electromagnetic field, Fermi's Golden Rule tells us that the cross section is proportional to

$$\sum_{mn} \frac{e^{-\beta \widehat{K}_m}}{Z} \frac{2\pi}{\hbar} \left| \langle n| \otimes \langle \mathbf{k}| \otimes \langle 0|_{em} \left(-\sum_{\mathbf{k}'} \mathbf{j}_{\mathbf{k}'} \cdot \mathbf{A}_{-\mathbf{k}'} \right) |m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em} \right|^2 \delta\left(\hbar\omega + \mu - (E_m - E_n)\right)$$

where $|m\rangle$ and $\langle n|$ denote many-body eigenstates of the system, $\langle \mathbf{k}|$ is the momentum eigenstate of the outgoing single electron with $|0\rangle$ the corresponding vacuum while $|1_{\mathbf{q}}\rangle_{em}$ is the one-photon eigenstate of the electromagnetic field with $\langle 0|_{em}$ the correponding vacuum. Note that we need to sum over all final states of the system $\langle n|$ since they are not measured. All we know about the initial state is that it is in a mixture described by the canonical ensemble.

The matrix element can be rearranged as follows

$$- \langle n| \otimes \langle \mathbf{k}| \otimes \langle 0|_{em} \left(\sum_{\mathbf{k}'} \mathbf{j}_{\mathbf{k}'} \cdot \mathbf{A}_{-\mathbf{k}'} \right) |m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em} . \tag{84.1}$$

$$= - \sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \mathbf{j}_{\mathbf{k}'} |m\rangle \otimes |0\rangle \cdot \langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle_{em} . \tag{84.2}$$

The vector potential is the analog of the position operator for harmonic vibration of the electromagnetic field. Hence, it is proportionnal to $a^\dagger_{-\mathbf{k}'} + a_{\mathbf{k}'}$ and $\mathbf{k}' = \mathbf{q}$ with the destruction operator will lead to a non-zero value of $\langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle$. For the range of energies of interest, the wave vector of the photon $\mathbf{k}' = \mathbf{q}$ can be

considered in the center of the Brillouin zone, $\mathbf{k}' \approx \mathbf{0}$. The current operator is a one-body operator. In the continuum, it is then given by

$$\mathbf{j}_{\mathbf{k}'=\mathbf{0}} = e \sum_{\mathbf{p}} \frac{\mathbf{p}}{m} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}. \tag{84.3}$$

The value $\mathbf{p} = \mathbf{k}_{||}$ will lead to a non-zero matrix element. Overall then, the matrix element is

$$- \langle n| \, c_{\mathbf{k}_{||}} \, |m\rangle \left(\langle \mathbf{k}| \, c_{\mathbf{k}_{||}}^{\dagger} \, |0\rangle \, e \frac{\mathbf{k}_{||}}{m} \cdot \langle 0|_{em} \, \mathbf{A}_{\mathbf{k}'=\mathbf{q}\sim\mathbf{0}} \, |1_{\mathbf{q}}\rangle_{em} \right). \tag{84.4}$$

The term in large parenthesis is a matrix element that does not depend on the state of the system. Without going into more details of the assumptions going into the derivation then, Fermi's golden rule suggests, (see first section of Chapter 2) that the differential cross section for ejecting an electron of momentum $\mathbf{k}_{||}$ and energy ω (measured with respect to μ) is proportional to

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} \left| \langle n| \, c_{\mathbf{k}_{||}} \, |m\rangle \right|^2 \delta \left(\omega + \mu - (E_m - E_n) \right) \tag{84.5}$$

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} \langle m| \, c_{\mathbf{k}_{||}}^{\dagger} \, |n\rangle \langle n| \, c_{\mathbf{k}_{||}} \, |m\rangle \, \delta \left(\omega - (K_m - K_n) \right). \tag{84.6}$$

Even if you miss some of the details, it is not important. We just want to suggest that it is important to compute correlation functions involving fermion creation and annihilation operators.

84.2 Definition of the Matsubara Green function

The most useful fermion correlation function, which can be used to obtain directly the above cross section as you will see, is the Matsubara Green function

$$\boxed{\mathcal{G}_{\alpha\beta}(\tau) = - \left\langle T_\tau c_\alpha(\tau) \, c_\beta^{\dagger}(0) \right\rangle} \tag{84.7}$$

$$= - \left\langle c_\alpha(\tau) \, c_\beta^{\dagger}(0) \right\rangle \theta(\tau) + \left\langle c_\beta^{\dagger}(0) \, c_\alpha(\tau) \right\rangle \theta(-\tau). \tag{84.8}$$

The last equation above defines the time ordering operator for fermions. It is very important to notice the minus sign associated with interchanging two fermion operators. This time-ordering operator is thus a slight generalization of the time-ordering operator we encountered before. One of the motivations for defining the Green function with a time-ordering operator is that T_τ appears naturally in perturbation theory as we have seen above. The time-ordering operator makes the perturbative evaluation of $\mathcal{G}_{\alpha\beta}$ natural.

Remark 377 *The time-ordering operator for quantities that are quadratic in fermions, i.e. bosonic quantities, such as $\widehat{K}_1$ that appeared in the perturbation expansion, never have a minus sign associated with the exchange of bosonic operators.*

Remark 378 *Physically, $\mathcal{G}_{\alpha\beta}(\tau)$ represents the amplitude that an excitation in a state β shows up as an excitation in state α after a "time" τ.*

We still need to specify a few things. First, the thermodynamic average is in the grand-canonical ensemble

$$\langle \mathcal{O} \rangle \equiv \frac{Tr\left[e^{-\beta \widehat{K}} \mathcal{O}\right]}{Tr\left[e^{-\beta \widehat{K}}\right]} \tag{84.9}$$

while the time evolution of the operators is defined by

$$\boxed{c_\alpha(\tau) \equiv e^{\widehat{K}\tau} c_\alpha e^{-\widehat{K}\tau}} \tag{84.10}$$

$$\boxed{c_\alpha^\dagger(\tau) \equiv e^{\widehat{K}\tau} c_\alpha^\dagger e^{-\widehat{K}\tau}} \tag{84.11}$$

Remark 379 *Note that $c_\alpha^\dagger(\tau)$ is not the Hermitian conjugate of $c_\alpha(\tau)$. The notation is somewhat abusive, but justified by the fact that if you replace immaginary time by real time, $\tau \to it/\hbar$, then we recover the usual case.*

Remark 380 *From now on, I set $\hbar = 1$. Sorry for the lazyness.*

84.3 The Matsubara frequency representation is convenient

Since we are working in time-translationally invariant systems, it is natural to think for Fourier transforms and enquire about a frequency representation. Since we work on a finite imaginary-time interval contained between $-\beta$ and β, it is in fact Fourier series that will come to the rescue.

The first thing to notice are the Kubo-Martin-Schwinger boundary conditions that tell us that $\mathcal{G}_{\alpha\beta}(\tau)$ is antiperiodic in imaginary time. What this means is the following.

$$\mathcal{G}_{\alpha\beta}(\tau) = -\mathcal{G}_{\alpha\beta}(\tau - \beta). \tag{84.12}$$

Proof: Take $\tau > 0$ for example.

$$\mathcal{G}_{\alpha\beta}(\tau) = -\frac{1}{Z} \operatorname{Tr}\left[e^{-\beta\widehat{K}} e^{\widehat{K}\tau} c_\alpha e^{-\widehat{K}\tau} c_\beta^\dagger\right] \tag{84.13}$$

The cyclic property of the trace then tells us that

$$\begin{aligned}
\mathcal{G}_{\alpha\beta}(\tau) &= -\frac{1}{Z} \operatorname{Tr}\left[c_\beta^\dagger e^{-\beta\widehat{K}} e^{\widehat{K}\tau} c_\alpha e^{-\widehat{K}\tau}\right] && (84.14)\\
&= -\frac{1}{Z} \operatorname{Tr}\left[e^{-\beta\widehat{K}} c_\beta^\dagger e^{-\beta\widehat{K}} e^{\widehat{K}\tau} c_\alpha e^{-\widehat{K}\tau} e^{\beta\widehat{K}}\right] \\
&= -\frac{1}{Z} \operatorname{Tr}\left[e^{-\beta\widehat{K}} c_\beta^\dagger c_\alpha(\tau - \beta)\right] \\
&= -\mathcal{G}_{\alpha\beta}(\tau - \beta). && (84.15)
\end{aligned}$$

where we have used $\tau - \beta < 0$ and the definition of the Green function.

The antiperiodicity that we just proved can be used in conjunction with the theorems on Fourier series to arrive to the useful representation

$$\boxed{\mathcal{G}_{\alpha\beta}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-ik_n\tau} \mathcal{G}_{\alpha\beta}(ik_n)} \tag{84.16}$$

where the so-called Matsubara frequencies for fermions are odd, namely

$$\boxed{k_n = (2n+1)\,\pi T = \frac{(2n+1)\pi}{\beta}} \quad ; \quad n \quad \text{integer} \tag{84.17}$$

The antiperiodicity property will be automatically fulfilled because $e^{-ik_n\beta} = e^{-i(2n+1)\pi} = -1$.

Choice of units Here and from now on, we have taken Boltzmann's constant k_B to be equal to unity.

The expansion coefficients are obtained as usual for Fourier series of antiperiodic functions from

$$\boxed{\mathcal{G}_{\alpha\beta}(ik_n) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}_{\alpha\beta}(\tau)} \tag{84.18}$$

84.4 Spectral weight and how it is related to $\mathcal{G}_{\mathbf{k}}(ik_n)$ and to photoemission

The quantity $-2\,\mathrm{Im}\,G^R(\omega)$ is called the spectral weight. To understand its general meaning, it suffices to start from the definition of the Matsubara Green function and to use a complete sets of states. More specifically,

$$\mathcal{G}_{\mathbf{k}}(ik_n) = -\int_0^\beta d\tau e^{ik_n\tau}\left\langle c_{\mathbf{k}}(\tau)\, c_{\mathbf{k}}^\dagger(0)\right\rangle \tag{84.19}$$

$$= -\int_0^\beta d\tau e^{ik_n\tau}\sum_{n,m}\frac{e^{-\beta K_n}}{Z}\langle n|\, e^{K_n\tau} c_{\mathbf{k}} e^{-K_m\tau}\,|m\rangle\,\langle m|\, c_{\mathbf{k}}^\dagger\,|n\rangle \tag{84.20}$$

The integral over imaginary time is now easy to do,

$$\boxed{\mathcal{G}_{\mathbf{k}}(ik_n) = \sum_{n,m}\frac{e^{-\beta K_n}}{Z}\frac{e^{\beta(K_n-K_m)}+1}{ik_n+K_n-K_m}\langle n|\, c_{\mathbf{k}}\,|m\rangle\,\langle m|\, c_{\mathbf{k}}^\dagger\,|n\rangle.} \tag{84.21}$$

We have used $e^{ik_n\beta} = -1$. This is the so-called Lehmann representation of $\mathcal{G}_{\mathbf{k}}(ik_n)$. This last result may be written in the so-called spectral representation

$$\boxed{\mathcal{G}_{\mathbf{k}}(ik_n) = \int \frac{d\omega}{2\pi}\frac{A_{\mathbf{k}}(\omega)}{ik_n-\omega}} \tag{84.22}$$

if we define the spectral weight by

$$A_{\mathbf{k}}(\omega) \equiv \sum_{n,m}\frac{1}{Z}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\langle n|\, c_{\mathbf{k}}\,|m\rangle\,\langle m|\, c_{\mathbf{k}}^\dagger\,|n\rangle \tag{84.23}$$

$$\times 2\pi\delta(\omega-(K_m-K_n)) \tag{84.24}$$

$$= \sum_{n,m}\frac{e^{-\beta K_m}}{Z}\left(1+e^{\beta\omega}\right)\langle n|\, c_{\mathbf{k}}\,|m\rangle\,\langle m|\, c_{\mathbf{k}}^\dagger\,|n\rangle\, 2\pi\delta(\omega-(K_m-K_n)).$$

Given this result, the differential photoemission cross section Eq.(84.6) may thus be obtained from

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto A_{\mathbf{k}}(\omega)\, f(\omega) \tag{84.25}$$

with $f(\omega) = \left(1+e^{\beta\omega}\right)^{-1}$ the Fermi function.

To find the physical meaning of the spectral weight, exchange the dummy summation indices m, n in the first term of Eq.(84.23) and you find

$$\begin{aligned} A_{\mathbf{k}}(\omega) &\equiv \sum_{n,m} \frac{1}{Z} e^{-\beta K_n} \langle n| c_{\mathbf{k}}^{\dagger} |m\rangle \langle m| c_{\mathbf{k}} |n\rangle 2\pi\delta(\omega - (K_n - K_m)) \\ &\quad + \frac{1}{Z} e^{-\beta K_n} \langle n| c_{\mathbf{k}} |m\rangle \langle m| c_{\mathbf{k}}^{\dagger} |n\rangle 2\pi\delta(\omega - (K_m - K_n)) \end{aligned} \tag{84.26}$$

This quantity is normalized since

$$\begin{aligned} \int \frac{d\omega}{2\pi} A_{\mathbf{k}}(\omega) &= \sum_{n,m} \frac{1}{Z} e^{-\beta K_n} \left(\langle n| c_{\mathbf{k}}^{\dagger} |m\rangle \langle m| c_{\mathbf{k}} |n\rangle + \langle n| c_{\mathbf{k}} |m\rangle \langle m| c_{\mathbf{k}}^{\dagger} |n\rangle \right) \\ &= \left\langle \left\{ c_{\mathbf{k}}^{\dagger}(0), c_{\mathbf{k}}(0) \right\} \right\rangle = 1. \end{aligned} \tag{84.27}$$

Clearly then, $A_{\mathbf{k}}(\omega)/(2\pi)$ can be interpreted as the probability that the state formed by adding to an eigenstate $|n\rangle$ a particle of momentum $\mathbf{k}$, i.e. $c_{\mathbf{k}}^{\dagger}|n\rangle$ or a hole $c_{\mathbf{k}}|n\rangle$, yields an eigenstate $\langle m|$ whose grand potential K has an energy ω compared with the original state $|n\rangle$. In the non-interacting case, for any given $\mathbf{k}$ there is only one frequency ω where there will be a non-zero contribution since $c_{\mathbf{k}}^{\dagger}|n\rangle$ or $c_{\mathbf{k}}|n\rangle$ are eigenstates. This is no-longer the case when there are interactions. Then, $c_{\mathbf{k}}^{\dagger}|n\rangle$ or $c_{\mathbf{k}}|n\rangle$ are not eigenstates and there are many states $\langle m|$ with different excitation energies ω whose overlap with $c_{\mathbf{k}}^{\dagger}|n\rangle$ or with $c_{\mathbf{k}}|n\rangle$ is non-vanishing (in other words where the quantum mechanical probability $|\langle m| c_{\mathbf{k}} |n\rangle|^2$ is non-vanishing). This is equivalent to saying that in the presence of interactions, the momentum $\mathbf{k}$ of a single particle is not conserved (or no-longer a good quantum number).

Remark 381 *It is important to recall once again that all the physical information is in the spectral weight* $A_{\mathbf{k}}(\omega)$.

84.5 $\mathcal{G}_{\mathbf{k}}(ik_n)$ for the non-interacting case $U = 0$

Before we see how the Green function is related to the photoemission cross section in general, it is useful to have a look at the non-interacting case to develop some intuition. This is our first occasion to write down the equation of motion for $\mathcal{G}_{\alpha\beta}$. You will notice that it is the kind of equation that one encounters with Green functions in general. Since we are considering the non-interacting case, take

$$\widehat{K}_0 = \sum_{\mathbf{p}} \zeta_{\mathbf{p}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}} \tag{84.28}$$

where $\zeta_{\mathbf{p}} = \varepsilon_{\mathbf{p}} - \mu$. Using the definition

$$\mathcal{G}_{\mathbf{k}}(\tau) = -\left\langle T_{\tau} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger}(0) \right\rangle \tag{84.29}$$

then

$$\frac{\partial \mathcal{G}_{\mathbf{k}}(\tau)}{\partial \tau} = -\delta(\tau) \left\langle \left\{ c_{\mathbf{k}}, c_{\mathbf{k}}^{\dagger} \right\} \right\rangle - \left\langle T_{\tau} \frac{\partial c_{\mathbf{k}}(\tau)}{\partial \tau} c_{\mathbf{k}}^{\dagger}(0) \right\rangle. \tag{84.30}$$

Since $\left\{c_{\mathbf{k}}, c_{\mathbf{k}}^{\dagger}\right\} = 1$ and using

$$\begin{aligned}[AB, C] &= ABC - CAB = ABC + (ACB - ACB) - CAB \\ &= A\{B, C\} - \{A, C\} B\end{aligned}$$

which yields

$$\frac{\partial c_{\mathbf{k}}(\tau)}{\partial \tau} = \left[\widehat{K}_0, c_{\mathbf{k}}(\tau)\right] \tag{84.31}$$

$$= -\zeta_{\mathbf{k}} c_{\mathbf{k}}(\tau) \tag{84.32}$$

we are left with

$$\frac{\partial \mathcal{G}_{\mathbf{k}}(\tau)}{\partial \tau} = -\delta(\tau) - \zeta_{\mathbf{k}} \mathcal{G}_{\mathbf{k}}(\tau). \tag{84.33}$$

Using Matsubara frequencies, as in Eq.(84.16) you find

$$(-ik_n + \zeta_{\mathbf{k}}) \mathcal{G}_{\mathbf{k}}(ik_n) = -1 \tag{84.34}$$

so that

$$\mathcal{G}_{\mathbf{k}}(ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}}}. \tag{84.35}$$

The replacement

$$ik_n \to \omega + i\eta \tag{84.36}$$

where ω is a real frequency and η is a positive infinitesimal, is called analytic continuation. We are about to see why we do this and why this is useful. But for now, let us just look at the result. Upon analytic continuation, $\mathcal{G}_{\mathbf{k}}(ik_n)$ becomes the so-called retarded Green function

$$\boxed{G^R(\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}}.} \tag{84.37}$$

Using the identity

$$\lim_{\eta \to 0} \frac{1}{x + i\eta} = \lim_{\eta \to 0} \frac{x - i\eta}{x^2 + \eta^2} = P\frac{1}{x} - i\pi\delta(x) \tag{84.38}$$

with P the principal part, we find

$$-2 \operatorname{Im} G^R(\omega) = 2\pi\delta(\omega - \zeta_{\mathbf{k}}), \tag{84.39}$$

which tells us that in a non-interacting system, in an eigenstate of momentum $\mathbf{k}$, the energy ω is $\zeta_{\mathbf{k}}$.

Remark 382 *When bands are calculated within DFT, one obtains $\zeta_{\mathbf{k},n}$ for each of the Bloch bands labeled by ν. In that case we have a band index so states must be labeled by both quantum numbers and*

$$A_{\mathbf{k},\nu}(\omega) = 2\pi\delta\left(\omega - \zeta_{\mathbf{k},\nu}\right). \tag{84.40}$$

84.6 Obtaining the spectral weight from $\mathcal{G}_{\mathbf{k}}(ik_n)$: the problem of analytic continuation

If we can compute $\mathcal{G}_{\mathbf{k}}(ik_n)$ by any means, we can obtain the spectral weight from its analytic continuation since, using the spectral representation Eq.(84.22) of $\mathcal{G}_{\mathbf{k}}(ik_n)$ we can simply do the analytic continuation $ik_n \to \omega + i\eta$ and find

$$\boxed{G^R_{\mathbf{k}}(\omega) = \int \frac{d\omega'}{2\pi} \frac{A_{\mathbf{k}}(\omega')}{\omega + i\eta - \omega'}.} \tag{84.41}$$

From this, the spectral weight $A_{\mathbf{k}}(\omega')$ is easy to find from

$$\boxed{A_{\mathbf{k}}(\omega) = -2\,\mathrm{Im}\,G^R_{\mathbf{k}}(\omega)\,.} \tag{84.42}$$

All this is very easy analytically, but with numerical data it turns into a nightmare. There are two methods that are widely used, Padé approximants and Maximum Entropy analytic continuation. These are whole subjects in themselves.

Remark 383 *We already mentioned that the physical information is in $A_{\mathbf{k}}(\omega)$. An equivalent way of saying this is that it is in the poles of $G^R_{\mathbf{k}}(\omega)$.*

85. SELF-ENERGY AND THE EFFECT OF INTERACTIONS

I begin by solving the Hubbard Hamiltonian when there are only interactions, no hopping. This is the so-called atomic limit. You will see that in this case the Green function takes a structure very different from the non-interacting case. This will be a natural occasion to introduce the notion of self-energy as a representation of the effect of interactions and to show that the self-energy is singular in the atomic limit, and more generally for Mott insulators. Also, we will see that in the case of a single interacting site in a sea of non-interacting electrons, the self-energy comes only from the interacting site. This is the Anderson impurity model, that happens to be very important in the context of Dynamical Mean-Field Theory. We will see Dyson's equation and a few general properties of the self-energy.

85.1 The atomic limit, $t = 0$

To see an extreme form of the effect of interactions, it suffices to consider the Hubbard model in the atomic limit, namely keeping only the interaction term:

$$\hat{K} = \sum_i \left(U n_{i\downarrow} n_{i\uparrow} - \mu n_{i\uparrow} - \mu n_{i\downarrow} \right). \tag{85.1}$$

In this problem, each site is independent and the Green relevant for photoemission becomes, restoring spin index

$$\begin{aligned} \left\langle c_{\mathbf{k}\sigma}(\tau)\, c^{\dagger}_{\mathbf{k}\sigma}(0) \right\rangle &= \frac{1}{N} \sum_{i,j} \left\langle c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_j\sigma}(0) \right\rangle e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} & (85.2) \\ &= \left\langle c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_i\sigma}(0) \right\rangle & (85.3) \end{aligned}$$

because $\left\langle c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_j\sigma}(0) \right\rangle = \left\langle c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_i\sigma}(0) \right\rangle \delta_{i,j}$. Indeed, even if the grand-canonical ensemble means that four possible states on each site will be considered, for a given number of particles on a site, the matrix element $\langle n_i| \langle n_j| e^{\beta K} c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_j\sigma}(0) |n_i\rangle |n_j\rangle$ vanishes if i and j are different because if I create an electron at site j with $c^{\dagger}_{\mathbf{R}_j\sigma}(0)$, the time evolution operator $e^{K\tau}$ cannot remove the electron from that site to make sure that the diagonal matrix elements of $c^{\dagger}_{\mathbf{R}_j\sigma}(0)$ do not vanish. Another way to say that is that $\langle n_i| \langle n_j| e^{\beta K} c_{\mathbf{R}_i\sigma}(\tau)\, c^{\dagger}_{\mathbf{R}_j\sigma}(0) |n_i\rangle |n_j\rangle$ vanishes in the trace for a given $|n_i\rangle |n_j\rangle$ if i is different from j, otherwise the number of electrons on a given site is not conserved despite the fact that $\hat{K}$ commutes with the number operator. The final result for $\mathcal{G}_{\mathbf{k}}(ik_n)$ will be momentum independent, as expected for a local problem.

