

PHY-892 Problème à N-corps (notes de cours)

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Part I

Introduction: Correlation functions and Green's functions.

1. INTRODUCTION

Physics is 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 at say, the tenth decimal place (?). 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 computed with perturbation theory. More generally, the “renormalization group” tells us how to construct effective theories that depend on the scale.

In addition, “More is different”, as emphasized by P.W. Anderson. 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} . Let us mention a few more scales, taken from lecture notes by P. Coleman. Take the time scale at the atomic level to be $\hbar/1 \text{ eV} \sim 10^{-15} \text{ s}$. If we take the characteristic macroscopic scale to be 1 s , the leap to go between the two scale is as big as that necessary to go from 1 s to the age of the universe. Length scales from the atom to the cm differ by 10^8 , and typically, the number of atoms we look at in an experiment done on a cm^3 of matter is 10^{23} . Clearly, this is an impossible task. What we need to proceed are new concepts, new principles, new laws if you want, that “emerge” from the basic theory. In the same way that entropy is a concept that emerges when one studies the statistical mechanics of matter, the concept of broken symmetry is necessary to study a 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 approximation for electron-phonon interaction.¹

This course is thus a course about principles, as well as a course on calculational approaches, although the latter will often appear to take the whole stage.

The first principle we will use is that of *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 the first part of these lecture notes, where we will develop the formalism of correlation functions

¹Note 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.

and perturbation theory. 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 will 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 adiabatically 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 be “guessed”, a Hamiltonian that breaks some of the symmetries present in the original phase. This will be the subject of the second part of these notes. And the underlying principle is 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.

Finally, the third part is concerned with modern problems and more recent calculational tools.

Yes, this course is also about calculational tools, about formalism. In quantum mechanics in general, what we normally call the “Physics” is very much tied to the calculational tools. These notes are also about calculational tools and about the Physics that comes out of these 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, in practice, this list of complex numbers grows exponentially with the number of degrees of freedom and it is not very illuminating. The density at a point, that we can extract from the wave function, 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 to 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 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. These quantities will, in a way, play the same role as viscosity in ordinary hydrodynamics. They are quantities where much of our ignorance about the exact solution to the problem can be hidden. Identifying these hiding 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 is work in progress. Many-body physics is an open frontier. Everyday new materials lead to new surprises, new phases, new phenomenon 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.

2. CORRELATION FUNCTIONS

Whenever the N -body problem can be solved exactly in d dimensions, the result is a function of Nd coordinates and of time, $\Psi(x_1, y_1, \dots, x_d, y_d, \dots; t)$. 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. In the cases where perturbation theory can be applied, Feynman diagrams help develop a physical intuition. Also, variational wave functions are usually chosen with a few physically motivated parameters.

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, we thus first discuss which quantities are observable, or in other words, what it is that we want to compute.

In this Chapter, we will introduce correlation functions. First, we show 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 in the linear response regime.

Whatever the appropriate microscopic description of the system, or whatever the underlying broken symmetry, the result of any given type of experiment can be expressed as a specific correlation function.

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

First, general properties, which are independent from the specific manner in which we compute correlation functions. 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

Second, we will need to develop techniques to compute specific correlation functions. Sometimes, phenomenological considerations suffice 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.

Microscopic approaches 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 Foster.[1]

In the present chapter, we 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 we discuss general properties of correlation functions
- Give a specific example of sum-rule calculation.

2.1 Relation between correlation functions and experiments

We want to illustrate the fact that scattering experiments with weak probes usually measure various equilibrium correlation functions of a system. What we 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. As an example, we will describe in detail 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 plan is simply to use Fermi’s Golden Rule to compute the cross section. We will obtain

$$\frac{d\sigma}{d\epsilon_f d\Omega_f} = \left[\frac{m^2}{(2\pi)^3 \hbar^5} \frac{k_f}{k_i} |V_{-\mathbf{q}}^c|^2 \right] \int dt e^{i\omega t} \langle \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \rangle \quad (2.1)$$

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...

Consider the experiment illustrated on figure (2-1). \mathcal{V} is the volume of the system, and Ω a quantization volume.