Here I take an unusual approach for the analytical solution of this model. This method is however very close to that used by some of the numerical approaches. Drop the site label for simplification and consider the correlation function for up spins only. I proceed by analogy with the steps used to derive the Lehmann

representation Eq.(84.21) for $\mathcal{G}_{\mathbf{k}}(ik_n)$. Taking into account the Pauli principle, only two terms survive in the trace and, similarly, for each of the states in the trace only one intermediate state gives a non-zero matrix element

$$\begin{aligned}\left\langle c_{\uparrow}(\tau)\, c_{\uparrow}^{\dagger}(0)\right\rangle &= \frac{1}{Z}\langle 0|\, e^{\hat{K}\tau} c_{\uparrow} e^{-\hat{K}\tau}\,|\uparrow\rangle\langle\uparrow|\, c_{\uparrow}^{\dagger}\,|0\rangle \\ &\quad + \frac{e^{\beta\mu}}{Z}\langle\downarrow|\, e^{\hat{K}\tau} c_{\uparrow} e^{-\hat{K}\tau}\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow|\, c_{\uparrow}^{\dagger}\,|\downarrow\rangle \qquad (85.4)\\ &= \frac{1}{Z}\langle 0|\, c_{\uparrow} e^{-(-\mu)\tau}\,|\uparrow\rangle\langle\uparrow|\, c_{\uparrow}^{\dagger}\,|0\rangle + \frac{e^{\beta\mu}}{Z}\langle\downarrow|\, e^{-\mu\tau} c_{\uparrow} e^{-(U-2\mu)\tau}\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow|\, c_{\uparrow}^{\dagger}\,|\downarrow\rangle \\ &= \frac{1}{Z} e^{\mu\tau} + \frac{e^{\beta\mu}}{Z} e^{-(U-\mu)\tau}. \qquad (85.5)\end{aligned}$$

We are now ready to compute the Matsubara Green function appropriate for photoemission using as usual $e^{ik_n\beta} = -1$

$$\begin{aligned}\mathcal{G}_{\mathbf{k}\sigma}(ik_n) &= -\int_0^{\beta} d\tau e^{ik_n\tau}\left\langle c_{\mathbf{k}\sigma}(\tau)\, c_{\mathbf{k}\sigma}^{\dagger}(0)\right\rangle = -\int_0^{\beta} d\tau e^{ik_n\tau}\left\langle c_{\uparrow}(\tau)\, c_{\uparrow}^{\dagger}(0)\right\rangle \\ &= -\int_0^{\beta} d\tau e^{ik_n\tau}\left[\frac{1}{Z} e^{\mu\tau} + \frac{e^{\beta\mu}}{Z} e^{-(U-\mu)\tau}\right] \\ &= -\frac{1}{Z}\left[\frac{-e^{\beta\mu}-1}{ik_n+\mu} + \frac{-e^{-\beta(U-\mu)}-1}{ik_n+\mu-U}\right]. \qquad (85.6)\end{aligned}$$

The partition function is easy to evaluate but to go directly to the point, take $\mu = U/2$. Then

$$\mathcal{G}_{\mathbf{k}\sigma}(ik_n) = \frac{e^{-\beta U/2}+1}{Z}\left[\frac{1}{ik_n+\frac{U}{2}} + \frac{1}{ik_n-\frac{U}{2}}\right].$$

The spectral weight $A_{\mathbf{k}}(\omega)$ is easily obtained from $A_{\mathbf{k}\sigma}(\omega) = -2\,\mathrm{Im}\, G^R_{\mathbf{k}\sigma}(\omega)$ by following the procedure outlined in the analytic continuation section 84.6:

$$G^R_{\mathbf{k}\sigma}(\omega) = \frac{e^{-\beta U/2}+1}{Z}\left[\frac{1}{\omega+i\eta+\frac{U}{2}} + \frac{1}{\omega+i\eta-\frac{U}{2}}\right]$$

Because of the normalization condition, the prefactor can only be 1/2 since

$$A_{\mathbf{k}\sigma}(\omega) = \frac{1}{2}\left[2\pi\delta\left(\omega+\frac{U}{2}\right) + 2\pi\delta\left(\omega-\frac{U}{2}\right)\right] \qquad (85.7)$$

Even though there would be a single band and correpondingly a single delta function in the non-interacting case, here you find two. In addition we realize that we have an interaction-induced insulator (Mott insulator) since there are no states at $\omega = 0$.

Remark 384 *The thermodynamics is easy to do. One finds* $Z = 1 + 2e^{\beta\mu} + e^{-\beta(U-2\mu)}$. *Similarly, one can compute* $\left\langle c_{\downarrow}(\tau)\, c_{\downarrow}^{\dagger}(0)\right\rangle = \langle n_{\downarrow}\rangle$ *and discover that in general,*

$$G^R_{\mathbf{k}\uparrow}(\omega) = \left[\frac{1-\langle n_{\downarrow}\rangle}{\omega+i\eta+\mu} + \frac{\langle n_{\downarrow}\rangle}{\omega+i\eta+\mu-U}\right]. \qquad (85.8)$$

The weight of the pole that is at U depends clearly depends on the number of states already occupied by down spins. Given that $1-\langle n_{\downarrow}\rangle = \langle n_{\uparrow}\rangle$, *the first term can similarly be understood.*

85.2 The self-energy and the atomic limit example (Mott insulators)

It follows from the spectral representation Eq.(84.41) for the retarded Green function that the effect of interactions is to introduce new poles or at least to shift them with respect to the non-interacting case. Hence, it is convenient to *define* the self-energy $\Sigma^R_{\mathbf{k}\sigma}(\omega)$ by

$$G^R_{\mathbf{k}\sigma}(\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}\boldsymbol{\sigma}} - \Sigma^R_{\mathbf{k}\sigma}(\omega)} \tag{85.9}$$

$$= \frac{1}{\left(G^{0R}_{\mathbf{k}\sigma}(\omega)\right)^{-1} - \Sigma^R_{\mathbf{k}\sigma}(\omega)}, \tag{85.10}$$

where $G^{0R}_{\mathbf{k}\sigma}(\omega)$ is the non-interacting Green function. The corresponding expression for the Matsubara Green function is

$$\mathcal{G}_{\mathbf{k}\sigma}(ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}\boldsymbol{\sigma}} - \Sigma_{\mathbf{k}\sigma}(ik_n)} \tag{85.11}$$

$$= \frac{1}{\left(\mathcal{G}^0_{\mathbf{k}\sigma}(ik_n)\right)^{-1} - \Sigma_{\mathbf{k}\sigma}(ik_n)}. \tag{85.12}$$

Simple algebra shows that the last form is equivalent to

$$\mathcal{G}_{\mathbf{k}\sigma}(ik_n) = \mathcal{G}^0_{\mathbf{k}\sigma}(ik_n) + \mathcal{G}^0_{\mathbf{k}\sigma}(ik_n)\,\Sigma_{\mathbf{k}\sigma}(ik_n)\,\mathcal{G}_{\mathbf{k}\sigma}(ik_n), \tag{85.13}$$

the so-called Dyson equation. Alternatively, the form that we generally obtain from the equations of motion is

$$\left(\mathcal{G}^0_{\mathbf{k}\sigma}(ik_n)\right)^{-1}\mathcal{G}_{\mathbf{k}\sigma}(ik_n) = 1 + \Sigma_{\mathbf{k}\sigma}(ik_n)\,\mathcal{G}_{\mathbf{k}\sigma}(ik_n). \tag{85.14}$$

The above definition of the self-energy is natural for several reasons. Perhaps the most compelling follows once we consider the expression for the spectral weight,

$$\frac{1}{2\pi}A_{\mathbf{k}\sigma}(\omega) = -\frac{1}{\pi}\operatorname{Im}G^R_{\mathbf{k}\sigma}(\omega) = \frac{1}{\pi}\frac{-\operatorname{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega)}{\left(\omega - \zeta_{\mathbf{k}\boldsymbol{\sigma}} - \operatorname{Re}\Sigma^R_{\mathbf{k}\sigma}(\omega)\right)^2 + \left(\operatorname{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega)\right)^2}. \tag{85.15}$$

It reduces to a Lorentzian if both $\operatorname{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega)$ and $\operatorname{Re}\Sigma^R_{\mathbf{k}\sigma}(\omega)$ are small constants. In general it is not a Lorentzian but it describes well the situation where an otherwise single delta function is replaced by a peak that has a width and is shifted from the position where the delta function would be if there were no interaction. All the effects of interactions are contained in $\Sigma^R_{\mathbf{k}\sigma}(\omega)$.

In the case where we have only weak electron-electron interactions, in other words for a Fermi liquid, we have that $\operatorname{Im}\Sigma^R_{\mathbf{k}\sigma}(\omega) \propto \left(\omega^2 + (\pi T)^2\right)$. In the atomic limit,

$$\mathcal{G}^R_\sigma(\omega) = \frac{1}{2}\left(\frac{1}{\omega + i\eta + U/2} + \frac{1}{\omega + i\eta - U/2}\right) = \frac{(\omega + i\eta)}{(\omega + i\eta)^2 - \left(\frac{U^2}{4}\right)} \tag{85.16}$$

$$= \frac{1}{(\omega + i\eta) - \frac{U^2}{4(\omega + i\eta)}} \tag{85.17}$$

so that clearly, the retarded self-energy $\Sigma^R(\omega) = \frac{U^2}{4(\omega+i\eta)}$ is singular at low frequency, not good news for perturbation theory. It gets rid of the pole that is at $\omega = 0$ when there is no interaction. Singular self-energies are a hallmark of Mott insulators.

85.3 A few properties of the self-energy

Given the spectral representation Eq.(84.41)

$$G^R_{\mathbf{k}\sigma}(\omega) = \int \frac{d\omega'}{2\pi} \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega + i\eta - \omega'} \tag{85.18}$$

and the positivity of $A_{\mathbf{k}\sigma}$, which can easily be seen from Eq.(84.23), it is clear that $G^R_{\mathbf{k}\sigma}(\omega)$ has poles only in the lower-half complex plane. It can be shown that this is a general consequence of causality. This implies that $\mathrm{Im}\,\Sigma^R_{\mathbf{k}\sigma}(\omega)$ is negative, as follows also from the positivity of $A_{\mathbf{k}\sigma}$ and its representation Eq.(85.15) in terms of the self-energy.

Also, the self-energy cannot grow with frequency since

$$\lim_{\omega\to\infty} \omega G^R_{\mathbf{k}\sigma}(\omega) = \omega \int \frac{d\omega'}{2\pi} \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega} = \int \frac{d\omega'}{2\pi} A_{\mathbf{k}\sigma}(\omega') = 1. \tag{85.19}$$

We have used the fact that $A_{\mathbf{k}\sigma}$ has to vanish at large frequency, as follows from Eq.(84.23) and the fact that the matrix elements between a true eigenstate and an eigenstate obtained from adding one excitation in a low energy state must vanish. In practice, the real part of the self-energy can at most be a constant at infinite frequency (This is the Hartree-Fock result).

85.4 Integrating out the bath in the quantum-impurity problem: The Anderson impurity model

Consider a single site with a Hubbard interaction U, connected to a bath of non-interacting electrons. This is the so-called Anderson impurity model. This problem plays a key role in the Dynamical Mean-Field Theory approach to correlated electrons. We will only set up the problem of quantum impurities without solving it. The Numerical Renormalization Group approach (NRG), Density Matrix Renormalization Group and, most prominently, Continuous Time Quantum Monte Carlo provide examples of methods that can be used to solve this problem.

We begin with the Anderson impurity problem. Including the chemical potential, the model is defined by

$$K_I = H_f + H_c + H_{fc} - \mu N \tag{85.20}$$

$$K_f \equiv \sum_\sigma (\varepsilon - \mu) f^\dagger_{i\sigma} f_{i\sigma} + U \left(f^\dagger_{i\uparrow} f_{i\uparrow}\right)\left(f^\dagger_{i\downarrow} f_{i\downarrow}\right) \tag{85.21}$$

$$K_c \equiv \sum_\sigma \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{85.22}$$

$$H_{fc} \equiv \sum_\sigma \sum_{\mathbf{k}} \left(V_{\mathbf{k}i} c^\dagger_{\mathbf{k}\sigma} f_{i\sigma} + V^*_{i\mathbf{k}} f^\dagger_{i\sigma} c_{\mathbf{k}\sigma}\right) \tag{85.23}$$

To physically motivate this model, think of a single f level on an atom where the on-site interaction is very large. That site is hybridized through $V_{i\mathbf{k}}$ with conduction electrons around it. The sum over $\mathbf{k}$ in the hybridization part of the Hamiltonian H_{fc} basically tells us that it is the local overlap of the conduction band with the impurity that produces the coupling.

Suppose we want to know the properties of the impurity, such as the local density of states. It can be obtained from the Green function

$$\mathcal{G}_{ff}(\tau) = -\left\langle T_\tau f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. \tag{85.24}$$

Let us proceed with the equation of motion method. We first write the equations of motion for $c_{\mathbf{k}\sigma}$ and $f_{i\sigma}$

$$\begin{aligned}
\frac{\partial}{\partial\tau} c_{\mathbf{k}\sigma} &= [K_I, c_{\mathbf{k}\sigma}] && (85.25)\\
&= -(\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma} - V_{\mathbf{k}i} f_{i\sigma} && (85.26)\\
\frac{\partial}{\partial\tau} f_{i\sigma} &= [K_I, f_{i\sigma}] && (85.27)\\
&= -(\varepsilon - \mu) f_{i\sigma} - U f^\dagger_{i-\sigma} f_{i-\sigma} f_{i\sigma} - \sum_{\mathbf{k}} V^*_{i\mathbf{k}} c_{\mathbf{k}\sigma} && (85.28)
\end{aligned}$$

Proceeding like our in our earlier derivation of the equations of motion we have

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{ff}(\tau) &= -\delta(\tau)\left\langle \left\{ f_{i\sigma}(\tau), f^\dagger_{i\boldsymbol{\sigma}} \right\} \right\rangle \\
&\quad - \left\langle T_\tau \left(-(\varepsilon - \mu) f_{i\sigma}(\tau) - U f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) - V^*_{\mathbf{k}i} c_{\mathbf{k}\sigma} \right) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle && (85.29)\\
&= -\delta(\tau) - (\varepsilon - \mu)\mathcal{G}_{ff}(\tau) + U\left\langle T_\tau f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle - \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \mathcal{G}_{cf}(\mathbf{k}, i, \tau)
\end{aligned}$$

where we defined

$$\mathcal{G}_{cf}(\mathbf{k}, i, \tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. \tag{85.30}$$

To eliminate this quantity, we write its equations of motion

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{cf}(\mathbf{k}, i, \tau) &= -\delta(\tau)\left\langle \left\{ c_{\mathbf{k}\sigma}(\tau), f^\dagger_{i\boldsymbol{\sigma}} \right\} \right\rangle \\
&\quad - \left\langle T_\tau \left(-(\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}(\tau) - V_{\mathbf{k}i} f_{i\sigma}(\tau) \right) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle \\
&= -(\varepsilon_{\mathbf{k}} - \mu)\mathcal{G}_{cf}(\mathbf{k}, i, \tau) - V_{\mathbf{k}i}\mathcal{G}_{ff}(\tau) && (85.31)
\end{aligned}$$

that follows because $\left\{ c_{\mathbf{k}\sigma}, f^\dagger_{i\boldsymbol{\sigma}} \right\} = 0$. It can be solved by going to Matsubara frequencies

$$\mathcal{G}_{cf}(\mathbf{k}, i, ik_n) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i}\mathcal{G}_{ff}(ik_n). \tag{85.32}$$

Substituting in the equation for $\mathcal{G}_{ff}(ik_n)$ we obtain

$$\begin{aligned}
&\left[ik_n - (\varepsilon - \mu) - \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i} \right] \mathcal{G}_{ff}(ik_n) \\
&= 1 - U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle. && (85.33)
\end{aligned}$$

The last term on the right-hand side is related to the self-energy as usual by

$$\Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) \equiv -U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f^\dagger_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^\dagger_{i\boldsymbol{\sigma}} \right\rangle \tag{85.34}$$

The equation to be solved has exactly the same Dyson equation structure as that which we would find for a single impurity

$$\begin{aligned}
\mathcal{G}^0_{ff}(ik_n)^{-1}\mathcal{G}_{ff}(ik_n) &= 1 + \Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) && (85.35)\\
\mathcal{G}_{ff}(ik_n) &= \mathcal{G}^0_{ff}(ik_n) + \mathcal{G}^0_{ff}(ik_n)\Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) && (85.36)
\end{aligned}$$

except that now the "non-interacting" Green function is

$$\mathcal{G}^0_{ff}\left(ik_n\right)^{-1} = ik_n - (\varepsilon - \mu) - \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i}. \tag{85.37}$$

This is in fact exactly the non-interacting Green function that we would find with $U = 0$. The last term reflects the fact that one can propagate from the impurity site back to the impurity site by going through the bath. One often defines the hybridization function $\Delta_{ff}\left(ik_n\right)$ by

$$\Delta_{ff}\left(ik_n\right) = \sum_{\mathbf{k}} V^*_{i\mathbf{k}} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}i}. \tag{85.38}$$

What is important to remember is that the self-energy affects only the site where there is an interaction U. Equations (85.29) and (85.31) for the Green's functions, written in Matsubara frequency, read:

$$\begin{pmatrix} ik_n - (\varepsilon - \mu) - \Sigma_{ff}\left(ik_n\right) & -V^*_{i\mathbf{k}} \\ -V_{\mathbf{k}i} & ik_n - (\varepsilon_{\mathbf{k}} - \mu) \end{pmatrix} \begin{pmatrix} \mathcal{G}_{ff}\left(ik_n\right) \\ \mathcal{G}_{cf}\left(\mathbf{k}, ik_n\right) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

In this equation, we imply the sum over $\mathbf{k}$. The structure of this equation is easy to remember and has a quite transparent meaning. What we have done, is used the second line of this equation to eliminate $\mathcal{G}_{cf}\left(\mathbf{k}, i, ik_n\right)$, i.e. the bath, completely. We are left with a single-site problem where the bath is replaced by a hybridization function. We are left with Dyson's equation for $\mathcal{G}_{ff}$ and and a new $\mathcal{G}^0_{ff}\left(ik_n\right)^{-1}$ which contains the bath as a hybridization function Eq.(85.37).

The solution to this impurity problem is complicated. The structure in imaginary time is highly non-trivial. Contrary to the atomic limit, the number of electrons on a site is not conserved, i.e. it is time-dependent, and the simplicity of the problem is lost. There is a complicated dynamics where electrons move in and out of the impurity site and what happens at a given time depends on what happened at earlier ones. For example, if there is a down electron on the impurity site, another down electron will not be able to come on the site unless the previous one comes out. The problem contains the rich Physics that goes under the name of Kondo and could be the subject of many chapters. It has been the focus of much attention in Condensed Matter Physics for decades. We will not, for now, expand further on this now.

Remark 385 *The self-energy will influence the value of* $\mathcal{G}_{cf}\left(\mathbf{k}, ik_n\right)$, *as we can see by inverting the matrix in the last equation. Nevertheless, the self-energy comes only from the site that has interactions. When particles propagate in the bath, they can step on the interacting site and that is where the effect of interactions show up.*

86. MANY-PARTICLE CORRELATION FUNCTIONS AND WICK'S THEOREM

To compute the many-particle correlation functions that arise directly in a non-interacting system or as intermediate steps in the perturbative calculations about a non-interacting (quadratic) Hamiltonian, Wick's theorem is extremely helpful. You can find a simple special case in Sec. C.3, a general proof in Sec. 33.1 that uses only the canonical formalism and finally a proof using coherent-state functional integrals in Sec. 80.4. There is also a simpler coherent-state functional integral proof that uses the diagonal basis in Sec. 80.3.

Wick's theorem takes the following form in the special case of spinless fermions:

$$\begin{aligned} & \left\langle T_\tau \psi(\tau_1)\psi(\tau_2)\cdots\psi(\tau_n)\psi^\dagger(\tau'_n)\cdots\psi^\dagger(\tau'_2)\psi^\dagger(\tau'_1)\right\rangle \\ = \quad & (-1)^n \det\begin{bmatrix} \mathcal{G}(\tau_1,\tau'_1) & \mathcal{G}(\tau_1,\tau'_2) & \cdots & \mathcal{G}(\tau_1,\tau'_n) \\ \mathcal{G}(\tau_2,\tau'_1) & \mathcal{G}(\tau_2,\tau'_2) & \cdots & \mathcal{G}(\tau_2,\tau'_n) \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{G}(\tau_n,\tau'_1) & \mathcal{G}(\tau_n,\tau'_2) & \cdots & \mathcal{G}(\tau_n,\tau'_n) \end{bmatrix}. \end{aligned} \tag{86.1}$$

Spatial indices and spin labels can easily be added. The antisymmetry of the time-ordered product under interchange of creation operators translates into the antisymmetry of the determinant under the interchange of columns. And similarly, the antisymmetry under interchange of destruction operators translates into antisymmetry under interchange of lines.

Another way to state the result is to say that

$$(-1)^n \left\langle T_\tau \psi(\tau_1)\psi(\tau_2)\cdots\psi(\tau_n)\psi^\dagger(\tau'_n)\cdots\psi^\dagger(\tau'_2)\psi^\dagger(\tau'_1)\right\rangle$$

is equal to the sum over of all complete sets of contractions, where a complete contraction is a configuration in which each ψ is contracted (paired) with a $\psi^\dagger$. A contraction of $\psi(\tau_1)$ with $\psi^\dagger(\tau'_1)$ is defined by $(-1)\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau'_1)\right\rangle = \mathcal{G}(\tau_1,\tau'_1)$. Each complete contraction has a sign that is determined by the signature of the permutation with respect to the original order. For example,

$$\begin{aligned} (-1)^2\left\langle T_\tau \psi(\tau_1)\psi(\tau_2)\psi^\dagger(\tau'_2)\psi^\dagger(\tau'_1)\right\rangle &= (-1)^2\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau'_1)\right\rangle\left\langle T_\tau \psi(\tau_2)\psi^\dagger(\tau'_2)\right\rangle \\ &\quad -(-1)^2\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau'_2)\right\rangle\left\langle T_\tau \psi(\tau_2)\psi^\dagger(\tau'_1)\right\rangle \\ &= \mathcal{G}(\tau_1,\tau'_1)\mathcal{G}(\tau_2,\tau'_2) - \mathcal{G}(\tau_2,\tau'_1)\mathcal{G}(\tau_1,\tau'_2) \end{aligned} \tag{86.2}$$

Remark 386 *To gain some insight into why correlation functions may factor for non interacting systems, consider the simple case where there are only two fermion states. In other words*

$$\hat{K}_0 = \zeta_1 c_1^\dagger c_1 + \zeta_2 c_2^\dagger c_2. \tag{86.3}$$

Then

$$e^{-\beta\hat{K}_0} = e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)} e^{-\beta\left(\zeta_2 c_2^\dagger c_2\right)} \tag{86.4}$$

and the partition function factors, i.e. in the occupation-number representation

$$Z = \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 n_2 | \, e^{-\beta \hat{K}_0} \, | n_1 n_2 \rangle = \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 n_2 | \, e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)} e^{-\beta\left(\zeta_2 c_2^\dagger c_2\right)} \, | n_1 n_2 \rangle \, . \tag{86.5}$$

Inserting a complete set of states in between the exponentials and using the fact that $e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)}$ *is diagonal in the occupation number basis, we are left with*

$$\begin{aligned} Z &= \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 n_2 | \, e^{-\beta \hat{K}_0} \, | n_1 n_2 \rangle = \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 n_2 | \, e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)} \, | n_1 n_2 \rangle \langle n_1 n_2 | \, e^{-\beta\left(\zeta_2 c_2^\dagger c_2\right)} \, | n_1 n_2 \rangle \\ &= \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 | \, e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)} \, | n_1 \rangle \langle n_2 | \, e^{-\beta\left(\zeta_2 c_2^\dagger c_2\right)} \, | n_2 \rangle = Z_1 Z_2 . \end{aligned} \tag{86.6}$$

Similarly, for any diagonal operator $\mathcal{O}_i$ *acting on state* i*, we have*

$$\begin{aligned} \langle \mathcal{O}_1 \mathcal{O}_2 \rangle &= \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \frac{\langle n_1 | \, e^{-\beta\left(\zeta_1 c_1^\dagger c_1\right)} \mathcal{O}_1 \, | n_1 \rangle}{Z_1} \frac{\langle n_2 | \, e^{-\beta\left(\zeta_2 c_2^\dagger c_2\right)} \mathcal{O}_2 \, | n_2 \rangle}{Z_2} & (86.7) \\ &= \langle \mathcal{O}_1 \rangle_1 \langle \mathcal{O}_2 \rangle_2 \, . & (86.8) \end{aligned}$$

Example 38 *The theorem is easy to understand in the diagonal basis for a given time order. In the end, this is the approach used to prove it.. Let us try to understand why the following equation is true:*

$$\left\langle c_\alpha c_\beta c_\gamma^\dagger c_\delta^\dagger \right\rangle = \left\langle c_\beta c_\gamma^\dagger \right\rangle \left\langle c_\alpha c_\delta^\dagger \right\rangle - \left\langle c_\alpha c_\gamma^\dagger \right\rangle \left\langle c_\beta c_\delta^\dagger \right\rangle . \tag{86.9}$$

Both sides of the equation vanish if we do not have $\beta = \gamma$ *and* $\alpha = \delta$ *OR* $\alpha = \gamma$ *and* $\beta = \delta$*. When either of these conditions is satisfied and* $\alpha \neq \beta$*, we can anticommute the operators when necessary and obtain the above formula. When either of the conditions is satisfied and* $\alpha = \beta$*, both sides of the equation vanish.*

87. SOURCE FIELDS TO CALCULATE MANY-BODY GREEN FUNCTIONS

In classical statistical mechanics, we are used to calculating observable quantities from derivatives of the free energy. There is an analogous procedure for the many-body problem. In this section, I will first introduce the notion of functional derivatives in the context of classical statistical mechanics and the proceed to show how the same paradigm can be used to formulate the general many-body problem. We will then encounter the so-called GW approximation that is natural for long-range Coulomb interactions and that is widely used to improve the results of band structure calculations.

87.1 A simple example in classical statistical mechanics

In elementary statistical mechanics, we can obtain the magnetization by differentiating the free energy with respect to the magnetic field and we can also obtain the magnetic susceptibility, related to the magnetization fluctuations, by differentiating once more. You can refresh your mind by checking Sec.35.1. Here I recall the less familiar results of this section.

Consider directly the more general problem of computing $\langle M(\mathbf{x}_1) M(\mathbf{x}_2)\rangle - \langle M(\mathbf{x}_1)\rangle \langle M(\mathbf{x}_2)\rangle$ in classical statistical mechanics. That can still be achieved if we impose a position dependent-external field:

$$Z[h] = \mathrm{Tr}\left[e^{-\beta\left(K - \int d^3\mathbf{x} h(\mathbf{x}) M(\mathbf{x})\right)}\right]. \tag{87.1}$$

It is as if at each position $\mathbf{x}$, there were an independent variable $h(\mathbf{x})$. The position is now just a label. The notation $Z[h]$ means that Z is a functional of $h(\mathbf{x})$.It takes a function and maps it into a scalar. To obtain the magnetization at a single point, we introduce the notion of functional derivative, which is just a simple generalization to the continuum of the idea of partial derivative. To be more specific,

$$\frac{\delta}{\delta h(\mathbf{x}_1)} \int d^3\mathbf{x} h(\mathbf{x}) M(\mathbf{x}) = \int d^3\mathbf{x} \frac{\delta h(\mathbf{x})}{\delta h(\mathbf{x}_1)} M(\mathbf{x}) \tag{87.2}$$

$$= \int d^3\mathbf{x} \delta(\mathbf{x}_1 - \mathbf{x}) M(\mathbf{x}) = M(\mathbf{x}_1). \tag{87.3}$$

In other words, the partial derivative $\partial y_1/\partial y_2 = \delta_{1,2}$ for two independent variables y_1 and y_2 is replaced by

$$\frac{\delta h(\mathbf{x})}{\delta h(\mathbf{x}_1)} = \delta(\mathbf{x}_1 - \mathbf{x}). \tag{87.4}$$

Very simple.

Armed with this notion of functional derivative, one finds that

$$\frac{\delta \ln Z\left[h\right]}{\beta \delta h\left(\mathbf{x}_1\right)} = \left\langle M\left(\mathbf{x}_1\right)\right\rangle_h \tag{87.5}$$

and the quantity we want is obtained from one more functional derivative

$$\frac{\delta^2 \ln Z\left[h\right]}{\beta^2 \delta h\left(\mathbf{x}_1\right)\delta h\left(\mathbf{x}_2\right)} = \left\langle M\left(\mathbf{x}_1\right)M\left(\mathbf{x}_2\right)\right\rangle_h - \left\langle M\left(\mathbf{x}_1\right)\right\rangle_h \left\langle M\left(\mathbf{x}_2\right)\right\rangle_h . \tag{87.6}$$

The $[h]$ near Z reminds us that Z is a functional of the function $h\left(\mathbf{x}\right)$, i.e. it maps this function to a scalar, namely Z. We can then evaluate everything at $h\left(\mathbf{x}\right)=0$ is that corresponds to the physical situation. The following generalization to Green functions is essentially a faithful copy of the one appearing in the main text.

87.2 Green functions and higher order correlations from source fields

Again, we follow the main text. In our case, we are interested in correlation functions that depend not only on space but also on real or imaginary time. In addition, we know that time-ordered products are relevant. Hence, you will not be surprized to learn that we use as our partition function with source fields

$$Z\left[\phi\right] = \mathrm{Tr}\left[e^{-\beta K}T_\tau \exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\right] \tag{87.7}$$

where we used the short-hand

$$\left(1\right) = \left(\mathbf{x}_1,\tau_1;\sigma_1\right) \tag{87.8}$$

with the overbar indicating integrals over space-time coordinates and spin sums. More specifically,

$$\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right) =$$

$$\sum_{\sigma_1,\sigma_2}\int d^3\mathbf{x}_1\int_0^\beta d\tau_1\int d^3\mathbf{x}_2\int_0^\beta d\tau_2\psi^\dagger_{\sigma_1}\left(\mathbf{x}_1,\tau_1\right)\phi_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1,\mathbf{x}_2,\tau_2\right)\psi_{\sigma_2}\left(\mathbf{x}_2,\tau_2\right).$$

We can think of $\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)$ as vector-matrix-vector multiplication. Some of the matrix or vector indices are continuous, but that should not confuse you I think. All the operators above evolve in imaginary time with the same $\hat{K}=\hat{H}-\mu\hat{N}$ that enters the Boltzmann weight $e^{-\beta\hat{K}}$.

With the definition,

$$\mathcal{S}\left[\phi\right] = \exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right) \tag{87.9}$$

we can write the Matsubara Green's function as a functional derivative of the generating function $\ln Z\left[\phi\right]$,

$$\begin{aligned} -\frac{\delta \ln Z\left[\phi\right]}{\delta\phi\left(2,1\right)} &= -\frac{\left\langle T_\tau \mathcal{S}\left[\phi\right]\psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle}{\left\langle T_\tau \mathcal{S}\left[\phi\right]\right\rangle} \\ &\equiv -\left\langle T_\tau \psi\left(1\right)\psi^\dagger\left(2\right)\right\rangle_\phi = \mathcal{G}\left(1,2\right)_\phi . \end{aligned} \tag{87.10}$$

To obtain this result, we used the fact that the functional derivative with respect to ϕ does not influence at all the time order, so one can differentiate the exponential inside the time-ordered product. (See Sec. 29.2) The thermal average on the first line is with respect to $e^{-\beta\hat{K}}$. In the average with a subscript, $\left\langle T_\tau \psi(1)\psi^\dagger(2)\right\rangle_\phi$, one does not write $\mathcal{S}[\phi]$ explicitly. Note the reversal in the order of indices in $\mathcal{G}$ and in ϕ.We have also used the fact that in a time ordered product we can displace operators as we wish, as long as we keep track of fermionic minus signs. Finally, the functional derivative with respect to ϕ is defined by

$$\frac{\delta\phi\left(\overline{1},\overline{2}\right)}{\delta\phi(1,2)} = \delta\left(\overline{1}-1\right)\delta\left(\overline{2}-2\right) \tag{87.11}$$

where the delta function is a mixture of Dirac and Kronecker delta functions

$$\delta\left(\overline{1}-1\right) = \delta^3\left(\mathbf{r}_{\overline{1}}-\mathbf{r}_1\right)\delta\left(\tau_{\overline{1}}-\tau_1\right)\delta_{\sigma_{\overline{1}},\sigma_1}. \tag{87.12}$$

Higher order correlation functions can be obtained by taking further functional derivatives

$$\begin{aligned}
\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= -\frac{\delta}{\delta\phi(3,4)}\frac{\left\langle T_\tau\mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\right\rangle}{\langle T_\tau\mathcal{S}[\phi]\rangle} \\
&= \frac{\left\langle T_\tau\mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle}{\langle T_\tau\mathcal{S}[\phi]\rangle} - \frac{\left\langle T_\tau\mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\right\rangle\left\langle T_\tau\mathcal{S}[\phi]\psi^\dagger(3)\psi(4)\right\rangle}{\langle T_\tau\mathcal{S}[\phi]\rangle^2} \\
&= \left\langle T_\tau\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\,\mathcal{G}(4,3)_\phi\,.
\end{aligned} \tag{87.13}$$

The first term is called a four-point correlation function. The last term comes from differentiating $\langle T_\tau\mathcal{S}[\phi]\rangle$ in the denominator. To figure out the minus signs in that last term note that there is one from $-1/Z^2$, one from the derivative of the argument of the exponential and one from ordering the field operators in the order corresponding to the definition of $\mathcal{G}_\sigma$. The latter is absorbed in the definition of $\mathcal{G}_\sigma$.

Remark 387 *The results of this section are independent of the explicit form of* $\hat{K}=\hat{H}-\mu\hat{N}$.

88. EQUATIONS OF MOTION TO FIND $\mathcal{G}_\phi$ AND Σ_ϕ

As we have seen before, if we have the equations of motion for $\psi(1)$, those for $\mathcal{G}_\phi$ will follow. And it is from the equations of motion that we find the self-energy.

88.1 Hamiltonian and equations of motion for $\psi(1)$

The Hamiltonian we consider contains the kinetic energy and the electron-electron interaction. Note that we now introduce spin indices denoted by Greek indices:

$$\begin{aligned}
\hat{K} &= \hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{V} + \hat{V}_n - \mu\hat{N} && (88.1)\\
\hat{H}_0 &= \frac{-1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\,\boldsymbol{\nabla}^2\psi_{\sigma_1}(\mathbf{x}_1) && (88.2)\\
\hat{V} &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\,\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1)\\
\hat{V}_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_2)\,n_0 && (88.3)
\end{aligned}$$

In the jellium model, the last piece, V_n represents the interaction between a "neutralizing background" of the same uniform density n_0 as the electrons, or we could use that actual attractive potential caused by the nuclei. The potential is the Coulomb potential

$$v(\mathbf{x}_1-\mathbf{x}_2) = \frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|} \tag{88.4}$$

The equations of motion are

$$\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} = \left[\hat{K},\psi_\sigma(\mathbf{x},\tau)\right], \tag{88.5}$$

which yields

$$\begin{aligned}
\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} &= \frac{\nabla^2}{2m}\psi_\sigma(\mathbf{x},\tau) + \mu\psi_\sigma(\mathbf{x},\tau) && (88.6)\\
&\quad -\sum_{\sigma_2}\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\,\psi^\dagger_{\sigma_2}(\mathbf{x}_2,\tau)\,\psi_{\sigma_2}(\mathbf{x}_2,\tau)\,\psi_\sigma(\mathbf{x},\tau)
\end{aligned}$$

The last term does not have the 1/2 factor that appeared in the Hamiltonian because $\psi_\sigma(\mathbf{x},\tau)$ can anticommute with one or the other $\psi^\dagger_\sigma$.

The equation of motion can be rewritten in the more matrix-like form

$$\frac{\partial\psi(1)}{\partial\tau_1} = \frac{\nabla_1^2}{2m}\psi(1) + \mu\psi(1) - \psi^\dagger(\overline{2})\,\psi(\overline{2})\,V(\overline{2}-1)\,\psi(1) \tag{88.7}$$

if we define a time and spin dependent potential

$$\boxed{V(1,2) = V_{\sigma_1,\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) \equiv \frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|}\delta(\tau_1-\tau_2).} \tag{88.8}$$

In reality the potential is independent of spin and is instantaneous but introducing these dependencies simplifies the notation.

88.2 Equations of motion for $\mathcal{G}_\phi$ and definition of $\sum_\phi$

We expect that the equation for motion for $\mathcal{G}(1,2)_\phi$

$$\mathcal{G}(1,2)_\phi = -\frac{\left\langle T_\tau \mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\right\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle}$$

will have the following structure $\mathcal{G}^{-1}(1,2)_\phi = \mathcal{G}_0^{-1}(1,2) - \phi(1,2) - \Sigma(1,2)_\phi$. In detail, it is obtained by taking an imaginary-time derivative. There will be three contributions. One from $\frac{\partial\psi(1)}{\partial\tau_1}$, that we found above, one from the time derivative of the two Heaviside functions $\theta(\tau_1-\tau_2)$ and $\theta(\tau_2-\tau_1)$ entering the definition of the time-ordered product (that gives the usual delta function), and one from the fact that terms in $\mathcal{S}[\phi]$ have to be ordered with respect to τ_1. The only unfamiliar contribution is the latter one. To understand how to compute it, we write explicitely the time integral associated with the creation operator in the exponential and order it properly:

$$\begin{aligned}\left\langle T_\tau \mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\right\rangle &= \left\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_1 \psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right)\right. \\ &\left.\psi(1)\exp\left(-\int_0^{\tau_1} d\tau_1 \psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right)\psi^\dagger(2)\right\rangle\end{aligned}$$

Since we moved an even number of fermion operators, we do not need to worry about sign. We do not need to worry about the destruction operator in the exponential either since it anticommutes with $\psi(1)$: The time-ordered product will eventually take care of the proper order (see also the first remark below). We thus have a contribution to the time derivative with respect to τ_1 that comes from acting on the exponentials and reads

$$\begin{aligned}&\left\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_1 \psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right)\int d^3\mathbf{x}_{1'}\left[\psi^\dagger(\mathbf{x}_{1'},\tau_1)\phi(\mathbf{x}_{1'},\tau_1,\overline{2})\psi(\overline{2}),\psi(\mathbf{x}_1,\tau_1)\right]\right. \\ &\left.\exp\left(-\int_0^{\tau_1} d\tau_1 \psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right)\psi^\dagger(2)\right\rangle \\ =\ &-\phi(1,\overline{2})\left\langle T_\tau \mathcal{S}[\phi]\psi(\overline{2})\psi^\dagger(2)\right\rangle.\end{aligned}$$

We had to take the derivative of the arguments of the exponentials and to be careful about order of operators at equal time. Collecting all the contributions, we can write

$$\begin{aligned}\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\mathcal{G}(1,2)_\phi &= -\delta(1-2) + \left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)V(1-\overline{2})\psi(\overline{2})\psi(1)\psi^\dagger(2)\right]\right\rangle_\phi \\ &\quad -\phi(1,\overline{2})\mathcal{G}(\overline{2},2)_\phi.\end{aligned} \tag{88.9}$$

Note that we had to specify $\psi^{\dagger}\left(\overline{2^{+}}\right)$ in the term with the potential energy. The superscrpt + specifies that the time in that field operator is later than the time in $\psi\left(\overline{2}\right)$. In other words

$$2^{+} \equiv \left(\mathbf{x}_2, \tau_2 + 0^{+}; \sigma_2\right)$$

Equal time does not mean anything in a time ordered product, we have to specify the order. The choice to take $\psi^{\dagger}\left(\overline{2^{+}}\right)$ keeps the field in the order it was in to begin with.

The equations of motion can be written in a compact form if we define

$$\boxed{\mathcal{G}_0^{-1}\left(1,\overline{2}\right) \equiv -\left(\frac{\partial}{\partial\tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\delta\left(1-\overline{2}\right).} \tag{88.10}$$

With this definition, the equation of motion Eq.(36.10) takes the form

$$\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right) - \phi\left(1,\overline{2}\right)\right)\mathcal{G}\left(\overline{2},2\right)_{\phi} = \delta\left(1-2\right) - V\left(1-\overline{2}\right)\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{2^{+}}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^{\dagger}\left(2\right)\right]\right\rangle_{\phi}.$$

Comparing with Dyson's equation, we have an explicit form for the self-energy,

$$\boxed{\Sigma\left(1,\overline{2}\right)_{\phi}\mathcal{G}\left(\overline{2},2\right)_{\phi} = -V\left(1-\overline{2}\right)\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{2^{+}}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^{\dagger}\left(2\right)\right]\right\rangle_{\phi}.} \tag{88.11}$$

The equation of motion can then also be written as

$$\boxed{\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right) - \phi\left(1,\overline{2}\right) - \Sigma\left(1,\overline{2}\right)_{\phi}\right)\mathcal{G}\left(\overline{2},2\right)_{\phi} = \delta\left(1-2\right)}$$

which also reads

$$\boxed{\mathcal{G}^{-1}\left(1,2\right)_{\phi} = \mathcal{G}_0^{-1}\left(1,2\right) - \phi\left(1,2\right) - \Sigma\left(1,2\right)_{\phi}.} \tag{88.12}$$

Remark 388 *You can work out a specifica example using the power series definition of the exponential to show that inside a time-ordered product, exponentials behave as ordinary exponential, $T_{\tau}\left[e^{A+B}\right] = T_{\tau}\left[e^{A}e^{B}\right]$ even when A and B are operators that do not commute, as long as A and B have bosonic commutation relations.*

Remark 389 *The self-energy is related to a four-point function and we note in passing that the trace of the defining equation 88.11 is related to the potential energy.*

$$\boxed{\Sigma\left(\overline{1},\overline{1'}\right)\mathcal{G}\left(\overline{1'},\overline{1^{+}}\right) = 2\left\langle V\right\rangle\beta = \left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{1^{+}}\right)\psi^{\dagger}\left(\overline{1'^{+}}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(\overline{1}\right)\right]\right\rangle} \tag{88.13}$$

Remark 390 *The 1^{+} on the left-hand side is absolutely necessary for this expression to make sense. Indeed, taken from the point of view of Matsubara frequencies, one knows that the self-energy goes to a constant at infinite frequency while the Green's function does not decay fast enough to converge without ambiguity. On the right-hand side of the above equation, all operators are at the same time, in the order explicitly given.*

89. THE GENERAL MANY-BODY PROBLEM

Since we need a four-point function to compute the self-energy and we know $\mathcal{G}_\phi$ if we know the self-energy, we can find a set of self-consistent equations if we can express the four-point function in terms of the self-energy. We begin by finding an integral equation for the four-point function to achieve this and then we use the result in the expression for the self-energy.

89.1 An integral equation for the four-point function

As we just saw in Eq.(87.13),

$$\frac{\delta \mathcal{G}\left(1,2\right)_\phi}{\delta\phi\left(3,4\right)} = \left\langle T_\tau \psi\left(1\right)\psi^\dagger\left(2\right)\psi^\dagger\left(3\right)\psi\left(4\right)\right\rangle_\phi + \mathcal{G}\left(1,2\right)_\phi \mathcal{G}\left(4,3\right)_\phi . \tag{89.1}$$

The equation for the functional derivative is then easy to find using $\mathcal{G}\mathcal{G}^{-1}=1$ and our matrix notation,

$$\frac{\delta\left(\mathcal{G}\mathcal{G}^{-1}\right)}{\delta\phi} = 0 \tag{89.2}$$

$$\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1} + \mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi} = 0 \tag{89.3}$$

$$\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}. \tag{89.4}$$

With Dyson's equation Eq. (88.12) for $\mathcal{G}^{-1}$ we find the right-hand side of that equation

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}. \tag{89.5}$$

Just to make sure what we mean, let us restore indices. This then takes the form

$$\begin{aligned}\frac{\delta \mathcal{G}\left(1,2\right)_\phi}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,\overline{1}\right)_\phi \frac{\delta\phi\left(\overline{1},\overline{2}\right)}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{2},2\right)_\phi + \mathcal{G}\left(1,\overline{5}\right)_\phi \frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_\phi}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{6},2\right)_\phi \\ &= \mathcal{G}\left(1,3\right)_\phi \mathcal{G}\left(4,2\right)_\phi + \mathcal{G}\left(1,\overline{5}\right)_\phi \frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_\phi}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{6},2\right)_\phi .\end{aligned} \tag{89.6}$$

We will see that Σ depends on ϕ only through its dependence on $\mathcal{G}$ so that this last equation can also be written in the form

$$\begin{aligned}\frac{\delta \mathcal{G}\left(1,2\right)_\phi}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,3\right)_\phi \mathcal{G}\left(4,2\right)_\phi \\ &\quad + \mathcal{G}\left(1,\overline{5}\right)_\phi \left(\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_\phi}{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_\phi}\frac{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_\phi}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_\phi .\end{aligned} \tag{89.7}$$

This general equation can also be written in short-hand notation

$$\frac{\delta \mathcal{G}}{\delta \phi} = \mathcal{G} \hat{\cdot} \mathcal{G} + \quad \mathcal{G} \quad \frac{\frac{\delta \Sigma}{\delta \mathcal{G}}}{\frac{\delta \mathcal{G}}{\delta \phi}} \quad \mathcal{G} \ , \tag{89.8}$$

where the caret $\hat{\cdot}$ reminds us that the indices adjacent to it are the same as those of ϕ and where the two terms on top of one another are matrix multiplied top down as well. Fig. 36-1 illustrates the equation with the indices. The diagrams go from top to bottom to remind ourselves of where the indices are in the algebraic equation, but we may rotate the diagrams in any direction we want.

89.2 Self-energy from functional derivatives

In short hand, what we want to achieve is the following. Starting from the general reult Eq.(88.11) written in terms of the four-point function which itself can be written as a functional derivative in Eq.(89.1), we have

$$\boxed{\Sigma = -V \left(\frac{\delta \mathcal{G}}{\delta \phi} - \mathcal{G}\mathcal{G} \right) \mathcal{G}^{-1}.} \tag{89.9}$$

Since the integral equation for $\frac{\delta \mathcal{G}}{\delta \phi}$ requires that we know both $\mathcal{G}$ and $\frac{\delta \Sigma}{\delta \mathcal{G}}$ there will be some iteration process involved.

One physical point that will become clearer when we put all indices back, is that the self-energy contains information about the fact that the medium is polarizable, i.e. it depends on the four-point correlation function $\frac{\delta \mathcal{G}}{\delta \phi}$ and hence on the density-density correlation function, or equivalently the longitudinal dielectric constant, as we shall verify.

We can also write an equation that looks as a closed functional equation for Σ by using the expression Eq.(89.5) relating $\frac{\delta \mathcal{G}}{\delta \phi}$ and $\frac{\delta \Sigma}{\delta \phi}$:

$$\begin{aligned} \Sigma &= -V \left(\mathcal{G} \frac{\delta \phi}{\delta \phi} \mathcal{G} + \mathcal{G} \frac{\delta \Sigma}{\delta \phi} \mathcal{G} - \mathcal{G}\mathcal{G} \right) \mathcal{G}^{-1}. \\ &= -V \left(\mathcal{G} \frac{\delta \phi}{\delta \phi} + \mathcal{G} \frac{\delta \Sigma}{\delta \phi} - \mathcal{G} \right) \end{aligned} \tag{89.10}$$

An alternate useful form that uses the fact that all the functional dependence of Σ on ϕ is implicit through its dependence on $\mathcal{G}$ is

$$\boxed{\Sigma = -V \left(\mathcal{G} \frac{\delta \phi}{\delta \phi} - \mathcal{G} + \mathcal{G} \frac{\delta \Sigma}{\delta \mathcal{G}} \frac{\delta \mathcal{G}}{\delta \phi} \right)} \tag{89.11}$$

Since Σ is already linear in V, it is tempting to use $\Sigma = -V \left(\mathcal{G} \frac{\delta \phi}{\delta \phi} - \mathcal{G} \right)$ as a first approximation. This is the Hartree-Fock approximation.