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

$$v(\mathbf{R}) = \sum_{\alpha=1}^N e_{\alpha} V^c(\mathbf{R} - \mathbf{r}_{\alpha}) = \int d^3r \rho(\mathbf{r}) V^c(\mathbf{R} - \mathbf{r}) \quad (2.2)$$

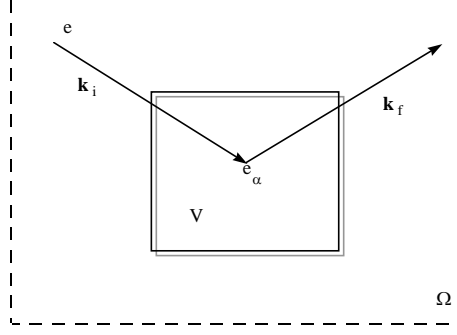


Figure 2-1 Electron scattering experiment. Ω is the quantization volume for the incoming and outgoing plane waves while V is the sample's volume. Each charge inside is labeled by e_α while the probe's charge is e and the incident and outgoing momenta are respectively \mathbf{k}_i and \mathbf{k}_f .

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

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^N e_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \quad (2.3)$$

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

$$P_{i \rightarrow f} = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta(E_f - E_i - \hbar\omega) \quad (2.4)$$

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,

$$\begin{aligned} \epsilon_f &= \epsilon_i - \hbar\omega \\ \hbar\mathbf{k}_f &= \hbar\mathbf{k}_i - \hbar\mathbf{q}. \end{aligned} \quad (2.5)$$

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:

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

Then, in the Born approximation, we have that

$$V_{fi} = \langle f | \otimes \langle \mathbf{k}_f | \int d^3r \rho(\mathbf{r}) V^c(\mathbf{R} - \mathbf{r}) | \mathbf{k}_i \rangle \otimes | i \rangle \quad (2.6)$$

where the plane-wave matrix element can easily be evaluated

$$\int d^3R \langle \mathbf{k}_f | R \rangle V^c(\mathbf{R} - \mathbf{r}) \langle R | \mathbf{k}_i \rangle = \Omega^{-1} \int d^3R e^{i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}} V^c(\mathbf{R} - \mathbf{r}) = \frac{V_{-\mathbf{q}}^c}{\Omega} e^{i\mathbf{q} \cdot \mathbf{r}} \quad (2.7)$$

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

$$V_{fi} = \frac{V_{-\mathbf{q}}^c}{\Omega} \int d^3r \langle f | \rho(\mathbf{r}) | i \rangle e^{i\mathbf{q} \cdot \mathbf{r}} = \frac{V_{-\mathbf{q}}^c}{\Omega} \langle f | \rho_{-\mathbf{q}} | i \rangle. \quad (2.8)$$

Substituting back in Fermi's Golden rule (2.4), we obtain

$$P_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \frac{V_{-\mathbf{q}}^c}{\Omega} \right|^2 \langle i | \rho_{\mathbf{q}} | f \rangle \langle f | \rho_{-\mathbf{q}} | i \rangle \delta(E_f - E_i - \hbar\omega). \quad (2.9)$$

Only the momentum and energy of the probe electron appear in this final expression, as we had set-up to do.

Definition 1 *Note in passing that we use the following definitions for Fourier transforms in the continuum*

$$f_{\mathbf{q}} = \int d^3r f(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \quad (2.10)$$

$$f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} f_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \quad (2.11)$$

$$g_{\omega} = \int dt g(t) e^{i\omega t} \quad (2.12)$$

$$g(t) = \int \frac{d\omega}{2\pi} g_{\omega} e^{-i\omega t} \quad (2.13)$$

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.([4]). The total cross section, whose units are those of a surface, is equal to

$$\sigma = \frac{\text{Number of transitions per unit time}}{\text{Number of incident particles per unit time per unit surface}} \quad (2.14)$$

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 $P_{i \rightarrow f}$ by the number of free electron states in this interval, namely

$$\Omega d^3k_f / (2\pi)^3 = \Omega k_f m d\epsilon_f d\Omega_f \hbar^{-2} / (2\pi)^3. \quad (2.15)$$

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,

$$\begin{aligned} \frac{d\sigma}{d\epsilon_f d\Omega_f} &= \frac{\text{Number of transitions per unit time in given solid angle and energy interval}}{\text{Number of incident particles per unit time per unit surface}} \\ &= \left[\frac{\Omega k_f m \hbar^{-2} / (2\pi)^3}{\hbar k_i / (m\Omega)} \right] \frac{\sum_i e^{-\beta E_i} \sum_f P_{i \rightarrow f}}{\sum_i e^{-\beta E_i}} \end{aligned} \quad (2.16)$$

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

$$\mathcal{O}(t) = e^{iHt/\hbar} \mathcal{O} e^{-iHt/\hbar} \quad (2.17)$$

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

$$2\pi\hbar \langle i|\rho_{\mathbf{q}}|f\rangle \delta(E_f - E_i - \hbar\omega) = \int dt e^{i\omega t} \langle i|\rho_{\mathbf{q}}|f\rangle e^{-i(E_f - E_i)t/\hbar} \quad (2.18)$$

$$= \int dt e^{i\omega t} \langle i|e^{iHt/\hbar} \rho_{\mathbf{q}} e^{-iHt/\hbar} |f\rangle = \int dt e^{i\omega t} \langle i|\rho_{\mathbf{q}}(t)|f\rangle. \quad (2.19)$$