Remark 391 $\frac{\delta \Sigma}{\delta \mathcal{G}}$ *in the equation for the functional derivative Eq.(89.7) is called the irreducible vertex in the particle-hole channel. The reason for this will become clear later. The term that contains this irreducible vertex is called a vertex correction. Note that* $\mathcal{G} \left(\frac{\delta \Sigma}{\delta \mathcal{G}} \right) \mathcal{G}$ *plays the role of a self-energy for the four-point function* $\frac{\delta \mathcal{G}}{\delta \phi}$*. For the same reason that it was profitable to resum infinite series for* $\mathcal{G}$ *by using the concept of a self-energy, it will be preferable to do the same here and use* $\mathcal{G} \left(\frac{\delta \Sigma}{\delta \mathcal{G}} \right) \mathcal{G}$ *as a self-energy instead of iterating the equation for* $\frac{\delta \mathcal{G}}{\delta \phi}$ *at some finite order.*

Let us do this restoring all indices. To compute the self-energy, according to Eq.(88.11), what we need to obtain the self-energy is

$$\Sigma\left(1,3\right)_{\phi}=-V\left(1-\overline{2}\right)\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{2^{+}}\right)\psi\left(\overline{2}\right)\psi\left(1\right)\psi^{\dagger}\left(\overline{4}\right)\right]\right\rangle_{\phi}\mathcal{G}_{\phi}^{-1}\left(\overline{4},3\right). \quad (89.12)$$

We write the four-point function with the help of the functional derivative Eq.(36.22) by replacing in the latter equation $3\rightarrow\overline{2^{+}}$, $4\rightarrow\overline{2}$, $1\rightarrow1$, $2\rightarrow\overline{4}$ so that

$$\begin{aligned}\Sigma\left(1,3\right)_{\phi} &= -V\left(1-\overline{2}\right)\left[\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(1,\overline{4}\right)_{\phi}\right]\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi}\\ &= -V\left(1-\overline{2}\right)\left[-\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\mathcal{G}^{-1}\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\right].\end{aligned}$$

where we used Eq.(36.24) $\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1}=-\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}$.This is the general expression that we need for Σ. Note that in $\delta\phi\left(\overline{2^{+}},\overline{2}\right)$ the spins are identical, in other words, in spin space that matrix is diagonal. This is not the only possibility but that is the only one that we need here as we can see from the four point correlation function that we need. This is the so-called longitudinal particle-hole channel.

Remark 392 *Mnemotechnic: The first index of the $V\left(1-\overline{2}\right)$ is the same as the first index of the upper line and is the same as the first index on the left-hand side of the equation. The second index is summed over and is the same as the index on the denominator of $\frac{\delta\mathcal{G}\left(1,\overline{4}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}$. The two Green's function in $\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\mathcal{G}\left(1,\overline{4}\right)_{\phi}$ can be arranged on top of one another so that this rule is preserved.*

To begin to do approximations, we use the equation relating $\frac{\delta\mathcal{G}^{-1}}{\delta\phi}$ Eq.(89.5) to $\frac{\delta\Sigma}{\delta\phi}$ to obtain a closed set of equation for Σ that will lend itself to approximations in power series of the potential

$$\begin{aligned}\Sigma\left(1,3\right)_{\phi} &= -V\left(1-\overline{2}\right)\left[\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\phi\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}+\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}\right.\\ &\quad\left.-\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\right] \quad (89.13)\\ &= -V\left(1-3\right)\mathcal{G}\left(1,3^{+}\right)_{\phi}+V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\\ &\quad -V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}. \quad (89.14)\end{aligned}$$

The last term is the only one that will give a frequency dependence, and hence an imaginary part, to the self-energy.

The first two terms in the above equation are the Hartree-Fock contribution, that we will discuss in the next section and at length later on. By the way, you may wonder about $\mathcal{G}\left(1,3^{+}\right)_{\phi}$. Where does the + come from? Well, note that

$$\begin{aligned}V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\phi\left(\overline{4},3\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)} &= V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\delta\left(3-\overline{2}\right)\delta\left(\overline{4}-\overline{2^{+}}\right) \quad (89.15)\\ &= V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{2^{+}}\right)_{\phi}\delta\left(3-\overline{2}\right) \quad (89.16)\end{aligned}$$

so that when we to the integrals over $\overline{2}$ and $\overline{4}$, the time that corresponds to $\overline{4}$ entering the Green's function has to be later than the time $\overline{2}$ entering the potential. That is relevant because $V\left(1-\overline{2}\right)$ is instantaneous, i.e. there is a delta function $\delta\left(\tau_1-\tau_{\overline{2}}\right)$ so whether we have $\mathcal{G}\left(1,\overline{2}\right)$ or $\mathcal{G}\left(1,\overline{2^+}\right)$ is relevant. The + reflects the fact that in the Hamiltonian, the creation operators are always to the left of the annihilation operators.

In general, the functional dependence of Σ on ϕ will be through the dependence on $\mathcal{G}$. Hence, using the chain rule, the above equation may be rewritten

$$\begin{aligned}\Sigma\left(1,3\right)_\phi &= -V\left(1-3\right)\mathcal{G}\left(1,3^+\right)_\phi + V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^+}\right)_\phi \delta\left(1-3\right) \\ &\quad -V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_\phi \frac{\delta\Sigma\left(\overline{4},3\right)_\phi}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_\phi}\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_\phi}{\delta\phi\left(\overline{2^+},\overline{2}\right)}. \end{aligned} \tag{89.17}$$

The equation for the self-energy is represented schematically in Fig. 36-2. Note that the diagrams are one-particle irreducible, i.e. they cannot be cut in two seperate pieces by cutting a single propagator.

Remark 393 *Connection between indices in the Green's function and the direction of the arrow in the diagram: We take the convention that for* $\mathcal{G}\left(1,2\right)_\phi$ *the arrow begins at the annihilation operator* 1 *and ends at the creation operator* 2*. It might have been natural to begin at the creation operator instead. In fact it does not matter, as long as one is consistent. Both conventions can be found in the literature.*

90. LONG-RANGE FORCES AND THE GW APPROXIMATION

Up to now, I have derived everything with space-time indices. In the first section below, we will see what happens if the irreducible vertex is evaluated in the Hartree-Fock approximation, again in space-time. Moving to momentum and frequency, an approximation known as the RPA approximation, or GW for the self-energy, will become obvious.

90.1 Equations in space-time

Since Σ is already linear in external potential, it is tempting to drop the last term of the last equation of the previous section since that will be of second order at least. If we do this, we obtain

$$\Sigma\left(1,3\right)_{\phi}=V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)-V\left(1-3\right)\mathcal{G}\left(1,3^{+}\right)_{\phi}. \tag{90.1}$$

This is the Hartree-Fock approximation. This can be used to compute $\frac{\delta\Sigma}{\delta\mathcal{G}}$ that appears both in the in the exact expression for the self-energy Eq.(89.17) and in the exact expression for the four-point function Eq.(89.7) that also appears in the self-energy. A look at the last two figures that we drew is helpful.

Refering to the exact expression for the four-point function Eq.(89.7), what we need is $\frac{\delta\Sigma(5,6)_{\phi}}{\delta\mathcal{G}(7,8)_{\phi}}$ which we evaluate from the the Hartree-Fock approximation Eq.(37.1),

$$\begin{aligned}\frac{\delta\Sigma\left(5,6\right)_{\phi}}{\delta\mathcal{G}\left(7,8\right)_{\phi}} &= V\left(5-\overline{9}\right)\delta\left(\overline{9}-7\right)\delta\left(\overline{9}-8\right)\delta\left(5-6\right)-V\left(5-6\right)\delta\left(7-5\right)\delta\left(8-6\right)\\ &= V\left(5-7\right)\delta\left(7-8\right)\delta\left(5-6\right)-V\left(5-6\right)\delta\left(7-5\right)\delta\left(8-6\right).\end{aligned}$$

It is easier to imagine the result by looking back at the illustration of the Hartree-Fock term in Fig. 36-1. The result of the functional derivative is illustrated in Fig. 37-3. When two coordinates are written on one end of the interaction line, it is because there is a delta function. For example, there is a $\delta\left(5-6\right)$ for the vertical line.

Substituting back in the equation for the exact found-point function $\frac{\delta\mathcal{G}}{\delta\phi}$ Eq.(89.7), we find

$$\begin{aligned}\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi}\\ &\quad+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta\mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{5},2\right)_{\phi} &(90.2)\\ &\quad-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_{\phi}. &(90.3)\end{aligned}$$

This expression is easy to deduce from the general diagrammatic representation of the general integral equation Fig. 36-1 by replacing the irreducible vertex by that in Fig. 37-3 that follows from the Hartree-Fock approximation. This is illustrated in Fig. 37-4.

To compute a better approximation for the self-energy we will need $\delta\phi\left(2^{+},2\right)$ instead of $\delta\phi\left(3,4\right)$, as can be seen from our exact result Eq.(89.17). Although one might guess it from symmetry, we will also see that all that we will need is, $\delta\mathcal{G}\left(1,1^{+}\right)$, although it is not obvious at this point. It is quite natural however that the density-density correlation function plays an important role since it is related to the dielectric constant. From the previous equation, that special case can be written

$$\frac{\delta\mathcal{G}\left(1,1^{+}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)} = \mathcal{G}\left(1,2\right)_{\phi}\mathcal{G}\left(2,1\right)_{\phi} \tag{90.4}$$

$$+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta\mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{5},1\right)_{\phi} \tag{90.5}$$

$$-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{6},1\right)_{\phi}. \tag{90.6}$$

This equation is refered to as the generalized RPA. When the last term is neglected, this is the RPA.

90.2 Equations in momentum space with $\phi = 0$

We are ready to set $\phi = 0$. Once this is done, we can use translational invariance so that $\Sigma\left(1,2\right) = \Sigma\left(1-2\right)$ and $\mathcal{G}\left(1,2\right) = \mathcal{G}\left(1-2\right)$. In addition, spin rotational invariance implies that these objects are diagonal in spin space. We then Fourier transform to take advantage of the translational invariance. In that case, restoring spin indices we can define

$$\mathcal{G}_{\sigma}\left(k\right) = \int d\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)\int_{0}^{\beta}d\left(\tau_{1}-\tau_{2}\right)e^{-i\mathbf{k}\cdot\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)}e^{ik_{n}\left(\tau_{1}-\tau_{2}\right)}\mathcal{G}_{\sigma}\left(1-2\right) \tag{90.7}$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. For clarity then, we have explicitly written a single spin label. We thus make the following rule:

- When in position space there is an arrow representing $\mathcal{G}\left(1-2\right)$ in the translationally invariant case, in momentum space, you can think of this arrow as carrying a momentum $\mathbf{k}$.

For the potential we define

$$V_{\sigma,\sigma'}\left(q\right) = \int d\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)\int_{0}^{\beta}d\left(\tau_{1}-\tau_{2}\right)e^{-i\mathbf{q}\cdot\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)}e^{iq_{n}\left(\tau_{1}-\tau_{2}\right)}V_{\sigma,\sigma'}\left(1-2\right) \tag{90.8}$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_{n} = 2n\pi T \tag{90.9}$$

with n and integer. Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}\left(1-2\right)$ is independent of spin.

- An interaction in a diagram is represented by a dotted line. Note that because $V(1-2) = V(2-1)$, in momentum space we are free to choose the direction of $\mathbf{q}$ on the dotted line at will. Once a convention is chosen, we stick with it.

Remark 394 *General spin-dependent interaction: In more general theories, there are four spin labels attached to interaction vertices. These labels correspond to those of the four fermion fields. Here the situation is simpler because the interaction not only conserves spin at each vertex but is also spin independent.*

Whether we compute $\mathcal{G}(1-2)$ or a susceptibility $\chi(1-2)$, when we go to momentum space, it is as if we were injecting a momentum (frequency) in the diagram. It is convenient to work completely in momentum space by starting from the above position space expressions, and their diagrammatic equivalent, and now write every $\mathcal{G}(1-2)$ and $V(1-2)$ entering the internal lines of a diagram also in terms of their Fourier-Matsubara transforms, Then we consider an internal vertex, as illustrated in Fig.(37-5), where one has to do the integral over the space-time position of the vertex, say $1'$ (in addition to the spin sum). Leaving aside the spin coordinates, that behave just as in position space, the integral to perform is

$$\int d\mathbf{x}_1' \int_0^\beta d\tau_1' e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_1'} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_1'} \tag{90.10}$$

$$= (2\pi)^3 \delta(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q}) \beta\delta_{(k_{2,n}-k_{1,n}),q_n} \tag{90.11}$$

$$= V\delta_{\mathbf{k}_1-\mathbf{k}_2,\mathbf{q}}\beta\delta_{(k_{2,n}-k_{1,n}),q_n} \tag{90.12}$$

$\delta_{\mathbf{k}_1-\mathbf{k}_2,\mathbf{q}}\delta_{(k_{2,n}-k_{1,n}),q_n}$ are Kronecker delta functions. The last line is for the discrete version of momentum. Note that the sum of two fermionic Matsubara frequencies is a bosonic Matsubara frequency since the sum of two odd numbers is necessarily even. This means that the integral over τ_1' is equal to β if $k_{1,n}-k_{2,n}+q_n = 0$ while it is equal to zero otherwise because $\exp(i(k_{1,n}-k_{2,n}+q_n)\tau_1')$is periodic in the interval 0 to β. The conclusion of this is that momentum and Matsubara frequencies are conserved at each interaction vertex. In other words, we obtain the following rule:

- *The sum of all wave vectors entering an interaction vertex vanishes. And similarly for Matsubara frequencies.*

This means that a lot of the momentum integrals and Matsubara frequency sums that occur can be done by simply using conservation of momentum and of Matsubara frequencies at each vertex. We are left with the following rules:

- *One must integrate over the momenta and Matsubara frequencies that are not determined by momentum conservation.* In general, there are as many integrals to perform as there are closed loops in a diagram.
- *We must also sum over spins that appear in internal indices, conserving spin at each interaction vertex when the interaction has this property.* The propagator $\mathcal{G}_\sigma$will then be diagonal in spin index.

Suppose we have $\mathcal{G}_\sigma(1-2)$ in terms of products of various $\mathcal{G}_\sigma$ and interactions. We want to write the corresponding expression in momentum space. This means that we take the Fourier-Matsubara transform of $\mathcal{G}_\sigma(1-2)$ to obtain $\mathcal{G}_\sigma(k)$. As mentioned above, a momentum k must flow in and out.

Example 39 *Writing*

$$k = (\mathbf{k}, ik_n), \tag{90.13}$$

the Hartree-Fock approximation for the self-energy Eq.(37.1) is

$$\Sigma(k) = -\frac{1}{\mathrm{V}}\sum_{\mathbf{q}} T \sum_{n=-\infty}^{\infty} V(q)\,\mathcal{G}(k+q)\,e^{ik_n 0^+} + V(q=0)\,\frac{1}{\mathrm{V}}\sum_{\mathbf{k}} T \sum_{n=-\infty}^{\infty} e^{ik_n 0^+}\,\mathcal{G}(k) \tag{90.14}$$

The sign of the wave vector q, or direction of the arrow in the diagram, must be decided once for each diagram but this choice is arbitrary since the potential is invariant under the interchange of coordinates, as mentioned above. This is illustrated in Fig. 37-6Note that here the $q = 0$ contribution in the Hartree (so-called tadpole diagram) is cancelled by the positive ion background since $\mathcal{G}\left(\overline{2}, \overline{2^+}\right)$ is just the electron density, which is the same as the ion density. You can convince yourself that $\mathcal{G}\left(\overline{2}, \overline{2^+}\right) = \frac{1}{\mathrm{V}}\sum_{\mathbf{k}} T \sum_{n=-\infty}^{\infty} e^{ik_n 0^+}\mathcal{G}(k)$. The same convergence factor appears in the Fock term. You can understand where it comes from by retuning to the discussion that surrounds Eq. (??) above.

Example 40 *For the four-point function, there are four outside coordinates so we would need three independent outside momenta. However, all that we will need, as we shall see, are the density-density fluctuations. In other words, as we can see from the general expression for the self-energy in Fig. 36-2, we can identify two of the space-time points at the bottom of the graph. We have already written the expression in coordinates in Eq.(37.11). Writing the diagrams for that expression and using our rules for momentum conservation with a four-momentum q flowing top down, the four-point function in Fig. 37-4 becomes as illustrated in Fig. 37-7.*

90.3 Density response in the RPA

We keep following our first step approach that gave us the Hartree-Fock approximation and corresponding susceptibility. Returning to our expression for the susceptibility in terms a functional derivative

$$\begin{aligned} -\sum_{\sigma_1,\sigma_2} \frac{\delta\mathcal{G}(1,1^+)}{\delta\phi(2^+,2)} &= \sum_{\sigma_1,\sigma_2} \left\langle T_\tau \psi^\dagger\left(1^+\right)\psi(1)\,\psi^\dagger\left(2^+\right)\psi(2)\right\rangle - n^2 && (90.15)\\ &= \langle T_\tau n(1)\,n(2)\rangle - n^2 && (90.16)\\ &= \langle T_\tau\,(n(1)-n)\,(n(2)-n)\rangle \\ &= \chi_{nn}(1-2). && (90.17) \end{aligned}$$

and Fourier transforming, we obtain in the case where the irreducible vertex is obtained from functional derivatives of the Hartree-Fock self-energy the set of diagrams in Fig. 37-7. In the middle diagram on the right-hand side of the equality, there is a sum over wave vectors k' because three of the original coordinates of the functional derivative at the bottom of the diagram were different. This means there are two independent momenta, contrary to the last diagram in the figure. One of the independent momenta can be taken as q by momentum conservation while the other one, k', must be integrated over. The contribution from that middle diagram is not singular at small wave vector because the Coulomb potential is integrated over. By contrast, the last diagram has a $1/q^2$ from the interaction potential, which is divergent. We thus keep only that last term. The integral equation, illustrated in Fig. 41-3, then takes an algebraic form

$$\chi_{nn}(q) = \chi^0_{nn}(q) - \chi^0_{nn}(q) V_{\mathbf{q}} \chi_{nn}(q). \tag{90.18}$$

To figure out the sign from the figure, recall that the green triangle stands for $\frac{\delta \mathcal{G}\left(1,1^{+}\right)}{\delta \phi\left(2^{+},2\right)}$, while there is a minus sign in the equation for the susceptibility Eq. (90.17). Since the integral equation (90.18) for $\chi_{nn}(q)$ has become an algebraic equation in Fourier-Matsubara space, it is easy to solve. We find,

$$\chi_{nn}(q)=\frac{\chi^{0}_{nn}(q)}{1+V_{\mathbf{q}}\chi^{0}_{nn}(q)}=\frac{1}{\chi^{0}_{nn}(q)^{-1}+V_{\mathbf{q}}}. \tag{90.19}$$

This is the so-called Random Phase Approximation, or RPA. The last form of the equality highlights the fact that the irreducible vertex, here $V_{\mathbf{q}}$, plays the role of an irreducible self-energy in the particle-hole channel. The analytic continuation will be trivial.

Note that we have written $\chi^{0}_{nn}(q)$ for the bubble diagram, i.e. the first term on the right-hand side of the equation in Fig. 37-7 even though everything we have up to now in the Schwinger formalism are dressed Green's functions. The reason is that neglecting the middle diagram on the right-hand side of the equality is like neglecting the contribution from the Fock, or exchange self-energy in Fig. 37-6. The only term left then is is the Hartree term that we argued should vanish because of the neutralizing background. Hence, the Green's functions are bare ones and the corresponding susceptibility is the Linhard function.

Remark 395 *Equivalence to an infinite set of bubble diagrams: The integral equation for the susceptibility has turned into an algebraic equation in 90.18. By recursively replacing $\chi_{nn}(q)$ on the right-hand side of that equation by higher and higher order approximations in powers of $V_{\mathbf{q}}$ we obtain*

$$\begin{aligned}\chi^{(1)}_{nn}(q) &= \chi^{0}_{nn}(q)-\chi^{0}_{nn}(q)V_{\mathbf{q}}\chi^{0}_{nn}(q)\\ \chi^{(2)}_{nn}(q) &= \chi^{0}_{nn}(q)-\chi^{0}_{nn}(q)V_{\mathbf{q}}\chi^{0}_{nn}(q)+\chi^{0}_{nn}(q)V_{\mathbf{q}}\chi^{0}_{nn}(q)V_{\mathbf{q}}\chi^{0}_{nn}(q)\end{aligned} \tag{90.20}$$

etc. By solving the algebraic equation then, it is as if we had summed an infinite series which diagrammatically would look, if we turn it sideways, like Fig. 41-2. The analogy with the self-energy in the case of the Green's function is again clear.

90.4 Self-energy and screening in the GW approximation

We have derived in Eq.(36.13) an expression for the product $\Sigma\mathcal{G}$. When $\phi=0$ and $2=1^{+}$, this equation reduces to

$$\boxed{\Sigma\left(1,\overline{2}\right)_{\phi}\mathcal{G}\left(\overline{2},1^{+}\right)_{\phi}=V\left(1-\overline{2}\right)\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{2^{+}}\right)\psi\left(\overline{2}\right)\psi^{\dagger}\left(1^{+}\right)\psi\left(1\right)\right]\right\rangle}. \tag{90.21}$$

It shows that we should have an approximation for the self-energy that, when multiplied by $\mathcal{G}$, gives the density-density correlation function. That is a very general result, or sum-rule, is a sort of consistency relation between one- and two-particle properties. It is equivalent to Eq.(43.23). This is a very important property that we will use also later in the context of non-perturbative treatments of the Hubbard model.

To obtain an approximation for the self-energy Σ that is consistent with the density-density correlation function that we just evaluated in the RPA approximation, we return to the general expression for the self-energy Eq.(89.17) and the

corresponding pictorial representation Eq.(36-2). We replace the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$ by the one shown in Fig. 41-3 that we used to compute the density-density correlation function illustrated in Fig. 37-7. Note however that, as we did before, we keep only the terms where $V_{\mathbf{q}}$ carries a momentum $\mathbf{q}$. We neglect the next to last diagram in Fig.37-7. The other way to justify why we keep only these terms is that they are the most divergent diagrams. Their sum to infinity is however finite. We also know that by summing all diagrams to infinity, we are calculating the two-particle equivalent of a self-energy, shifting poles of the non-interacting density-density correlation function, as we should.

The final result is illustrated in Fig. 44-5. We just need to replace the functional derivative of the Green function appearing at the bottom right by the RPA series illustrated in Fig. 41-3. Recalling that the Hartree term vanishes, the final result is equivalent, when looked at sideways, to the series of bubble diagrams illustrated in Fig. 44-2.

The algebraic expression for this second level of approximation for the self-energy can be read off the figure. It takes the explicit form

$$\begin{aligned}\Sigma_{RPA}\left(\mathbf{k},ik_n\right) &= \Sigma^{(2)}\left(\mathbf{k},ik_n\right) \\ &= -\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}V_{\mathbf{q}}\left[1-\frac{V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\right]\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\end{aligned} \tag{90.22}$$

where the first term comes from the Fock contribution. The two terms can be combined into the single expression

$$\Sigma^{(2)}\left(\mathbf{k},ik_n\right)=-\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right). \tag{90.23}$$

Using our result for the longitudinal dielectric constant that follows from the density fluctuations in the RPA approximation Eq. (41.9), the last result can be written as

$$\Sigma^{(2)}\left(\mathbf{k},ik_n\right)=-\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{\varepsilon_L\left(\mathbf{q},iq_n\right)/\varepsilon_0}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right) \tag{90.24}$$

which has the very interesting interpretation that the effective interaction entering the Fock term should be the screened one instead of the bare one. The two are equal only at very high frequency. The screened potential $\frac{V_{\mathbf{q}}}{\varepsilon_L(\mathbf{q},iq_n)/\varepsilon_0}$ is often denoted W which means that the integrand is $W\mathcal{G}^0$, hence the name GW approximation. We discuss this further below.

Remark 396 *To see that this deminition makes sense, we rederive the expression for the longitudinal dielectric constant. The electric field depends on the total charge, including the induced one*

$$i\mathbf{q}\cdot\mathbf{E}=\frac{\left(\rho_e+\delta\left\langle\rho\right\rangle\right)}{\varepsilon_0}. \tag{90.25}$$

The longitudinal dielectric constant is defined by

$$i\mathbf{q}\cdot\overleftrightarrow{\epsilon^L}\cdot\mathbf{E}=\rho_e. \tag{90.26}$$

$\overleftrightarrow{\epsilon^L}$ *depends on* $\mathbf{q}$ *and* ω*, it is a retarded response function. With a longitudinal applied field, the previous two equations lead to*

$$\left(\epsilon^L\right)^{-1}=\frac{\rho_e+\delta\left\langle\rho\right\rangle}{\varepsilon_0\rho_e}. \tag{90.27}$$

The linear response to an external charge can be computed from the response to the scalar potential $\phi_e(\mathbf{q},\omega) = \rho_e/\left(q^2\varepsilon_0\right)$ *it induces*

$$\delta\left\langle\rho(\mathbf{q},\omega)\right\rangle = -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi_e(\mathbf{q},\omega) \tag{90.28}$$

so that simple substitution in the equation for $\left(\epsilon^L\right)^{-1}$ *gives,*

$$\boxed{\frac{1}{\epsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - \frac{1}{q^2\varepsilon_0}\chi^R_{\rho\rho}(\mathbf{q},\omega)\right)}. \tag{90.29}$$

The above results are recovered with $\chi^R_{\rho\rho}(q) = e^2\chi_{nn}(q)$ *and Eq.(90.19).*

90.5 Hedin's equations

How do we keep the structure of the final formula that we obtained for the self-energy, that contains an effective interaction and the dielectric constant? It is posible to formulate the general many-body problem in such a way that an effective interaction appears. The final result is the Hedin formulation. One simply separates the Irreducible vertex into a part that comes from the Hartree term, and gave RPA, and the rest. The final equations are presented pictorially in Fig.51-3 and derived in Chapter 51. The self-energy takes the general form

$$\Sigma\left(1,3\right) = -\mathcal{G}\left(1,\overline{4}\right)W\left(1,\overline{2}\right)\Gamma\left(\overline{2}^+,\overline{2};\overline{4},3\right) \tag{90.30}$$

where W is the effective interaction and Γ contains vertex corrections. These vertex corrections appear also in the expression for W. The GW approximation discussed above corresponds to approximating Γ by unity.

91. LUTTINGER-WARD FUNCTIONAL AND RELATED FUNCTIONALS

There is a very elegant formulation of the Many-Body problem that focuses on a functional of the interacting Green function instead of on a functional of source fields. The two approaches are related by a Legendre transform. This is where one encounters the so-called Luttinger-Ward functional, that plays a prominent role in defining approximations that satisfy conservation laws and in deriving Dynamical Mean-Field Theory.

The free energy as a functional of the source field ϕ is given by

$$F[\phi] = -T \ln Z[\phi] = -T \ln \mathrm{Tr}\left[e^{-\beta K} T_\tau \exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\right]. \quad (91.1)$$

The physical free energy is $F[\phi = 0]$. The derivative with respect to the source field is simply related to the Green function

$$\frac{1}{T}\frac{\delta F[\phi]}{\delta \phi(1,2)} = \mathcal{G}(2,1). \quad (91.2)$$

The last two equations can be used to define a Legendre transform where $\mathcal{G}$ is the natural variable:

$$\Omega[\mathcal{G}] = F[\phi] - \mathrm{Tr}[\phi\mathcal{G}]. \quad (91.3)$$

The trace contains a factor of temperature. More specifically, when there is time and space translational invariance,

$$\mathrm{Tr}[\cdots] = T\sum_{ik_n}\sum_{\mathbf{k}}[\cdots] \quad (91.4)$$

while in general,

$$\mathrm{Tr}[\phi\mathcal{G}] = T\phi\left(\overline{1},\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{1}\right). \quad (91.5)$$

Remark 397 *Legendre transform are usually defined between convex functions. We cannot prove continuty in our case. The best we can hope is that the Legendre transform is defined locally and check that the results make sense.*

The functional $\Omega[\mathcal{G}]$ is the so-called Kadanoff-Baym functional. As expected for Legendre transforms

$$\frac{1}{T}\frac{\delta\Omega[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = -\phi(2,1). \quad (91.6)$$

The proof is easy and can be found in Chapter 72.3.

Using the equations of motion, we have that the relation between ϕ and $\mathcal{G}$ is given by

$$\mathcal{G}^{-1}(1,2)_\phi = \mathcal{G}_0^{-1}(1,2) - \phi(1,2) - \Sigma(1,2)_\phi \quad (91.7)$$

which means that

$$\frac{1}{T}\frac{\delta\Omega[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = -\phi(2,1) = \mathcal{G}^{-1}(2,1)_\phi - \mathcal{G}_0^{-1}(2,1) + \Sigma(2,1)_\phi \quad (91.8)$$

and Dyson's equation in its usual form is satisfied only for $\phi = 0$ where the extremum principle

$$\frac{1}{T}\frac{\delta\Omega\left[\mathcal{G}\right]}{\delta G\left(1,2\right)} = 0 \tag{91.9}$$

is satisfied and where the functional $\Omega[\mathcal{G}]$ is simply equal to the free energy as follows from the definition Eq.(91.3) with $\phi = 0$.

We can guess an explicit expression for $\Omega\left[\mathcal{G}\right]$ by starting from its derivative Eq.(91.8). We obtain the so-called Baym-Kadanoff functional,

$$\Omega\left[\mathcal{G}\right] = \Phi\left[\mathcal{G}\right] - \mathrm{Tr}\left[\left(\mathcal{G}_0^{-1} - \mathcal{G}^{-1}\right)\mathcal{G}\right] + \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] \tag{91.10}$$

which gives the correct result in the non-interacting case (for the definition of $\mathcal{G}_\infty$ see Eq.(80.18)) and reduces to Eq.(91.8) when functionally differentiated, as long as

$$\frac{1}{T}\frac{\delta\Phi\left[\mathcal{G}\right]}{\delta\mathcal{G}\left(1,2\right)} = \Sigma\left(2,1\right). \tag{91.11}$$

We also need to prove that $\frac{1}{T}\frac{\delta}{\delta\mathcal{G}(1,2)}\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] = \mathcal{G}^{-1}\left(2,1\right)$. The proof evaluates the logarithm in the diagonal basis as you can see in Chapter **??**.

The functional $\Phi\left[\mathcal{G}\right]$ is the so-called Luttinger-Ward functional. We can obtain an explicit form for it by using the basic property of Legendre transforms exemplified by our example with pressure in ordinary statistical mechanics, Eq.(A.17). More specifically, multiply the potential energy term in the Hamiltonian by λ, then the physical case corresponds to $\lambda = 1$ and the general properties of Legendre transforms tell us that

$$\left.\frac{\partial\Omega_\lambda\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}} = \left.\frac{\partial F_\lambda\left[\phi\right]}{\partial\lambda}\right|_{\phi}. \tag{91.12}$$

But the explicit form of the Baym-Kadanoff functional Eq.(91.10) tells us that

$$\left.\frac{\partial\Omega_\lambda\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}} = \left.\frac{\partial\Phi_\lambda\left[\mathcal{G}\right]}{\partial\lambda}\right|_{\mathcal{G}} \tag{91.13}$$

while the derivative of the free energy is

$$\left.\frac{\partial F_\lambda\left[\phi\right]}{\partial\lambda}\right|_{\phi} = \frac{1}{\lambda}\left\langle\lambda\hat{V}\right\rangle_\lambda. \tag{91.14}$$

The average $\langle\rangle_\lambda$ means that the potential energy is averaged with the Hamiltonian where the coupling constant is multiplied by λ so that $\hat{V} \to \lambda\hat{V}$. Hence, we can obtain the Luttinger-Ward functional by a coupling constant integration

$$\Phi_\lambda\left[\mathcal{G}\right] = \int_0^1 d\lambda\frac{1}{\lambda}\left\langle\lambda\hat{V}\right\rangle_\lambda. \tag{91.15}$$

Note that since the equality of the two potentials with respect to λ, Eq.(91.12), is valid for any $\mathcal{G}$ and the corresponding ϕ, the coupling constant integration for the Luttinger-Ward functional may be evaluated for $\phi = 0$ and for $\mathcal{G}$ that satisfies the usual Dyson equation or for any $\mathcal{G}$ we wish. The average of the potential energy in the last equation is related to the density-density correlation function. The resulting integral over coupling constant gives for $\Phi_\lambda\left[\mathcal{G}\right]$ the same result that we would have obtained from the linked cluster theorem. There is a $1/n$ factor for a term of order n.

Remark 398 *Since* $\frac{1}{T}\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = \Sigma(2,1)$ *with* Σ *the sum of all one-particle irreducible skeleton diagrams,* $\Phi[\mathcal{G}]$ *is the sum of two-particle irreducible skeleton diagrams.*

For more on functionals and their relation to dynamical mean-field theory, see Chapter 77.

92. A GLANCE AT COHERENT STATE FUNCTIONAL INTEGRALS

In modern treatments of the many-body problem, one often writes an action instead of a Hamiltonian. To understand this, one first need to grasp the general idea of path integral. This is discussed in the one-particle context in Chapter 22. In this approach, one divides the time-evolution operator e^{-iHt} into infinitesimal time steps. This allows to write $e^{-iT\Delta t - iV\Delta t} \simeq e^{-iT\Delta t}e^{-iV\Delta t}$ with T and V the kinetic and potential energies respectively. Then, the amplitude to go between initial and final space-time points is proportional to the exponential of the action. Recall that the action is the time-integral of the Lagrangian.

One can do something analogous in second quantization. First, fermion coherent states are introduced in Chapter 79. To define these states, one needs the notion of anticommuting numbers, known as Grassmann numbers. Integrals and derivatives over these numbers can also be defined and all the results that involve quadratic Hamiltonians can be obtained from Gaussian integrals and derivatives over Grassmann numbers. Then in Chapter 80 you will find functional integrals where the action appears. Below, only some of the main results are mentioned.

92.1 Fermion coherent states

Let c be a fermion destruction operator, then $c\,|0\rangle = 0$ while the fermion coherent state $|\eta\rangle$ is defined as an eigenstate of the destruction operator,

$$c\,|\eta\rangle = \eta\,|\eta\rangle\,. \tag{92.1}$$

Since $c_1c_2\,|\eta_1,\eta_2\rangle = -c_2c_1\,|\eta_1,\eta_2\rangle$ the eigenvalues η must be numbers that anticommute. Namely,

$$\{\eta_1,\eta_2\} = 0. \tag{92.2}$$

Since Grassmann numbers occur only inside time-ordered products, it turns out that it suffices to define the adjoint in such a way that it also anticommutes, there is no delta function:

$$\left\{\eta,\eta^\dagger\right\} = 0. \tag{92.3}$$

Given the definition of Grassmann numbers, one can write an explicit definition of fermion coherent states in the Fock basis if we add the definition that Grassmann numbers and fermion operators also anticommute:

$$|\eta\rangle = \left(1-\eta c^\dagger\right)|0\rangle \tag{92.4}$$

Given that $\eta^2 = 0$, one can verify the defining property $c\,|\eta\rangle = \eta\,|\eta\rangle$ Eq.(92.1):

$$c\,|\eta\rangle = c\,|0\rangle + \eta cc^\dagger\,|0\rangle = \eta\,|0\rangle = \eta\left(1-\eta c^\dagger\right)|0\rangle = \eta\,|\eta\rangle\,. \tag{92.5}$$

Also, again since $\eta^2 = 0$, we can use the definition

$$|\eta\rangle = e^{-\eta c^\dagger}\,|0\rangle \tag{92.6}$$

that has the same structure as a boson coherent state.

Note that while η and $\eta^\dagger$ must be considered independent, they are nevertheless adjoint from each other. Namely, we have that

$$\langle \eta | = \langle 0 | \left(1 - c\eta^\dagger \right). \tag{92.7}$$

92.2 Grassmann calculus

All functions can only be linear in Grassmann variables. The integral over Grassmann variables resembles derivatives, namely

$$\boxed{\int d\eta = 0.} \tag{92.8}$$

$$\boxed{\int d\eta \eta = 1.} \tag{92.9}$$

The most important identity is

$$\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta} - \boldsymbol{\eta}^\dagger \mathbf{J} - \mathbf{J}^\dagger \boldsymbol{\eta}} = \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\left(\boldsymbol{\eta}^\dagger + \mathbf{J}^\dagger \mathbf{A}^{-1}\right)\mathbf{A}\left(\boldsymbol{\eta} + \mathbf{A}^{-1}\mathbf{J}\right) + \left(\mathbf{J}^\dagger \mathbf{A}^{-1} \mathbf{J}\right)}$$

$$\boxed{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-\boldsymbol{\eta}^\dagger \mathbf{A} \boldsymbol{\eta} - \boldsymbol{\eta}^\dagger \mathbf{J} - \mathbf{J}^\dagger \boldsymbol{\eta}} = \det\left(A\right) \exp\left(\mathbf{J}^\dagger \mathbf{A}^{-1} \mathbf{J}\right)} \tag{92.10}$$

where $\mathbf{A}$ is an invertible matrix while $\boldsymbol{\eta}$ and $\mathbf{J}$ are vectors of Grassmann numbers and the measure is

$$\boxed{\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta \equiv \prod_i \int d\eta_i^\dagger \int d\eta_i.} \tag{92.11}$$

Each space and imaginary-time slice has a Grassmann number associated with it. Wick's theorem can be derived rather systematically with this approach.

92.3 Recognizing the Hamiltonian in the action

As an example, let us seem how the Anderson impurity problem looks like in action formalism. We need to evaluate

$$\int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta e^{-S}$$

where the total action is

$$S = S_I + S_{Ib} + S_b \tag{92.12}$$

with the impurity action

$$\begin{aligned} S_I &= \int_0^\beta d\tau \left[\sum_\sigma \left(\psi_\sigma^\dagger(\tau) \frac{\partial}{\partial \tau} \psi_\sigma(\tau) + \varepsilon_I \psi_\sigma^\dagger(\tau) \psi_\sigma(\tau) \right) + U \psi_\uparrow^\dagger(\tau) \psi_\downarrow^\dagger(\tau) \psi_\downarrow(\tau) \psi_\uparrow(\tau) \right] \\ &= \int_0^\beta d\tau \left[\sum_\sigma \left(\psi_\sigma^\dagger(\tau) \left(-\mathcal{G}_0^{-1} \right) \psi_\sigma(\tau) \right) + U \psi_\uparrow^\dagger(\tau) \psi_\downarrow^\dagger(\tau) \psi_\downarrow(\tau) \psi_\uparrow(\tau) \right] \end{aligned} \tag{92.13}$$

and the action of the bath

$$S_b = \int_0^\beta d\tau \sum_{\mathbf{k}} \sum_\sigma \left[\eta_\sigma^\dagger (\mathbf{k},\tau) \frac{\partial}{\partial \tau} \eta_\sigma (\mathbf{k},\tau) + \varepsilon (\mathbf{k}) \eta_\sigma^\dagger (\mathbf{k},\tau) \eta_\sigma (\mathbf{k},\tau) \right] \quad (92.14)$$

$$= \int_0^\beta d\tau \sum_{\mathbf{k}} \sum_\sigma \eta_\sigma^\dagger (\mathbf{k},\tau) \left(-\mathcal{G}_b^{-1} (\mathbf{k},\tau) \right) \eta_\sigma (\mathbf{k},\tau) \quad (92.15)$$

and the contribution to the action coming from the hybridization between impurity and bath

$$S_{Ib} = \int_0^\beta d\tau \sum_{\mathbf{k}} \sum_\sigma \left[V_\sigma (\mathbf{k}) \psi_\sigma^\dagger (\tau) \eta_\sigma (\mathbf{k},\tau) + V_\sigma^* (\mathbf{k}) \eta_\sigma^\dagger (\mathbf{k},\tau) \psi_\sigma (\tau) \right]. \quad (92.16)$$

Remark 399 *In general, we change from the Hamiltonian to the above action formalism, simply by using the recipe*

$$S_I = \int_0^\beta d\tau \left[\left(\sum_\sigma \psi_\sigma^\dagger (\tau) \frac{\partial}{\partial \tau} \psi_\sigma (\tau) \right) + H \left(\psi_\sigma^\dagger (\tau), \psi_\sigma (\tau) \right) \right] \quad (92.17)$$

where we simply replace the creation operators in the original H by $\psi_\sigma^\dagger (\tau)$ and the destruction operators by $\psi_\sigma (\tau)$. In the classical formalism, $L = p\dot{q} - H$ with

$$p = \frac{\partial L}{\partial \dot{q}}. \quad (92.18)$$

For the corresponding quantum fields then, $\psi_\sigma^\dagger (\tau)$ is the conjugate field and

$$\psi_\sigma^\dagger (\tau) = \frac{\partial L}{\partial \dot{\psi}_\sigma (\tau)}. \quad (92.19)$$

Since ψ and $\psi^\dagger$ obey $\left\{ \psi (\mathbf{r}), \psi^\dagger (\mathbf{r}') \right\} = \delta (\mathbf{r} - \mathbf{r}')$ it is natural to expect that they are conjugate variables and that they should appear in the combination $\psi_\sigma^\dagger (\tau) \frac{\partial}{\partial \tau} \psi_\sigma (\tau)$ when changinf from Hamiltonian to Lagrangian.

Remark 400 *It is now clear that $-\mathcal{G}_0^{-1}$ instead of H_0 is now the basic object since it appears in the quadratic term of the action. In addition to $\partial/\partial\tau$, other imaginary-time dependent single-particle quantities can appear in $\mathcal{G}_0^{-1}$.*

Part X

Appendices

A. STATISTICAL PHYSICS AND DENSITY MATRIX

A.1 Density matrix in ordinary quantum mechanics

Quantum mechanics tells us that the expectation value of an observable O in a *normalized* state $|\psi\rangle$ is given by $\langle\psi| O |\psi\rangle$. Expanding over complete sets of states, we obtain

$$\begin{aligned} \langle\psi| O |\psi\rangle &= \sum_{i,j} \langle\psi|\ i\rangle \langle i| O |j\rangle \langle j\ |\psi\rangle & \text{(A.1)} \\ &= \sum_{i,j} \langle j\ |\psi\rangle \langle\psi|\ i\rangle \langle i| O |j\rangle & \text{(A.2)} \\ &= \sum_{i,j} \langle j| \rho |i\rangle \langle i| O |j\rangle & \text{(A.3)} \\ &= \mathrm{Tr}\,[\rho O] & \text{(A.4)} \end{aligned}$$

where the *Density Matrix* ρ is defined, as an operator, by

$$\rho \equiv |\psi\rangle \langle\psi| . \tag{A.5}$$

This is when we have a *pure* state. If the state is prepared in a statistical superposition, in other words, if we have a certain probability p_n that the state that is prepared is $|\psi_n\rangle$, then the expectation value of an observable will be given by the weighted sum of the results in each state, in other words, in the above formula for the average we should use

$$\rho \equiv \sum_n p_n |\psi_n\rangle \langle\psi_n| . \tag{A.6}$$

This is the density matrix for a *mixed state.* Note that

$$\rho^2 = \sum_{n,m} p_n p_m |\psi_n\rangle \langle\psi_n|\ \psi_m\rangle \langle\psi_m| . \tag{A.7}$$

We have the property $\rho^2 = \rho$ only for a *pure* state.

When a system of interest is in contact with an environment, it is very useful to work with an effective density matrix obtained by taking the trace first over the degrees of freedom of the environment. This idea is common in particular in the field of quantum information. By considering part of a large system as the environment, we can greatly reduce the size of the Hilbert space that needs to be considered to diagonalize a Hamiltonian, especially in one dimension. The optimal way of doing this was found by Steve White and is discussed in the context of the "Density Matrix Renormalization Group". Not so surprisingly, quantum information theory has helped to improve even further this approach. Uli Schollwöck will explain this.

A.2 Density Matrix in Statistical Physics

Statistical Physics tells us that conserved quantities play a special role. Indeed, at equilibrium, the density matrix cannot depend on time, so it depends only on conserved quantities. This means that generally, the density matrix is diagonal in the energy and number basis for example. All that is left to do is to specify p_n. The basic postulate of statistical physics is that in an isolated system, all microscopic states consistent with the value of the conserved quantities are equiprobable. This is the microcanonical ensemble where p_n is identical for all energy eigenstates $|\psi_n\rangle$. The other ensembles are derived in the usual way by considering the microcanonical system as including the system of interest and various reservoirs. In the canonical ensemble for example, $p_n = e^{-\beta E_n}/Z$ where Z is the partition function $\sum_n e^{-\beta E_n}$ and $\beta = (k_B T)^{-1}$.

Alternatively, the various ensembles are obtained by maximizing the entropy

$$S \equiv -k_B \mathrm{Tr}\left[\rho \ln \rho\right] \tag{A.8}$$

subject to constraints such as fixed average energy and normalization in the case of the canonical ensemble. Important properties of the entropy include extensivity and concavity. The entropy also plays a major role in quantum information.

A.3 Legendre transforms

Legendre transforms are encountered in mechanics when going from a Lagrangian to a Hamiltonian formulation. That transformation is extremely useful in statistical physics as well and it will be used for example by Gabi Kotliar at this School.

The important idea of statistical physics that we start with is that of potentials. If you know the entropy as a function of mechanical quantities, like energy volume and number of particles for example, then you know all the thermodynamics. Indeed,

$$dE = TdS - pdV + \mu dN \tag{A.9}$$

$$dS = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dN \tag{A.10}$$

so you can obtain temperature T, pressure p and chemical potential μ simply by taking partial derivatives of the entropy. $(1/T, S)\,(p/T, V)\,(-\mu/T, N)$ are pairs of conjugate variables. Instead of using E, V, N as independent variables, given the concavity of the entropy and the uniqueness of the equilibrium state, you can write S as a function of any three other variables. Nevertheless, the purely mechanical variables E, V, N are the most natural ones for the entropy. The entropy plays the role of a thermodynamic potential. As a function of all microscopic variables not fixed by E, V, N, it is maximum at equilibrium.

Remark 401 *When there are broken symmetries, additional variables must be added. For example, for a ferromagnet with magnetization* $\mathbf{M}$ *in a magnetic field* $\mathbf{H}$,

$$dE = TdS - pdV + \mu dN + \mathbf{M}\cdot d\mathbf{H} \tag{A.11}$$

There are other potentials. For example, if a system is in contact with a heat reservoir, the work that will be done at constant temperature will be modified by the presence of the reservoir that can absorb and give internal energy through thermal contact, i.e. in the form of heat. It is thus physically motivated to define for example the Helmholtz free energy

$$F = E - TS \tag{A.12}$$

$$T = \left(\frac{\partial E}{\partial S}\right)_{V,N} \tag{A.13}$$

In this case

$$dF = dE - SdT - TdS = -SdT - pdV + \mu dN. \tag{A.14}$$

The Helmholtz free energy F can be written in terms of any three thermodynamical variables, but T, V, N are the most natural ones. At fixed T, V, N it is the free energy that is a minimum instead of the energy because we have to take into account the reservoir. The change from S to T as a natural variable has been done through the pair of equations (A.12,A.13). This is the general structure of a Legendre transform. F and E are potentials, and the subtraction of the product of the conjugate variables $-\left(\frac{\partial E}{\partial S}\right)_{V,N} S$ does the trick of relating the two potentials

Remark 402 *Note that* $\left(\partial^2 E/\partial S^2\right) = (\partial T/\partial S) = 1/\left(\partial S/\partial T\right) = -1/\left(\partial^2 F/\partial T^2\right)$.

There is another useful definition of Legendre transform. Omitting the variables N and V that appear on both sides of the equation, we have the Legendre-Fenchel transform

$$F(T) = \min_S \widetilde{F}(E, S) \equiv \min_S \left(E(S) - TS\right). \tag{A.15}$$

This definition is valid even in the context of phase transitions where $\left(\frac{\partial E}{\partial S}\right)_{V,N}$ might not be well defined. Its equivalent is used also in the context of Luttinger-Ward and other functionals.

One of the main motivations for the definition of Legendre transforms is to find various thermodynamic quantity from a potential that reflects the actual physical situation. For example, mechanically pressure is a derivative with respect to volume. If one wants to find the pressure from the internal energy E then one needs to fix the entropy since

$$p = -\left(\frac{\partial E}{\partial V}\right)_{S,N}. \tag{A.16}$$

But if the system is not thermally isolated to keep S fixed, but is instead in contact with a heat reservoir that fixes the temperature, then the pressure must be also be computed from a derivative with respect to volume but of a different thermodynamic potential, namely

$$p = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = -\left(\frac{\partial E}{\partial V}\right)_{S,N}. \tag{A.17}$$

Analogous results hold for the chemical potential and any other thermodynamic quantity that is a derivative with respect to entropy or temperature.