Substituting this expression in the equation for the transition probability, (2.9)

$$\sum_f P_{i \rightarrow f} = \left| \frac{V_{-\mathbf{q}}^c}{\Omega\hbar} \right|^2 \int dt e^{i\omega t} \langle i|\rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)|i\rangle \quad (2.20)$$

the cross section is proportional to

$$\frac{\sum_i e^{-\beta E_i} \int dt e^{i\omega t} \langle i|\rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)|i\rangle}{\sum_i e^{-\beta E_i}} = \frac{\sum_i \int dt e^{i\omega t} \langle i|e^{-\beta H} \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)|i\rangle}{\sum_i e^{-\beta E_i}} \quad (2.21)$$

$$= \int dt e^{i\omega t} \frac{\text{Tr} [e^{-\beta H} \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)]}{\text{Tr} [e^{-\beta H}]} = \int dt e^{i\omega t} \langle \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0) \rangle. \quad (2.22)$$

More explicitly, we find Eq.(2.1) 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!

Definition 2 *In the last equation, we have also introduced what we mean by the thermal average $\langle \rangle$. Here we used the canonical ensemble, but we will mostly use the grand-canonical one. The only change implied is $e^{-\beta H} \rightarrow e^{-\beta(H - \mu N)}$. Note also that the quantity*

$$\rho \equiv \frac{e^{-\beta H}}{\text{Tr}[e^{-\beta H}]} \quad (2.23)$$

is often called the density matrix. The fact that thermal averages are traces is an important fact that we will often use later.

2.2 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 thermal gradient etc... The result will be again an equilibrium correlation function. We will be able to relate this correlation function to equilibrium correlation functions of the type just calculated at the end of the last section by developing the so-called ‘‘fluctuation-dissipation theorem’’. 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_0 as the unperturbed Hamiltonian.

Let

$$\mathcal{H}(t) = H_0 + \delta\mathcal{H}(t) \quad (2.24)$$

where H_0 is the Hamiltonian of the system under study and $\delta\mathcal{H}(t)$ is the perturbation given by the time-dependent Hamiltonian

$$\boxed{\delta\mathcal{H}(t) = - \int d^3r A_i(\mathbf{r}) a_i(\mathbf{r}, t)}. \quad (2.25)$$

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 the 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}/c through a current \mathbf{j} , ($A_i(\mathbf{r}) = j_x(\mathbf{r})\delta_{i,x}$; $a_i(\mathbf{r}, t) = A_x(\mathbf{r}, t)\delta_{i,x}/c$) 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. We 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.

2.2.1 Schrödinger and Heisenberg pictures.

Since the Hamiltonian is the infinitesimal generator of time translations, Schrödinger's equation for a time-dependent Hamiltonian takes the same form as usual,

$$i\hbar \frac{\partial \psi_S}{\partial t} = \mathcal{H}(t) \psi_S. \quad (2.26)$$

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

$$\psi_S(t) = U(t, t_0) \psi_S(t_0) \quad (2.27)$$

where $U(t, t_0)$ is a unitary operator satisfying

$$U(t_0, t_0) = 1 \quad (2.28)$$

while by time-reversal symmetry

$$U(t_0, t) U(t, t_0) = 1. \quad (2.29a)$$

Conservation of probability gives

$$U(t, t_0)^\dagger U(t, t_0) = 1 \quad (2.30)$$

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

$$U(t, t_0)^{-1} = U(t, t_0)^\dagger. \quad (2.31)$$

Furthermore, when we can use time-reversal invariance, Eq.(2.29a), we also have

$$U(t, t_0)^{-1} = U(t, t_0)^\dagger = U(t_0, t). \quad (2.32)$$

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

$$\boxed{\langle \psi_S(t) | \mathcal{O}_S | \psi_S(t) \rangle = \langle \psi_H | \mathcal{O}_H(t) | \psi_H \rangle}. \quad (2.33)$$

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

$$\mathcal{O}_S(t=0) = \mathcal{O}_H(t=0) \equiv \mathcal{O}_S \quad (2.34)$$

$$\psi_S(t=0) = \psi_H(t=0) \equiv \psi_S \quad (2.35)$$

Using the expression for the time-dependent wave function, and the equality of matrix elements Eq.(2.33), we obtain

$$\mathcal{O}_H(t) = U^\dagger(t, 0)\mathcal{O}_S U(t, 0). \quad (2.36)$$

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

$$\boxed{U(t, t_0) = e^{-i\mathcal{H}(t-t_0)/\hbar}} \quad (2.37)$$

Remark 1 *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.(2.36) becomes*

$$\mathcal{O}_H(t) = U(0, t)\mathcal{O}_S U(t, 0). \quad (2.38)$$

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.(2.36) but in much of the later chapters, the above representation will be used.