Remark 403 *Connection with classical statistical mechanics: Legendre transforms are always defined between pairs of thermodynamically conjugate variables.*

In ordinary classical mechanics, let p be momentum and q be position. Then with L the Lagrangian, function of q and $\dot{q}$ the Euler Lagrange equations yield

$$\left(\frac{\partial L}{\partial \dot{q}}\right)_q = p \tag{A.18}$$

$$\left(\frac{\partial L}{\partial q}\right)_{\dot{q}} = \dot{p} \tag{A.19}$$

so that p is conjugate to $\dot{q}$ and $\dot{p}$ is conjugate to q, namely

$$dL = pd\dot{q} + \dot{p}dq. \tag{A.20}$$

A Legendre transform allows us to define a function of p and q instead of $\dot{q}$ and q, namely the Hamiltonian.

$$H = p\dot{q} - L \tag{A.21}$$

Note that derivatives with respect to the variable that is not involved in the transformation, namely q, allow us to find $\dot{p}$ from a derivative with respect to q but with different potentials and variables held constant, just as in thermodynamics, namely

$$\dot{p} = \left(\frac{\partial L}{\partial q}\right)_{\dot{q}} = -\left(\frac{\partial H}{\partial q}\right)_p. \tag{A.22}$$

A.4 Legendre transform from the statistical mechanics point of view

Note that since

$$-\frac{F}{T} = S - \frac{E}{T} \tag{A.23}$$

$$= S - \left(\frac{\partial S}{\partial E}\right)_{V,N} E \tag{A.24}$$

the quantity $-F/T$ can be seen as the Legendre transform of the microcanonical entropy. From the point of view of statistical mechanics, if we define $\Omega(E)$ as the number of microstate n corresponding to a given energy, then $p_n = 1/\Omega(E)$ for every microstate and

$$S(E) = -k_B \mathrm{Tr}\left[\rho \ln \rho\right] = -k_B \sum_n \frac{1}{\Omega(E)} \ln \frac{1}{\Omega(E)} \tag{A.25}$$

$$= k_B \ln \Omega(E) \tag{A.26}$$

So, from the point of view of statistical mechanics, the Legendre transform of the entropy is obtained from

$$-\frac{F}{T} = k_B \ln Z = k_B \ln \sum_n e^{-\beta E_n} \tag{A.27}$$

$$= k_B \ln \sum_E \Omega(E) e^{-\beta E} \tag{A.28}$$

$$= k_B \ln \sum_E e^{\ln \Omega(E)} e^{-\beta E} \tag{A.29}$$

$$= k_B \ln \sum_E e^{(S(E) - E/T)/k_B} \tag{A.30}$$

Whereas the microcanonical entropy is a function of the energy of microstates, its Legendre transform is summed over energy and is a function of $1/T$, the coefficient of E in both the thermodynamical expression of the Legendre transform Eq.(A.25) and the statistical one Eq.(A.30).

We know that

$$\begin{aligned} \langle E \rangle &= -\frac{\partial \ln Z}{\partial \beta} \\ &= -\frac{\partial \left(-F/T\right)}{\partial \left(1/T\right)} \end{aligned} \tag{A.31}$$

which clarifies the connection between the statistical mechanical and thermodynamical definitions of Legendre transform. E in the case of thermodynamics is really the average energy from the statistical mechanical point of view. The last equation could have been written down directly from the statistical expression for $-F/T$.

Finally, note that a saddle point evaluation of the sum over energy appearing in the partition function Eq.(A.30) leads to

$$\frac{-F\left(T\right)}{T} = \sup_{E} \left(S\left(E\right) - \frac{E}{T} \right) \tag{A.32}$$

which is another version of Eq.(A.15).

B. SECOND QUANTIZATION

B.1 Describing symmetrized or antisymmetrized states

States that describe identical particles must be either symmetrized, for bosons, or antisymmetrized, for fermions. To simplify the calculations, it is useful to use second quantization. As its name suggest, there is also an axiomatic way to introduce this method as a quantization of fields but here we will just introduce it as a calculational tool. The approach will be familiar already if you master ladder operators for the harmonic oscillator.

For definiteness, let us concentrate on fermions. This can be translated for bosons. Define the operator $\psi^\dagger(\mathbf{r})$ that creates a particle in a position eigenstate $|\mathbf{r}\rangle$ and antisymmetrizes the resulting wave function. Define also the vacuum state $|0\rangle$ that is destroyed by the adjoint, namely $\psi(\mathbf{r})|0\rangle = 0$. In this language

$$\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')|0\rangle = \frac{1}{\sqrt{2}}\left(|\mathbf{r}\rangle|\mathbf{r}'\rangle - |\mathbf{r}'\rangle|\mathbf{r}\rangle\right) \tag{B.1}$$

$$\equiv |\mathbf{r},\mathbf{r}'\rangle = -|\mathbf{r}',\mathbf{r}\rangle\,. \tag{B.2}$$

The state to the right is clearly normalized and antisymmetric. There are two copies of the one-particle Hilbert space. In one component of the wave function, the particle in the first copy is at $|\mathbf{r}\rangle$, in the other component the particle in the first copy is at $|\mathbf{r}'\rangle$. Clearly, that can become quite complicated. The two body-wave function $\langle\mathbf{r},\mathbf{r}'|\varphi\rangle$ is antisymmetric and in the case where there are only two one-particle states occupied it is a Slater determinant. Clearly, that becomes a mess. In terms of the creation-annihilation operators however, all we need to know is that by definition of these operators,

$$\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}') + \psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r}) = 0. \tag{B.3}$$

We use the short-hand for anticommutation

$$\left\{\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\} = 0. \tag{B.4}$$

Taking the adjoint,

$$\{\psi(\mathbf{r}),\psi(\mathbf{r}')\} = 0. \tag{B.5}$$

The only thing missing is that

$$\left\{\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}')\,. \tag{B.6}$$

That is a bit more complicated to show, but let us take it for granted. It is clear that if $\psi^\dagger(\mathbf{r})$ creates a particle, then $\psi(\mathbf{r})$ removes one (or destroys it). If the particles are at different positions, that can be done in any order. If $\mathbf{r} = \mathbf{r}'$, then it will matter if we create a particle before destroying it. If the creation occurs before the destruction, there will be one more particle to destroy. The Dirac delta function comes from normalization in the continuum. For discrete basis, we would have unity on the right.

B.2 Change of basis

A key formula for the "field" operators $\psi^{\dagger}(\mathbf{r})$ is the formula for basis change. Suppose that one has a new complete basis of one-particle states $|\alpha\rangle$. Then, we can change basis as follows:

$$|\mathbf{r}\rangle = \sum_{\alpha} |\alpha\rangle \langle\alpha| \mathbf{r}\rangle \tag{B.7}$$

Given the definition of creation operators, the creation operator $\psi^{\dagger}(\mathbf{r})$ for a particle in state $|\mathbf{r}\rangle$ is related to the creation operator $c_{\alpha}^{\dagger}$ for a particle in state $|\alpha\rangle$ by the analogous formula, namely

$$\psi^{\dagger}(\mathbf{r}) = \sum_{\alpha} c_{\alpha}^{\dagger} \langle\alpha| \mathbf{r}\rangle . \tag{B.8a}$$

This formula is quite useful.

B.3 Second quantized version of operators

B.3.1 One-body operators

If we know the matrix elements of an operator in the one-particle basis, the calculation of any observable can be reduced to some algebra with the creation-annihilation operators. In other words, not only states, but also operators corresponding to observables can be written using creation-annihilation operators. The expression for these operators is independent of the number of particles and formally analogous to the calculation of averages of operators in first quantized notation.

To be more specific, consider the operator for the density of particles at position $|\mathbf{r}\rangle$. It can be written as $\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})$ as we prove now. Since $ABC - CAB = ABC + ACB - ACB - CAB$ the commutator ot this operator with $\psi^{\dagger}(\mathbf{r}')$ is,

$$\begin{aligned}\left[\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}), \psi^{\dagger}(\mathbf{r}')\right] &= \psi^{\dagger}(\mathbf{r})\left\{\psi(\mathbf{r}), \psi^{\dagger}(\mathbf{r}')\right\} - \left\{\psi^{\dagger}(\mathbf{r}), \psi^{\dagger}(\mathbf{r}')\right\}\psi(\mathbf{r}) &\text{(B.9)}\\ &= \delta(\mathbf{r}-\mathbf{r}')\psi^{\dagger}(\mathbf{r}) &\text{(B.10)}\end{aligned}$$

We can now use the following little "theorem" on commutator of ladder operators:

Theorem 41 *If $[A,B] = \beta B$ and $|\alpha\rangle$ is an eigenstate of A with eigenvalue α, then $B|\alpha\rangle$ is an eigenstate of A with eigenvalue $\alpha+\beta$, as follows from $AB|\alpha\rangle - BA|\alpha\rangle = A(B|\alpha\rangle) - \alpha(B|\alpha\rangle) = \beta(B|\alpha\rangle)$.*

Since $\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})|0\rangle = 0$, the above implies that $\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})\left(\psi^{\dagger}(\mathbf{r}_1)|0\rangle\right) = \delta(\mathbf{r}-\mathbf{r}_1)\left(\psi^{\dagger}(\mathbf{r}_1)|0\rangle\right)$, and generally a state $\psi^{\dagger}(\mathbf{r}_1)\psi^{\dagger}(\mathbf{r}_2)\ldots|0\rangle$ is an eigenstate of $\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})$ with eigenvalue $\delta(\mathbf{r}-\mathbf{r}_1) + \delta(\mathbf{r}-\mathbf{r}_2) + \ldots$ Clearly, the potential energy of identical electrons in a potential $V(\mathbf{r})$ can be written

$$\int \psi^{\dagger}(\mathbf{r}) V(\mathbf{r}) \psi(\mathbf{r}) d^3\mathbf{r}. \tag{B.11}$$

The same reasoning leads to the kinetic energy in the momentum basis, where it is diagonal

$$\int c^{\dagger}(\mathbf{k}) \frac{\hbar^2 \mathbf{k}^2}{2m} c(\mathbf{k}) \frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{B.12}$$

Returning to the position-space basis, we obtain

$$\int \psi^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m}\right) \psi(\mathbf{r}) d^3\mathbf{r}. \tag{B.13}$$

In other words, for any one-body operator, we can always obtain its second-quantized form in the one-particle basis $|\alpha\rangle$ where it is diagonal:

$$\sum_{\alpha} c_{\alpha}^{\dagger} \langle\alpha| O |\alpha\rangle c_{\alpha} = \sum_{\alpha,\beta} c_{\alpha}^{\dagger} \langle\alpha| O |\beta\rangle c_{\beta}. \tag{B.14}$$

If we change to an arbitrary basis

$$|\alpha\rangle = \sum_{i} |i\rangle \langle i| \alpha\rangle \tag{B.15}$$

the operator takes the form

$$\sum_{\alpha,\beta} c_{\alpha}^{\dagger} \langle\alpha| O |\beta\rangle c_{\beta} = \sum_{\alpha,i,j} c_{\alpha}^{\dagger} \langle\alpha| i\rangle \langle i| O |j\rangle \langle j| \alpha\rangle c_{\alpha} = \sum_{i,j} c_{i}^{\dagger} \langle i| O |j\rangle c_{j}. \tag{B.16}$$

Example 42 *Let $\psi_{\alpha}^{\dagger}(\mathbf{r})$ be the creation operator for the position state $|\mathbf{r}\rangle$ with the spin $\alpha = \uparrow, \downarrow$. We know the matrix elements of all component of the spin operators in the basis where S_z is diagonal. Thus, from the last formula, we see that the three components of the spin operator are*

$$\int \psi_{\alpha}^{\dagger}(\mathbf{r}) \left(\frac{\hbar}{2} \boldsymbol{\sigma}_{\alpha\beta}\right) \psi_{\beta}(\mathbf{r}) d^3\mathbf{r} \tag{B.17}$$

where, as usual, the Pauli matrices are given by $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

B.3.2 Two-body operators

Let us now consider a two-body operator such as the potential energy. It is diagonal in position-space. The Coulomb interaction

$$V_c(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \tag{B.18}$$

is an example. The second quantized Coulomb energy takes the form

$$\int V_c(\mathbf{r} - \mathbf{r}') \frac{1}{2} \left(\rho(\mathbf{r}) \rho(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r})\right) d^3\mathbf{r} d^3\mathbf{r}' \tag{B.19}$$

where the $1/2$ comes from avoiding double-counting and $\delta(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r})$ is necessary not to count the interaction of an electron with itself. Including spin, the density operator is

$$\rho(\mathbf{r}) = \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}). \tag{B.20}$$

Substituting in the expression for the Coulomb interaction and using anti-commutation relations, we obtain

$$\frac{1}{2}\sum_{\sigma,\sigma'}\int V_c\left(\mathbf{r}-\mathbf{r}'\right)\psi_\sigma^\dagger\left(\mathbf{r}\right)\psi_{\sigma'}^\dagger\left(\mathbf{r}'\right)\psi_{\sigma'}\left(\mathbf{r}'\right)\psi_\sigma\left(\mathbf{r}\right)d^3\mathbf{r}d^3\mathbf{r}'. \tag{B.21}$$

It is an interesting and not very long exercise to prove that formula (which happens to have the same form for bosons and fermions).

Let us change to some arbitrary basis. First notice that in terms of the potential energy operator $\hat{V}_c$

$$V_c\left(\mathbf{r}-\mathbf{r}'\right)=\left\langle\mathbf{r}\right|\left\langle\mathbf{r}'\right|\hat{V}_c\left|\mathbf{r}\right\rangle\left|\mathbf{r}'\right\rangle. \tag{B.22}$$

Then, the change of basis

$$\psi_\sigma^\dagger\left(\mathbf{r}\right)=\sum_i c_{i\sigma}^\dagger\left\langle i\right|\left.\mathbf{r}\right\rangle. \tag{B.23a}$$

leads to the following two-particle analog of the one-body operator Eq.(B.16) in an arbitrary basis

$$\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\left\langle i\right|\left\langle j\right|\hat{V}_c\left|k\right\rangle\left|l\right\rangle c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma'}c_{k\sigma}. \tag{B.24}$$

C. HARTREE-FOCK APPROXIMATION

The Hartree-Fock approximation is the simplest approximation to the many-body problem. It is a mean-field theory of the full Hamiltonian, that we will call "The theory of everything". We will begin by writing it explicitely then proceed with two theorems that form the basis of this approximation.

C.1 The theory of everything

Gathering the results of the previous section, an electron gas interacting with a *static* lattice takes the form

$$\begin{aligned} H_{toe} &= \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V_{c,e-i}(\mathbf{r}) \right) \psi_{\sigma}(\mathbf{r}) \, d^3\mathbf{r} \\ &\quad + \frac{1}{2} \sum_{\sigma,\sigma'} \int V_c(\mathbf{r}-\mathbf{r}') \, \psi_{\sigma}^{\dagger}(\mathbf{r}) \, \psi_{\sigma'}^{\dagger}(\mathbf{r}') \, \psi_{\sigma'}(\mathbf{r}') \, \psi_{\sigma}(\mathbf{r}) \, d^3\mathbf{r} d^3\mathbf{r}' \end{aligned} \quad \text{(C.1)}$$

where $V_{c,e-i}(\mathbf{r})$ is the electron-ion Coulomb potential. The dynamics of the ions (phonons) can be added to this problem, but until the rest of these introductory notes, we shall take the lattice as static. We need the to allow the lattice to move and to include spin-orbit interactions to have the complete "theory of everything" we want to solve. But the above is certainly a non-trivial start.

C.2 Variational theorem

The Ritz variational principle states that any normalized wave function satisfies

$$\langle \psi | H | \psi \rangle \geq \langle \psi_0 | H | \psi_0 \rangle \quad \text{(C.2)}$$

where $|\psi_0\rangle$ is the ground state wave function.
Proof. That follows easily by expanding $|\psi\rangle = \sum_i a_i |\psi_i\rangle$, where $H|\psi_i\rangle = E_i |\psi_i\rangle$, and using $E_0 \leq E_i$:

$$\begin{aligned} \langle \psi | H | \psi \rangle &= \sum_{i,j} a_j^* a_i \langle \psi_j | H | \psi_i \rangle = \sum_i |a_i|^2 E_i \\ &\geq E_0 \sum_i |a_i|^2 = \langle \psi_0 | H | \psi_0 \rangle \end{aligned} \quad \text{(C.3)}$$

■

In the Hartree Fock approximation, we use the variational principle to look for the best one-body Green function for H_{toe}. In other words, we use our formula

for a change of basis (there is no sum on repeated spin index here)

$$\psi_{\sigma}^{\dagger}(\mathbf{r}) = \sum_{i} c_{i\sigma}^{\dagger} \langle i,\sigma|\, \mathbf{r},\sigma\rangle = \sum_{i} c_{i\sigma}^{\dagger} \phi_{i\sigma}^{*}(\mathbf{r}) \tag{C.4}$$

$$c_{i\sigma}^{\dagger} = \int d^{3}\mathbf{r}\psi_{\sigma}^{\dagger}(\mathbf{r}) \langle \mathbf{r},\sigma|\, i,\sigma\rangle = \int d^{3}\mathbf{r}\psi_{\sigma}^{\dagger}(\mathbf{r}) \phi_{i\sigma}(\mathbf{r}) \tag{C.5}$$

and write our ground state wave function as

$$|\psi_{HF}\rangle = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} \ldots c_{N/2\uparrow}^{\dagger} c_{N/2\downarrow}^{\dagger} |0\rangle . \tag{C.6}$$

Our variational parameters are the one-particle Green functions $\phi_{\sigma}^{*}(\mathbf{r})$. Note that the most general wave function would be a linear combination of wave functions of the type $|\psi_{HF}\rangle$, each with different one-particle states occupied.

C.3 Wick's theorem

To compute $\langle\psi_{HF}| H |\psi_{HF}\rangle$, we expand each of the creation-annihilation operators in the Hamiltonian Eq.(C.1) in the basis we are looking for, using the change of basis formula Eq.(C.4). Consider first the quadratic term and focus on the second quantized operators. We need to know

$$\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle \tag{C.7}$$

The key to compute such matrix elements is to simply use the anticommutation relations for the creation-annihilation operators and the fact that annihilation operators acting on the vacuum give zero. Let us do this slowly.

The anticommutation relations for the operators $c_{i\sigma}^{(\dagger)}$ are as follows:

$$\left\{c_{i\sigma}, c_{j\sigma'}^{\dagger}\right\} = \int d^{3}\mathbf{r} \int d^{3}\mathbf{r}' \phi_{i\sigma}^{*}(\mathbf{r}) \left\{\psi_{\sigma}(\mathbf{r}), \psi_{\sigma'}^{\dagger}(\mathbf{r}')\right\} \phi_{j\sigma'}(\mathbf{r}') \tag{C.8}$$

$$= \int d^{3}\mathbf{r} \phi_{i\sigma}^{*}(\mathbf{r}) \phi_{j\sigma'}(\mathbf{r}) = \delta_{i,j}\delta_{\sigma,\sigma'} \tag{C.9}$$

so

$$\langle 0| c_{i\uparrow} c_{i\uparrow}^{\dagger} |0\rangle = 1 - \langle 0| c_{i\uparrow}^{\dagger} c_{i\uparrow} |0\rangle = 1. \tag{C.10}$$

Generalizing this reasoning, we see that $\langle\psi_{HF}|\, \psi_{HF}\rangle = 1$. Now, $\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle$ will vanish if either i or j are not in the list of occupied states in $|\psi_{HF}\rangle$ since $c_{i\uparrow}^{\dagger}$ also annihilates the vacuum in the bra. If i and j are both in the list of occupied states, $\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle = \delta_{i,j}$ since $c_{j\uparrow}$ will remove a particle in state j in $|\psi_{HF}\rangle$ while $c_{i\uparrow}^{\dagger}$ will remove a particle in state i in $\langle\psi_{HF}|$. If the list of particles is not the same in the bra and in the ket, the annihilation operators can be anticommuted directly to the vacuum and will destroy it. With this, we have that

$$\langle\psi_{HF}| \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^{2}\boldsymbol{\nabla}^{2}}{2m} + V_{c,e-i}(\mathbf{r})\right) \psi_{\sigma}(\mathbf{r})\, d^{3}\mathbf{r} |\psi_{HF}\rangle \tag{C.11}$$

$$= \sum_{\sigma} \sum_{i=1}^{N/2} \int \phi_{i\sigma}^{*}(\mathbf{r}) \left(-\frac{\hbar^{2}\boldsymbol{\nabla}^{2}}{2m} + V_{c,e-i}(\mathbf{r})\right) \phi_{i\sigma}(\mathbf{r})\, d^{3}\mathbf{r}. \tag{C.12}$$

To compute the expectation value of the interacting part of H_{toe} we need

$$\langle\psi_{HF}| c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{k\sigma'} c_{l\sigma} |\psi_{HF}\rangle . \tag{C.13}$$

Since $|\psi_{HF}\rangle$ is a direct product of wave functions for up and down spins, if the spins are different, we obtain

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k}. \tag{C.14}$$

If the spins are identical, something new happens. If the conditions $k = l$ or $i = j$ are satisfied, the expectation value vanishes because of the anticommutation relations (Pauli principle). Consider k different from l. Since all we need is that the list of states created be the same as the list of states destroyed there are two possibilities

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma}c_{k\sigma}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l}. \tag{C.15}$$

The last contribution is known as the exchange contribution. The difference in sign comes from the anticommutation. All these results, including the cases $k = l$ or $i = j$ for same spin, can be summarized by

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l}\delta_{\sigma,\sigma'}. \tag{C.16}$$

The last result can be written as

$$\begin{aligned}\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle \;&=\; \langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c_{l\sigma}\,|\psi_{HF}\rangle\,\langle\psi_{HF}|\, c^{\dagger}_{j\sigma'}c_{k\sigma'}\,|\psi_{HF}\rangle &\text{(C.17)}\\ &\quad - \langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c_{k\sigma'}\,|\psi_{HF}\rangle\,\langle\psi_{HF}|\, c^{\dagger}_{j\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle. &\text{(C.18)}\end{aligned}$$

A four point correlation function has been factored into a product of two-point correlation functions. For states such as $|\psi_{HF}\rangle$ that are single-particle states, creation operators are "contracted" in all possible ways with the destruction operators. This elegant form is a special case of Wick's theorem. It applies to expectation values of any number of creation and annihilation operators. The signs follow from anticommutation.

C.4 Minimization and Hartree-Fock equations

Using Wick's theorem Eq.(C.16) and proceeding with the Coulomb interaction between electrons as we did with the one-body part of the Hamiltonian in Eq.(C.12) we obtain

$$\begin{aligned}\langle\psi_{HF}|\, H_{toe}\,|\psi_{HF}\rangle &= \sum_{\sigma}\sum_{i=1}^{N/2}\int \phi^{*}_{i\sigma}(\mathbf{r})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V_{c,e-i}(\mathbf{r})\right)\phi_{i\sigma}(\mathbf{r})\,d^3\mathbf{r}\\ &+ \sum_{\sigma,\sigma'}\sum_{i=1}^{N/2}\sum_{j=1}^{N/2}\frac{1}{2}\int V_c(\mathbf{r}-\mathbf{r}')\left[\phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r})\,\phi^{*}_{j\sigma'}(\mathbf{r}')\,\phi_{j\sigma'}(\mathbf{r}')\right. &\text{(C.19)}\\ &\left. - \delta_{\sigma,\sigma'}\phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r}')\,\phi^{*}_{j\sigma'}(\mathbf{r}')\,\phi_{j\sigma'}(\mathbf{r})\right]d^3\mathbf{r}d^3\mathbf{r}'. &\text{(C.20)}\end{aligned}$$

To find our variational parameters, namely the functions $\phi_{i\sigma}(\mathbf{r})$, we minimize the above, subject to the constraint that the wave functions must be orthonormalized. This means that we take partial derivatives with respect to all variables in the above expression. We satisfy the constraints

$$\int \phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{j\sigma'}(\mathbf{r})\,d^3\mathbf{r} - \delta_{i,j}\delta_{\sigma,\sigma'} = 0 \tag{C.21}$$

using Lagrange multipliers. We have to think of $\phi^{*}_{i\sigma}(\mathbf{r})$ and $\phi_{i\sigma}(\mathbf{r})$ as independent variables defined at each different position $\mathbf{r}$ and for each index i, σ. To take the

partial derivatives carefully, one should discretize space and take the limit but the final result is pretty obvious. All we need to know is that what replaces the partial derivative in the continuum version is the functional derivative

$$\frac{\delta\phi_{i\sigma}(\mathbf{r})}{\delta\phi_{j\sigma'}(\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}')\,\delta_{i,j}\delta_{\sigma,\sigma'} \tag{C.22}$$

$$\frac{\delta\phi^*_{i\sigma}(\mathbf{r})}{\delta\phi_{j\sigma'}(\mathbf{r}')} = 0. \tag{C.23}$$

The result of the minimization with respect of $\phi^*_{i\sigma}(\mathbf{r})$ is straightforward. One obtains

$$\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+V_{c,e-i}(\mathbf{r})\right)\phi_{i\sigma}(\mathbf{r})+V_H(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r})-\int d^3\mathbf{r}'V_{ex}(\mathbf{r},\mathbf{r}')\,\phi_{i\sigma}(\mathbf{r}')$$

$$= \sum_{i=1}^{N/2}\gamma_{ij}\phi_{j\sigma}(\mathbf{r}) \tag{C.24}$$

$$V_H(\mathbf{r}) = \int d^3\mathbf{r}'V_c(\mathbf{r}-\mathbf{r}')\sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r})\right|^2 \tag{C.25}$$

$$V_{ex}(\mathbf{r},\mathbf{r}') = V_c(\mathbf{r}-\mathbf{r}')\sum_{j=1}^{N/2}\phi^*_{j\sigma}(\mathbf{r}')\,\phi_{j\sigma}(\mathbf{r}). \tag{C.26}$$

The matrix γ_{ij} is a real symmetric matrix of Lagrange multipliers. Diagonalizing γ_{ij} and writing the eigenvalues ε_i, the above equation looks like a Schrödinger equation. The Hartree contribution $V_H(\mathbf{r})$ has the physical interpretation that each electron interacts with the average density of the other electrons

$$n(\mathbf{r}) = \sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r})\right|^2. \tag{C.27}$$

The exchange contribution $V_{ex}(\mathbf{r},\mathbf{r}')$ has no classical analog. It comes from the anticommutation of indistinguishible particles. The ε_i can be interpreted as single-particle excitation energies only if removing a particle does not modify too much the effective potentials.

D. MODEL HAMILTONIANS

D.1 Heisenberg and t-J model

Consider the Hubbard Hamiltonian, supposing that we are in the limit where U is much larger than the bandwidth. One expects that in low energy eigenstates, single-particle Wannier states will be either empty or occupied by a spin up or a spin down electron and that double occupation will be small. If we could write an effective Hamiltonian valid at low energy, that means that we would reduce the size of the Hilbert space from roughly 4^N to 3^N for an N site lattice. This is possible. The effective Hamiltonian that one obtains in this case is the $t-J$ model, which becomes the Heisenberg model at half-filling.

To obtain this model, one can use canonical transformations or equivalently degenerate perturbation theory. Although both approches are equivalent, the one that is most systematic is the canonical transformation approach. Nevertheless, we will see a simplified version of the degenerate perturbation theory approach since it is sufficient for our purpose and simpler to use.

We start from the point of view that the unperturbed part of the Hamiltonian is the potential energy. If there is no hopping, the ground state has no double occupancy and it is highly degenerate since the spins can take any orientation. Hopping will split this degeneracy. Let us write the eigenvalue problem for the Hubbard Hamiltonian in the block form

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E \begin{pmatrix} X \\ Y \end{pmatrix} \tag{D.1}$$

where H_{11} contains only terms that stay within the singly occupied subspace, H_{12} and H_{21} contains hopping that links the singly occupied subspace with the other ones and H_{22} contains terms that connect states where there is double occupancy. Formally, this separation can be achieved using projection operators. To project a state in the singly occupied subspace, one uses $H_{11} = PHP$ where the projector P is

$$P = \prod_{i=1}^{N} \left(1 - n_{i\uparrow} n_{i\downarrow}\right). \tag{D.2}$$

Returning to the block form of the Hamiltonian, we can solve for $Y = \left(E - H_{22}\right)^{-1} H_{21} X$ and write

$$\left(H_{11} + H_{12} \left(E - H_{22}\right)^{-1} H_{21}\right) X = EX. \tag{D.3}$$

What save us here is that the eigenstates we are looking for are near $E = 0$ whereas H_{22} will act on states where there is one singly occupied state since the hopping term in H_{12} can at most create one doubly occupied state from a state with no double occupation. The leading term in H_{22} will thus simbply give a contribution U which is large compared to E. We are left with the eigenvalue problem

$$\left(H_{11} - \frac{H_{12} H_{21}}{U}\right) X = EX. \tag{D.4}$$

The first part of the Hamiltonian H_{11} contains only hopping between states where no site is doubly occupied. The potential energy in those states vanishes.

The quantity $H_{12}H_{21}$ can be computed as follows. The only term of the original Hamiltonian that links singly and doubly occupied states is the hopping part. Let us consider only nearest neighbor hopping with $t_{ij} = -t$. Then

$$H_{12}H_{21} = t^2 \sum_{\langle ij\rangle\sigma} \sum_{\langle kl\rangle\sigma'} \left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right)\left(c^\dagger_{k\sigma'}c_{l\sigma'} + h.c.\right) \tag{D.5}$$

where each nearest-neighbor bond $\langle ij\rangle$ is counted only once in the sum. Since we leave from a state with singly occupied sites and return to a state with singly occupied sites, $\langle kl\rangle = \langle ij\rangle$ survives as well as cases such as $\langle kl\rangle = \langle il\rangle$ if one of the sites i is empty in the initial state. The latter contribution is called correlated hopping. It describes second-neighbor hopping through a doubly occupied state. In the $t-J$ model, this term is often neglected on the grounds that it is proportional to t^2/U whereas H_{11} is of order t. That is not necessarily a good reason to neglect this term.

Let us return to the contribution coming from $\langle kl\rangle = \langle ij\rangle$. Discarding terms that destroy two particles on the same site, we are left with only

$$-\frac{H_{12}H_{21}}{U} = -\frac{t^2}{U}\sum_{\langle ij\rangle\sigma\sigma'}\left(c^\dagger_{i\sigma}c_{j\sigma}Qc^\dagger_{j\sigma'}c_{i\sigma'} + i \leftrightarrow j\right) \tag{D.6}$$

where Q is the projection operator that makes sure that the intermediate state is doubly occupied. We have to consider four spin configurations for the neighboring sites i and j . The configurations $|i\uparrow\rangle\ |j\uparrow\rangle$ and $|i\downarrow\rangle\ |j\downarrow\rangle$ do not contribute since the intermediate state is prohibited by the Pauli principle. The configuration $|i\uparrow\rangle\ |j\downarrow\rangle$ when acted upon by the first term in the last equation Eq.(D.6) has non-zero matrix elements with two possible finite states, $\langle i\uparrow|\langle j\downarrow|$ and $\langle i\downarrow|\langle j\uparrow|$. The matrix element has the value $-t^2/U$ for the first case and t^2/U for the configuration where the spins have been exchanged because of the fermionic nature of the states. The configuration $|i\downarrow\rangle\ |j\uparrow\rangle$ has the corresponding possible final states. And the $i \leftrightarrow j$ term in Eq.(D.6) just doubles the previous results, in other words the magnitude of the non-zero matrix elements is $2t^2/U$. Since only spins are involved, all we need to do is to find spin operators that have exactly the same matrix elements.

What we are looking for is

$$\frac{4t^2}{U\hbar^2}\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{\hbar^2}{4}n_in_j\right) = J\sum_{\langle ij\rangle}\left(S^z_iS^z_j + \frac{1}{2}\left(S^+_iS^-_j + S^-_iS^+_j\right) - \frac{\hbar^2}{4}n_in_j\right) \tag{D.7}$$

where $J \equiv 4t^2/U\hbar^2$. Indeed, if the neighboring spins are parallel, the quantity $S^+_iS^-_j + S^-_iS^+_j$ has zero expectation value while the expectation of $S^z_iS^z_j$, namely $\hbar^2/4$, is cancelled by the expectation of $-\hbar^2n_in_j/4$. For antiparallel spins, $S^z_iS^z_j - \hbar^2n_in_j/4$ has expectation value $-\hbar^2/2$ between configurations where the spins do not flip while $\frac{1}{2}\left(S^+_iS^-_j + S^-_iS^+_j\right)$ has vanishing matrix elements. In the case where the spins flip between the initial and final state, only $\frac{1}{2}\left(S^+_iS^-_j + S^-_iS^+_j\right)$ has non-zero expectation value and it is equal to $\hbar^2/2$. With the definition of J given, this corresponds to the matrix elements we found above.

This is the form of the Heisenberg Hamiltonian. Including the correlated hopping term, the $t-J$ Hamiltonian takes the following form

$$\begin{aligned} H &= P\left[\sum_{\langle ij\rangle\sigma} t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{\hbar^2}{4}n_in_j\right)\right]P \\ &\quad + P\left[-\frac{J}{4}\sum_{i,k\neq k'}\left(c^\dagger_{i,-\sigma}c_{j,-\sigma}c^\dagger_{j+k,\sigma}c_{j+k',\sigma} + c^\dagger_{j+k,-\sigma}c^\dagger_{i,-\sigma}c_{j,-\sigma}c_{j+k',\sigma}\right)\right]P \end{aligned} \tag{D.8}$$

where the last term is the three-site hopping term that is usually neglected.

It is remarkable, but expected, that at half-filling the effective Hamiltonian is a spin-only Hamiltonian (The first term in the above equation does not contribute when there is no hole because of the projection operators). From the point of view of perturbation theory, the potential energy is the large term. We are in an insulating phase and hopping has split the spin degeneracy.

Classically, the ground state on a hypercubic lattice would be an antiferromagnet. This mechanism for antiferromagnetism is known as *superexchange*.

In closing, one should remember that to compute the expectation value of any operator in the singly occupied space, one must first write it in block form, in other words, one should not forget the contribution from the Y component of the wave function. *For example, the kinetic energy $\langle K\rangle$ of the Hubbard model calculated in the low energy subspace will be equal to minus twice the potential energy $\langle V\rangle$.* That can be seen from

$$\langle K\rangle = (X\ Y)\,K\begin{pmatrix} X \\ Y \end{pmatrix} = (XKY)+(YKX) = -\frac{2}{U}\,(X\ KK\ X) \quad \text{(D.9)}$$

$$\langle V\rangle = (X\ Y)\,V\begin{pmatrix} X \\ Y \end{pmatrix} = (YVY) = +\frac{1}{U}\,(X\ KK\ X) \quad \text{(D.10)}$$

since in the intermediate state, V gives the eigenvalue U in all intermediate states.

D.2 Anderson lattice model

In the Anderson lattice model, on purely phenomenological grounds one considers localized states $\left(f^\dagger_{i\sigma}\right)$ with a Hubbard U, hybridized with a conduction band $\left(c^\dagger_{\mathbf{k}\sigma}\right)$ of non-interacting electrons. This model is particularly useful for heavy fermions, for example, where one can think of the localized states as being f electrons:

$$H_A = H_f + H_c + H_{fc} \quad \text{(D.11)}$$

$$H_f \equiv \sum_\sigma \sum_i \varepsilon f^\dagger_{i\sigma} f_{i\sigma} + \sum_i U\left(f^\dagger_{i\uparrow} f_{i\uparrow}\right)\left(f^\dagger_{i\downarrow} f_{i\downarrow}\right) \quad \text{(D.12)}$$

$$H_c \equiv \sum_\sigma \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \quad \text{(D.13)}$$

$$H_{fc} \equiv \sum_\sigma \sum_i V_i c^\dagger_{i\sigma} f_{i\sigma} + h.c. \quad \text{(D.14)}$$

In the case where there is only one site with f electrons, one speaks of the Anderson impurity model. When U is large, one can proceed as for the $t-J$ Hamiltonian and obtain an effective model where there is no double occupancy of the impurity and where the spin of the conduction electrons interacts with the spin of the impurity. The transformation is called the Schrieffer-Wolf transformation and the effective Hamiltonian is the Kondo Hamiltonian.

E. BROKEN SYMMETRY AND CANONICAL TRANSFORMATIONS

The occurence of broken symmetry can be obtained from mathematical arguments only in very few situations, such as the Ising model in two dimensions. A simple paramagnetic state and a state with broken symmetry are separated by a phase transition, in other words by singularities in the free energy. Hence, the broken symmetry state cannot be obtained perturbatively. One postulates a one-body Hamiltonian where the symmetry is broken its stability verified using variational arguments. In this and many other contexts, canonical transformations are key tools to understand and solve the problem. We have seen examples above. Basis changes obtained from unitary transformations preserve the (anti)commutation relations. Such transformations are called canonical. We will illustrate these concepts with the example of superconductivity.

E.1 The BCS Hamiltonian

The general idea of Cooper pairs is that $c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}$ almost plays the role of a boson $b^\dagger_{\mathbf{p}}$. Commutation relations are not the same, but we want to use the general idea that superconductivity will be described by a non-zero expectation value of $b^\dagger_{\mathbf{p}}$ by analogy to superfluidity. The expectation value $\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle$ occurs in the Ginzburg-Landau theory as a pair wave function. The mean-field state will be described by a coherent state.

We first write the general Hamiltonian in momentum space and, in the spirit of Weiss, the trial Hamiltonian for the mean-field takes the form

$$\begin{aligned} H_E-\mu N &= H_0-\mu N+\frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow} \\ &\quad +\frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle \\ &= H_0-\mu N+\sum_{\mathbf{p}}\left(\Delta^*_{\mathbf{p}}c_{-\mathbf{p}\downarrow}c_{\mathbf{p}\uparrow}+c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\Delta_{\mathbf{p}}\right) \end{aligned} \tag{E.1}$$

where we defined

$$\Delta_{\mathbf{p}}=\frac{1}{V}\sum_{\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle. \tag{E.2}$$

The potential $U\left(\mathbf{p}-\mathbf{p}'\right)$ is an effective attraction that comes from phonons in standard BCS theory. We take this for granted. The states within an energy shell of size $\hbar\omega_D$ around the Fermi level are those that are subject to that attraction.The kinetic part of the Hamiltonian is given by

$$H_0-\mu N = \sum_{\mathbf{p},\boldsymbol{\sigma}}\left(\varepsilon_{\mathbf{p}}-\mu\right)c^\dagger_{\mathbf{p},\boldsymbol{\sigma}}c_{\mathbf{p},\boldsymbol{\sigma}} \tag{E.3}$$

$$\equiv \sum_{\mathbf{p},\boldsymbol{\sigma}}\zeta_{\mathbf{p}}c^\dagger_{\mathbf{p},\boldsymbol{\sigma}}c_{\mathbf{p},\boldsymbol{\sigma}}. \tag{E.4}$$

In the so-called jellium model, $\varepsilon_{\mathbf{p}} = \hbar^2\mathbf{p}^2/2m_e$ but one can take a more general dispersion relation. In matrix form, the combination of all these terms gives, within a constant

$$H_E - \mu N = \sum_{\mathbf{p}} \begin{pmatrix} c^\dagger_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{-\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix}. \tag{E.5}$$

One is looking for a canonical transformation that diagonalize the Hamiltonian. When this will be done, the $c^{(\dagger)}_{-\mathbf{p}\downarrow}$ will be linear combinations of eigenoperators. These linear combinations will involve $\Delta_{\mathbf{p}}$. To find the value of $\Delta_{\mathbf{p}}$, it will suffice to substitute the eigenoperator expression for $c_{\mathbf{p}\boldsymbol{\sigma}}$ in the definition of $\Delta_{\mathbf{p}}$, Eq.(E.2). This will give a self-consistent expression for $\Delta_{\mathbf{p}}$.

Let us define the Nambu spinor

$$\Psi_{\mathbf{p}} = \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \tag{E.6}$$

whose anticommutator is

$$\left\{\Psi_{\mathbf{p},i}, \Psi^\dagger_{\mathbf{p}',j}\right\} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{i,j} \tag{E.7}$$

where i and j identiby the components of the Nambu spinor. Any unitary transformation of the Nambu spinors will satisfy the anticommutation relations, as one can easily check. Since the Hamiltonian matrix is Hermitian, it can be diagonalized by a unitary transformation.

Eigenvalues $E_{\mathbf{p}}$ are obtained from the characteristic equation

$$\left(\lambda_{\mathbf{p}} - \zeta_{\mathbf{p}}\right)\left(\lambda_{\mathbf{p}} + \zeta_{\mathbf{p}}\right) - \left|\Delta_{\mathbf{p}}\right|^2 = 0 \tag{E.8}$$

where one used $\zeta_{\mathbf{p}} = \xi_{-\mathbf{p}}$ valid for a lattice with inversion symmetry. The solutions are

$$\lambda_{\mathbf{p}} = \pm E_{\mathbf{p}} = \pm\sqrt{\zeta^2_{\mathbf{p}} + \left|\Delta_{\mathbf{p}}\right|^2} \tag{E.9}$$

and the eigenvectors obey

$$\begin{pmatrix} \pm E_{\mathbf{p}} - \zeta_{\mathbf{p}} & -\Delta_{\mathbf{p}} \\ -\Delta^*_{\mathbf{p}} & \pm E_{\mathbf{p}} + \zeta_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} a_{1\mathbf{p}} \\ a_{2\mathbf{p}} \end{pmatrix} = 0. \tag{E.10}$$

whose solution is

$$\left(\pm E_{\mathbf{p}} - \zeta_{\mathbf{p}}\right) a_{1\mathbf{p}} = \Delta_{\mathbf{p}} a_{2\mathbf{p}} \tag{E.11}$$

The constraint of normalization for a unitary transformation is

$$\left|a_{1\mathbf{p}}\right|^2 + \left|a_{2\mathbf{p}}\right|^2 = 1. \tag{E.12}$$

The unitary transformation U

$$U = \begin{pmatrix} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v^*_{\mathbf{p}} & u^*_{\mathbf{p}} \end{pmatrix} \tag{E.13}$$

$$U^\dagger = \begin{pmatrix} u^*_{\mathbf{p}} & v_{\mathbf{p}} \\ -v^*_{\mathbf{p}} & u_{\mathbf{p}} \end{pmatrix} \tag{E.14}$$

where

$$\begin{pmatrix} u_{\mathbf{p}} \\ v^*_{\mathbf{p}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \left(1 + \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{-i\phi_{1\mathbf{p}}} \\ \left(1 - \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{i\phi_{2\mathbf{p}}} \end{pmatrix}$$

diagonalizes the Hamiltonian

$$\begin{pmatrix} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{pmatrix} = U^{\dagger} \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^{*} & -\zeta_{\mathbf{p}} \end{pmatrix} U.$$

Using this result, we can write

$$\begin{aligned} H_E - \mu N &= \sum_{\mathbf{p}} \begin{pmatrix} c_{\mathbf{p}\uparrow}^{\dagger} & c_{-\mathbf{p}\downarrow} \end{pmatrix} UU^{\dagger} \begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^{*} & -\zeta_{\mathbf{p}} \end{pmatrix} UU^{\dagger} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} && \text{(E.15)} \\ &= \sum_{\mathbf{p}} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow}^{\dagger} & \alpha_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} && \text{(E.16)} \\ &= \sum_{\mathbf{p},\boldsymbol{\sigma}} E_{\mathbf{p}} \alpha_{\mathbf{p},\sigma}^{\dagger} \alpha_{\mathbf{p},\boldsymbol{\sigma}} + cte. && \text{(E.17)} \end{aligned}$$

where the new operators are related to the old by the Bogoliubov-Valentin (1958) transformation

$$\begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} = U^{\dagger} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{p}}^{*} & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^{*} & u_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}. \tag{E.18}$$

The ground state is the state that is annihilated by these new operators

$$\alpha_{\mathbf{p}\boldsymbol{\sigma}} \left| BCS \right\rangle = 0.$$

The new operators are linear combination of creation-annihilation operators since the eigenstate is a linear combination of states having different numbers of particles. At zero temperature for example, one can check explicitely that the following state is indeed annihilated by $\alpha_{\mathbf{p}\boldsymbol{\sigma}}$

$$\left| BCS \right\rangle = \prod_{\mathbf{k}} \left(1 + \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^{*}} c_{-\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow}^{\dagger} \right) \left| 0 \right\rangle.$$

The value of the gap $\Delta_{\mathbf{p}}$ is obtained from the self-consistency equation Eq.(E.2). It suffices to write the $c_{\mathbf{p}\uparrow}$ en as a function of the diagonal operators $\alpha_{\mathbf{p}\boldsymbol{\sigma}}$. Inverting the Bogoliubov transformation Eq.(E.18) gives

$$\begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v_{\mathbf{p}}^{*} & u_{\mathbf{p}}^{*} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix} \tag{E.19}$$

whose adjoint is

$$\begin{pmatrix} c_{\mathbf{p}\uparrow}^{\dagger} & c_{-\mathbf{p}\downarrow} \end{pmatrix} = \begin{pmatrix} \alpha_{\mathbf{p}\uparrow}^{\dagger} & \alpha_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} u_{\mathbf{p}}^{*} & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^{*} & u_{\mathbf{p}} \end{pmatrix}. \tag{E.20}$$

We also note that

$$n\left(E_{\mathbf{p}}\right) \equiv \left\langle \alpha_{\mathbf{p}\uparrow}^{\dagger} \alpha_{\mathbf{p}\uparrow} \right\rangle = \frac{1}{e^{\sigma' E_{\mathbf{p}}} + 1}. \tag{E.21}$$

The Fermi-Dirac distribution arises from the fact the the Hamiltonian is diagonal and quadratic when written as a function of fermionic operators $\alpha_{\mathbf{p}}^{(\dagger)}$. We can now

compute the mean value of the pair operator.

$$\begin{aligned}
\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle &= \left\langle \left(v_{\mathbf{p}'} \alpha^{\dagger}_{\mathbf{p}'\uparrow} + u_{\mathbf{p}'} \alpha_{-\mathbf{p}'\downarrow} \right) \left(u_{\mathbf{p}'} \alpha_{\mathbf{p}'\uparrow} - v_{\mathbf{p}'} \alpha^{\dagger}_{-\mathbf{p}'\downarrow} \right) \right\rangle && \text{(E.22)} \\
&= v_{\mathbf{p}'} u_{\mathbf{p}'} \left\langle \alpha^{\dagger}_{\mathbf{p}'\uparrow} \alpha_{\mathbf{p}'\uparrow} - \alpha_{-\mathbf{p}'\downarrow} \alpha^{\dagger}_{-\mathbf{p}'\downarrow} \right\rangle && \text{(E.23)} \\
&= -v_{\mathbf{p}'} u_{\mathbf{p}'} \left(1 - 2n \left(E_{\mathbf{p}'} \right) \right) && \text{(E.24)} \\
&= -\frac{1}{2} \left(1 - \frac{\zeta^2_{\mathbf{p}'}}{E^2_{\mathbf{p}'}} \right)^{1/2} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2n \left(E_{\mathbf{p}'} \right) \right) && \text{(E.25)} \\
&= -\frac{1}{2} \frac{|\Delta_{\mathbf{p}'}|}{E_{\mathbf{p}'}} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2n \left(E_{\mathbf{p}'} \right) \right). && \text{(E.26)} \\
&= -\frac{1}{2} \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n \left(E_{\mathbf{p}'} \right) \right) && \text{(E.27)}
\end{aligned}$$

Substituting in self-consistency equation, we Eq.(E.2) on obtain

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U \left(\mathbf{p} - \mathbf{p}' \right) \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n \left(E_{\mathbf{p}'} \right) \right). \tag{E.28}$$

where $\Delta_{\mathbf{p}}$ is in general complex. This is known as the BCS equation.

Remark 404 *Even when the interaction depends on* $\mathbf{p} - \mathbf{p}'$*, the phase is necessarily independent of* $\mathbf{p}$*. Indeed, the gap equation can be rewritten in the form*

$$\left[C_{\mathbf{p}} \Delta_{\mathbf{p}} \right] = -\frac{1}{2V} \sum_{\mathbf{p}'} C_{\mathbf{p}} U \left(\mathbf{p} - \mathbf{p}' \right) C_{\mathbf{p}'} \left[C_{\mathbf{p}'} \Delta_{\mathbf{p}'} \right]. \tag{E.29}$$

where

$$C_{\mathbf{p}} = \left(\frac{\left(1 - 2n \left(E_{\mathbf{p}} \right) \right)}{E_{\mathbf{p}}} \right)^{1/2}. \tag{E.30}$$

The gap equation can then be reinterpreted as an eigenvalue equation. The eigenvectors are in brackets and the eigenvalue is unity. Since the matrix $-C_{\mathbf{p}} U \left(\mathbf{p} - \mathbf{p}' \right) C_{\mathbf{p}'} / \left(2V \right)$ *whose eigenvalues we are looking for is real and symmetric, the eigenvector is real within a global phase, i.e. a complex number* $e^{i\phi}$ *that multiplies all components of the eigenvector. This independence of* $\mathbf{p}$ *of the phase is known as "phase coherence". It is key to superconductivity, If the eigenvalue of the gap equation is degenerate, something new can happen. One obvious degeneracy is associated with time-reversal symmetry. When this symmetry is broken, there is still an overall* $\mathbf{p}$ *independent phase, but the order parameter is complex in a way that does not correspond to a global phase. This in general gives, for example, a non-trivial value of the orbital angular momentum.*

Remark 405 *Coherence: Since* $\phi_{1\mathbf{p}} + \phi_{2\mathbf{p}} = \phi$ *for all values of* $\mathbf{p}$*, all the pairs are added to the wave function with exactly the same phase. This can be seen from the BCS wave function at zero temperature*

$$\prod_{\mathbf{k}} \left(1 + \frac{v_{\mathbf{k}}}{u^*_{\mathbf{k}}} c^{\dagger}_{-\mathbf{k}\downarrow} c^{\dagger}_{\mathbf{k}\uparrow} \right) |0\rangle .$$

It is the interactions that impose that phase coherence that is at the origin of the phenomenon of superconductivity. Only the overall $\mathbf{p}$ *independent phase of* Δ *is arbitrary. The global gauge symmetry is broken by fixing the phase since phase and number obey an uncertainty relation. Fixing the phase thus corresponds to making the total number of particles uncertain.*

F. FEYNMAN'S DERIVATION OF THE THERMODYNAMIC VARIATIONAL PRINCIPLE FOR QUANTUM SYSTEMS

For quantum systems, the general result Eq.(33.74) applies but it is more difficult to prove because there is in general no basis that diagonalizes simultaneously each and every term in the expansion of $T_\tau \exp\left[-\int_0^\beta d\tau \widetilde{V}(\tau)\right]$. If $\widetilde{V}$ was not time dependent, as in the classical case, then matters would be different since $\widetilde{V}^n$ would be diagonal in the same basis as $\widetilde{V}$ and one could apply our inequality Eq.(33.75) in this diagonal basis and prove the theorem. The proof of the variational principle in the quantum case is thus more complicated because of the non-commutation of operators. The proof given in Sec. 33.3.1 is simpler than this one. As far as I know, the following proof is due to Feynman [12].

Proof: First, let

$$H(\alpha) = \widetilde{H}_0 + \alpha\left(H - \widetilde{H}_0\right) \tag{F.1}$$

$$= \widetilde{H}_0 + \alpha\widetilde{V} \tag{F.2}$$

then

$$H(0) = \widetilde{H}_0 \tag{F.3}$$

and

$$H(1) = H \tag{F.4}$$

The exact free energy corresponding to $H(\alpha)$ is then written as $F(\alpha)$. If for any α we can prove that $\partial^2 F(\alpha)/\partial\alpha^2 \leq 0$ then the function $F(\alpha)$ is concave downward and we can write

$$F(1) \leq F(0) + \left.\frac{\partial F(\alpha)}{\partial\alpha}\right|_{\alpha=0} \tag{F.5}$$

as illustrated in Fig.(F-1). Eq.(F.5) is the variational principle that we want Eq.(33.74). Indeed, let us compute the first derivative of $F(\alpha)$ by going to the interaction representation where $\widetilde{H}_0$ plays the role of the unperturbed Hamiltonian and use the result for F in terms of connected graphs Eq.(33.69) to obtain

$$\left.\frac{\partial F(\alpha)}{\partial\alpha}\right|_{\alpha=0} = \frac{\partial}{\partial\alpha}\left\{-T\left[\left\langle T_\tau\left[e^{-\alpha\int_0^\beta d\tau\left(\widehat{H}(\tau)-\widetilde{H}_0\right)}\right]\right\rangle_{\widetilde{0}c} - 1\right]\right\}_{\alpha=0} \tag{F.6}$$

$$= T\left\langle\int_0^\beta d\tau\left(\widehat{H}(\tau) - \widetilde{H}_0\right)\right\rangle_{\widetilde{0}} \tag{F.7}$$

$$= \left\langle H - \widetilde{H}_0\right\rangle_{\widetilde{0}} \tag{F.8}$$

The second line follows simply by expanding the time-ordered product to first order while the last line follows if we use the cyclic property of the trace

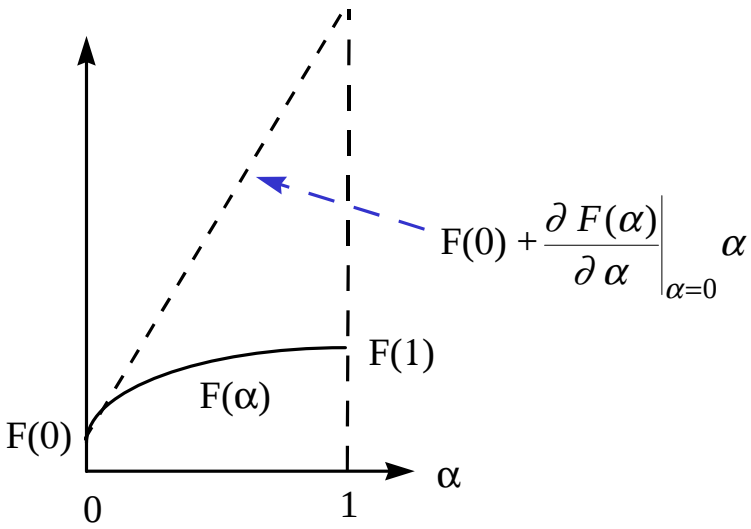

Figure F-1 Geometrical significance of the inequalities leading to the quantum thermodynamic variational principle.

to eliminate the imaginary-time dependence of the Hamiltonian. All that we have to do now is to evaluate the second derivative $\partial^2 F(\alpha)/\partial\alpha^2 \leq 0$ for an arbitrary value of α. This is more painful and will occupy us for the rest of this proof. It is important to realize that this concavity property of the free-energy is independent on the form of the Hamiltonian in general and of the interactions in particular, as long as the Hamiltonian is time-independent. The generalization to the time-dependent case is not obvious. The second derivative may be evaluated by going to the interaction representation where $H(\alpha)$ is the unperturbed Hamiltonian and $\gamma\left(H-\widetilde{H}_0\right)$ is the perturbation. Then,

$$F(\alpha+\gamma) = -T\left[\left\langle T_\tau\left[e^{-\gamma\int_0^\beta d\tau\left(\widehat{H}(\tau)-\widetilde{H}_0\right)}\right]\right\rangle_{\alpha,c} - 1\right] - T\ln Z(\alpha) \qquad \text{(F.9)}$$

and the second derivative of $F(\alpha)$ may be obtained from the second-order term in γ in the above expression. Note that the average is taken with the density matrix $\exp(H(\alpha)-\mu N)/Z(\alpha)$. Expanding the exponential to second order in γ and returning to our definition of $\widetilde{V}$ Eq.(F.2) we find

$$\begin{aligned} F(\alpha+\gamma) &= F(\alpha)+\gamma\left\langle\widetilde{V}\right\rangle_\alpha - \frac{1}{2}\gamma^2\left(\frac{1}{\beta}\left\langle T_\tau\left[-\gamma\int_0^\beta d\tau\widetilde{V}(\tau)\right]^2\right\rangle_{\alpha,c}\right)+\ldots \\ F(\alpha+\gamma) &= F(\alpha)+\frac{\partial F(\alpha)}{\partial\alpha}+\frac{1}{2}\gamma^2\frac{\partial^2 F(\alpha)}{\partial\alpha^2}+\ldots \end{aligned} \qquad \text{(F.10)}$$

so that the second derivative, using the expression we found above for the second cumulant Eq.(33.67) is,

$$\begin{aligned} \frac{\partial^2 F(\alpha)}{\partial\alpha^2} &= -\frac{1}{\beta}\left\langle T_\tau\left[\left(-\int_0^\beta d\tau\widetilde{V}(\tau)\right)^2\right]\right\rangle_{\alpha,c} \qquad \text{(F.11)} \\ &= -\frac{1}{\beta}\left\langle T_\tau\left[\left(-\int_0^\beta d\tau\widetilde{V}(\tau)\right)^2\right]\right\rangle_\alpha + \frac{1}{\beta}\left\langle\int_0^\beta d\tau\widetilde{V}(\tau)\right\rangle_\alpha^2 \end{aligned}$$

This is where we need to roll up our sleeves and do a bit of algebra. Using the cyclic property of the trace and the definition of time-ordered product, we can rewrite the above result as follows,

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} = -2\frac{1}{\beta}\left\langle \int_0^\beta d\tau \widetilde{V}(\tau) \int_0^\tau d\tau' \widetilde{V}(\tau') \right\rangle_\alpha + \beta \left\langle \widetilde{V} \right\rangle_\alpha^2 \tag{F.12}$$

Let us work a bit on the first term by going to the basis where $H(\alpha)$ is diagonal. We obtain, using also the cyclic property of the trace,

$$\left\langle \int_0^\beta d\tau \widetilde{V}(\tau) \int_0^\tau d\tau' \widetilde{V}(\tau') \right\rangle_\alpha \tag{F.13}$$

$$= \frac{1}{Z(\alpha)} \sum_{m,n} e^{-K_n\beta} \int_0^\beta d\tau \int_0^\tau d\tau' e^{K_n(\tau-\tau')} e^{-K_m(\tau-\tau')} \left| \langle n| \widetilde{V} |m\rangle \right|^2$$

$$= \frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \int_0^\beta d\tau e^{(K_n-K_m)\tau} \left. \frac{e^{(K_m-K_n)\tau'}}{K_m-K_n} \right|_0^\tau \left| \langle n| \widetilde{V} |m\rangle \right|^2$$

$$+ \frac{1}{Z(\alpha)} \sum_n e^{-K_n\beta} \int_0^\beta d\tau\tau \left| \langle n| \widetilde{V} |n\rangle \right|^2 \tag{F.14}$$

$$= \frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \int_0^\beta d\tau \frac{1-e^{(K_n-K_m)\tau}}{K_m-K_n} \left| \langle n| \widetilde{V} |m\rangle \right|^2 \tag{F.15}$$

$$+ \frac{\beta^2}{2Z(\alpha)} \sum_n e^{-K_n\beta} \left| \langle n| \widetilde{V} |n\rangle \right|^2 \tag{F.16}$$

The first term on the right-hand side is easily evaluated as follows

$$\frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \left[\frac{\beta}{K_m-K_n} + \frac{e^{(K_n-K_m)\beta}-1}{(K_m-K_n)^2} \right] \left| \langle n| \widetilde{V} |m\rangle \right|^2$$

$$= \frac{\beta}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \frac{\left| \langle n| \widetilde{V} |m\rangle \right|^2}{K_m-K_n} \tag{F.17}$$

where we have used the fact that the term with the denominator $(K_m-K_n)^2$ goes into minus itself under a change of dummy summation variables $m \longleftrightarrow n$. Substituting all we have done in the expression for the second derivative Eq.(F.12) we finally obtain

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} = -\frac{2}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \frac{\left| \langle n| \widetilde{V} |m\rangle \right|^2}{K_m-K_n} \tag{F.18}$$

$$-\beta \left(\frac{\sum_n e^{-K_n\beta} \left| \langle n| \widetilde{V} |n\rangle \right|^2}{Z(\alpha)} - \left(\frac{\sum_n e^{-K_n\beta} \langle n| \widetilde{V} |n\rangle}{Z(\alpha)} \right)^2 \right)$$

The terms on the last line gives a negative contribution, as can be seen from the Cauchy-Schwarz inequality

$$\left[\sum_n |a_n|^2 \right] \left[\sum_n |b_n|^2 \right] \geq \left| \sum_n a_n b_n \right|^2 \tag{F.19}$$

when we substitute

$$a_n = \sqrt{\frac{e^{-K_n\beta}}{Z\left(\alpha\right)}} \tag{F.20}$$

$$b_n = \sqrt{\frac{e^{-K_n\beta}}{Z\left(\alpha\right)}}\left\langle n\right|\widetilde{V}\left|n\right\rangle \tag{F.21}$$

This allows us to prove that the sign of the second derivative is negative for any α. It suffices to rewrite the first term in Eq.(F.18) in the form

$$-\frac{2}{Z\left(\alpha\right)}\sum_{m\neq n}e^{-K_n\beta}\frac{\left|\left\langle n\right|\widetilde{V}\left|m\right\rangle\right|^2}{K_m-K_n}=-\frac{1}{Z\left(\alpha\right)}\sum_{m\neq n}\frac{e^{-K_n\beta}-e^{-K_m\beta}}{K_m-K_n}\left|\left\langle n\right|\widetilde{V}\left|m\right\rangle\right|^2 \tag{F.22}$$

and to use the Cauchy-Schwartz inequality to obtain

$$\frac{\partial^2 F\left(\alpha\right)}{\partial\alpha^2}\leq-\frac{1}{Z\left(\alpha\right)}\sum_{m\neq n}\frac{e^{-K_n\beta}-e^{-K_m\beta}}{K_m-K_n}\left|\left\langle n\right|\widetilde{V}\left|m\right\rangle\right|^2\leq 0 \tag{F.23}$$

QED

G. DEFINITIONS

1. Dirac's delta $\delta(\omega)$ and Heaviside's theta

$$\theta(\omega) = \begin{cases} 1 \text{ if } \omega > 0 \\ \frac{1}{2} \text{ if } \omega = 0 \\ 0 \text{ if } \omega < 0 \end{cases} \tag{G.1}$$

2. Grand-canonical average

$$\frac{\sum_i e^{-\beta(E_i-\mu N_i)} \langle i| \mathcal{O} |i\rangle}{\sum_i e^{-\beta(E_i-\mu N_i)}} = \frac{\sum_i \langle i| e^{-\beta(H-\mu N)} \mathcal{O} |i\rangle}{\sum_i e^{-\beta(E_i-\mu N_i)}} = \frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]} = \langle \mathcal{O} \rangle \tag{G.2}$$

3. We often define the density matrix by

$$\widehat{\varrho} = e^{-\beta H} / \mathrm{Tr}\left[e^{-\beta H}\right]. \tag{G.3}$$

Then, we can write

$$\langle A_s(t) A_s \rangle = \mathrm{Tr}\left[\widehat{\varrho} A_s(t) A_s\right] \tag{G.4}$$

4. Conductivity sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left[\sigma_{xx}(q_x,\omega)\right] = \frac{ne^2}{2m} = \frac{\omega_p^2}{8\pi} \tag{G.5}$$

5. Dielectric constants

$$\overleftrightarrow{\epsilon^T}(\mathbf{q},\omega) = \left(1 - \frac{\omega_p^2}{(\omega+i\eta)^2}\right) \overleftrightarrow{I} + \frac{4\pi}{(\omega+i\eta)^2} \left(\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)\right)^T. \tag{G.6}$$

$$\frac{1}{\epsilon^L(\mathbf{q},\omega)} = 1 - \frac{4\pi}{q^2} \chi^R_{\rho\rho}(\mathbf{q},\omega). \tag{G.7}$$

6. Equalities.

$$\approx \text{ Asymptotically equal to} \tag{G.8}$$

$$\sim \text{ Scales as} \tag{G.9}$$

$$\equiv \text{ Is equal by definition} \tag{G.10}$$

$$\simeq \text{ Is approximately equal to} \tag{G.11}$$

7. f sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi"_{nn}(\mathbf{k},\omega) = \frac{n\mathbf{k}^2}{m}. \tag{G.12}$$

8. Fluctuation-dissipation theorem

$$S_{A_iA_j}(\omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \chi"_{A_iA_j}(\omega) \tag{G.13}$$

9. Fourier transforms

$$f_{\mathbf{k}} = \int d^3r\ f(\mathbf{r})\mathbf{e}^{-i\mathbf{k}\cdot\mathbf{r}}$$

$$f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} f_{\mathbf{k}}\mathbf{e}^{i\mathbf{k}\cdot\mathbf{r}}$$

$$g_\omega = \int dt\ g(t)e^{i\omega t}$$

$$g(t) = \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t}$$

(note the difference in sign in the exponent for space and time Fourier transforms.)

Convolution theorem:

$$\int dt e^{i\omega t}\left[\int dt' a(t')b(t-t')\right] \equiv a_\omega b_\omega$$

Parseval's theorem is obtained by taking $\int \frac{d\omega}{2\pi}$ on both sides of the previous equality

$$\int dt' a(t')b(-t') \equiv \int \frac{d\omega}{2\pi} a_\omega b_\omega$$

The above two theorems may also be written in a reciprocal manner

$$\int \frac{d\omega}{2\pi} e^{-i\omega t}\left[\int \frac{d\omega'}{2\pi} a_{\omega'} b_{\omega-\omega'}\right] = a(t)b(t)$$

$$\int \frac{d\omega'}{2\pi} a_{\omega'} b_{-\omega'} = \int dt e^{i\omega t} a(t)b(t)$$

For a translationally invariant system, note that with $\mathcal{V}$ the volume,

$$\int d\left(\mathbf{r}-\mathbf{r}'\right) e^{-i\mathbf{q}\cdot\left(\mathbf{r}-\mathbf{r}'\right)} f(\mathbf{r}-\mathbf{r}') = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{q}\cdot r} \int d\mathbf{r}' e^{-i\mathbf{q}\cdot r'} f(\mathbf{r}-\mathbf{r}') \tag{G.14}$$

10. Heisenberg representation

$$\mathcal{O}(t) = e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar}$$

11. Interaction representation

$$\begin{aligned} \mathcal{O}_I(t) &= e^{iH_0t/\hbar}\mathcal{O}_S e^{-iH_0t/\hbar} \\ i\hbar\frac{\partial}{\partial t}U_I(t,t_0) &= \mathcal{H}_I(t)U_I(t,t_0) \\ U_I(t,0) &= T_c e^{-i\int_0^t \mathcal{H}_I(t')dt'} \end{aligned} \tag{G.15}$$

$$U_I(t_0,t_0) = 1$$

1. Kramers-Krönig relations

$$\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}$$

$$\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}.$$

2. Kubo formula for longitudinal conductivity

$$\sigma_{xx}(q_x,\omega)=\frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega)-\frac{ne^2}{m}\right]=\left[\frac{1}{iq_x}\chi^R_{j_\mu\rho}(q_x,\omega)\right]. \quad \text{(G.16)}$$

for transverse conductivity

$$\sigma_{yy}(q_x,\omega)=\frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_yj_y}(q_x,\omega)-\frac{ne^2}{m}\right]. \quad \text{(G.17)}$$

3. Mathematical identities (Sokhatsky-Weierstrass formula)

$$\lim_{\eta\to0}\frac{1}{\omega+i\eta}=\lim_{\eta\to0}\frac{\omega-i\eta}{\omega^2+\eta^2}=\lim_{\eta\to0}\left[\frac{\omega}{\omega^2+\eta^2}-\frac{i\eta}{\omega^2+\eta^2}\right]=\mathcal{P}\frac{1}{\omega}-i\pi\delta(\omega)$$

$$\lim_{\eta\to0}\frac{1}{\omega-i\eta}=\lim_{\eta\to0}\frac{\omega+i\eta}{\omega^2+\eta^2}=\lim_{\eta\to0}\left[\frac{\omega}{\omega^2+\eta^2}+\frac{i\eta}{\omega^2+\eta^2}\right]=\mathcal{P}\frac{1}{\omega}+i\pi\delta(\omega)$$

4. Normalization:

Continuum normalization for plane waves:

$$\langle\mathbf{R}\,|\mathbf{k}_i\rangle=\frac{1}{\Omega^{1/2}}e^{i\mathbf{k}_i\cdot\mathbf{R}} \quad \text{(G.18)}$$

$$\int\frac{d\mathbf{k}}{(2\pi)^3}=\frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\quad;\quad\mathcal{V}=L_xL_yL_z\quad;\quad k_x=\frac{\pi n_x}{L_x}...\quad;\quad n_x=-\frac{L_x}{a}+1,...,-1,0,1,...,\frac{L_x}{a} \quad \text{(G.19)}$$

This is another consistent normalization

$$\int d\mathbf{r}\,|\mathbf{r}\rangle\langle\mathbf{r}|=1 \quad \text{(G.20)}$$

$$\langle\mathbf{r}\,|\mathbf{r}'\rangle=\delta(\mathbf{r}-\mathbf{r}') \quad \text{(G.21)}$$

$$\langle\mathbf{r}\,|\mathbf{k}\rangle=e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{(G.22)}$$

$$\int\frac{d\mathbf{k}}{(2\pi)^3}\,|\mathbf{k}\rangle\langle\mathbf{k}|=1 \quad \text{(G.23)}$$

$$\langle\mathbf{k}\,|\mathbf{k}'\rangle=(2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right) \quad \text{(G.24)}$$

1. Plasma frequency

$$\omega_p^2=\frac{4\pi ne^2}{m} \quad \text{(G.25)}$$

2. Response function (Susceptibility)

$$\chi^R_{AB}(\mathbf{r},\mathbf{r}';t,t')=\frac{i}{\hbar}\langle[A(\mathbf{r},t),B(\mathbf{r}',t')]\rangle\,\theta(t-t')$$

or in short hand,

$$\chi"_{A_iA_j}(t-t')=\frac{1}{2\hbar}\langle[A_i(t),A_j(t')]\rangle.$$

$$\chi^R_{A_iA_j}(t-t')=2i\chi"_{A_iA_j}(t-t')\theta(t-t').$$

For operators with the same signature under time reversal,

$$\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = \chi"_{A_iA_j}(\omega)$$

while two operators A_i, A_j with opposite signatures under time reversal

$$\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = \chi"_{A_iA_j}(\omega).$$

Spectral representation

$$\chi_{A_iA_j}(z) = \int \frac{d\omega'}{\pi} \frac{\chi"_{A_iA_j}(\omega')}{\omega' - z} \tag{G.26}$$

3. Minimal coupling to the electromagnetic field. N.B. e is the charge of the particle. It can be positive or negative

$$\mathbf{p}_\alpha = \frac{\hbar}{i}\nabla_\alpha \to \frac{\hbar}{i}\nabla_\alpha - e\mathbf{A}(\mathbf{r}_\alpha, t) \tag{G.27}$$

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\phi(\mathbf{r}_\alpha, t). \tag{G.28}$$

4. Tensors. Multiplication by a vector

$$\left(\overleftrightarrow{\sigma^T} \cdot \mathbf{A}\right)_\mu = \sum_\nu \sigma^T_{\mu\nu} A_\nu. \tag{G.29}$$

Unit vector

$$\widehat{\mathbf{q}} = \mathbf{q}/\left|\mathbf{q}\right|$$

Transverse part

$$\overleftrightarrow{\sigma^T}(\mathbf{q},\omega) = \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \cdot \overleftrightarrow{\sigma}(\mathbf{q},\omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \tag{G.30}$$

Dyadic product represention of a matrix

$$(\widehat{\mathbf{q}}\widehat{\mathbf{q}})_{ab} = \widehat{q}_a \widehat{q}_b \tag{G.31}$$

Longitudinal part

$$\overleftrightarrow{\sigma^L}(\mathbf{q},\omega) = \widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q},\omega) \cdot \widehat{\mathbf{q}}\widehat{\mathbf{q}} \tag{G.32}$$

5. Thermal average (see canonical average)

6. Theta function (Heaviside function)

$$\theta(t) = \frac{1 \text{ if } t > 0}{0 \text{ if } t < 0} \tag{G.33}$$

7. Kronecker delta function

$$\delta_{k,0} = \frac{1 \text{ if } k = 0}{0 \text{ otherwise}} \tag{G.34}$$

8. Electromagnetic constants: $\varepsilon_0 = 8.85\times10^{-12}$ farad/meter is the permittivity of vacuum and $\mu_0 = 4\pi \times 10^{-7}$ henry/meter its permeability.

$$\varepsilon_0\mu_0 = \frac{1}{c^2}.$$

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