2.2.2 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

$$\boxed{\mathcal{H}(t) = H_0 + \delta\mathcal{H}(t)} \quad (2.39)$$

where H_0 is time-independent as above, but the proof can be generalized to time-dependent H_0 simply by replacing $e^{iH_0 t/\hbar}$ everywhere below by the appropriate evolution operator.

The definition of the evolution operator in the interaction representation $U_I(t, 0)$ is given by

$$U(t, 0) \equiv e^{-iH_0 t/\hbar} U_I(t, 0). \quad (2.40)$$

and

$$U(0, t) \equiv U_I(0, t)e^{iH_0 t/\hbar}. \quad (2.41)$$

so that for example

$$\boxed{U(t, t_0) \equiv e^{-iH_0 t/\hbar} U_I(t, t_0) e^{iH_0 t_0/\hbar}} \quad (2.42)$$

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 $t = 0$. The justification for the definition of U_I above is that when the external perturbation $\delta\mathcal{H}(t)$ is small,

$U_I(t, t_0)$ is close to unity. If we write again the equality of matrix elements in the general case, we obtain

$$\langle \psi_S(t) | \mathcal{O}_S | \psi_S(t) \rangle = \langle \psi_S | U^\dagger(t, 0) \mathcal{O}_S U(t, 0) | \psi_S \rangle \quad (2.43)$$

$$= \langle \psi_S | U_I^\dagger(t, 0) e^{iH_0 t/\hbar} \mathcal{O}_S e^{-iH_0 t/\hbar} U_I(t, 0) | \psi_S \rangle \quad (2.44)$$

$$= \langle \psi_S | U_I^\dagger(t, 0) \mathcal{O}_I(t) U_I(t, 0) | \psi_S \rangle \quad (2.45)$$

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

$$\boxed{\mathcal{O}_I(t) = e^{iH_0 t/\hbar} \mathcal{O}_S e^{-iH_0 t/\hbar}} \quad (2.46)$$

while the wave functions obey

$$\boxed{|\psi_I(t)\rangle = U_I(t, 0) |\psi_S\rangle} \quad (2.47)$$

In other words, in the interaction picture both the operators and the wave function evolve. 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,

$$i\hbar \frac{\partial U(t, t_0)}{\partial t} = \mathcal{H}(t) U(t, t_0) \quad (2.48)$$

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

$$H_0 e^{-iH_0 t/\hbar} U_I(t, 0) + e^{-iH_0 t/\hbar} i\hbar \frac{\partial}{\partial t} U_I(t, 0) = \mathcal{H}(t) e^{-iH_0 t/\hbar} U_I(t, 0) \quad (2.49)$$

$$i\hbar \frac{\partial}{\partial t} U_I(t, 0) = e^{iH_0 t/\hbar} \delta\mathcal{H}(t) e^{-iH_0 t/\hbar} U_I(t, 0). \quad (2.50)$$

so that using the definition of time evolution of an arbitrary operator in the interaction representation as above (2.46) the equation for the time evolution operator $U_I(t, 0)$ in the interaction representation may be written,

$$i\hbar \frac{\partial}{\partial t} U_I(t, 0) = \delta\mathcal{H}_I(t) U_I(t, 0) \quad (2.51)$$

with the initial condition

$$U_I(0, 0) = 1. \quad (2.52)$$

As expected, Eq.(2.51) 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 $U_I(0, t_0)$ we have for an arbitrary initial time

$$\boxed{i\hbar \frac{\partial}{\partial t} U_I(t, t_0) = \delta\mathcal{H}_I(t) U_I(t, t_0)} \quad (2.53)$$

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 (2.53) and using the initial condition, we have

$$\boxed{U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \delta\mathcal{H}_I(t') U_I(t', t_0)} \quad (2.54)$$

which, iterated to first order, gives,

$$U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \quad (2.55)$$

and correspondingly

$$U_I^\dagger(t, t_0) = 1 + \frac{i}{\hbar} \int_{t_0}^t dt' \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \quad (2.56)$$

2.2.3 Linear response

Returning to our general considerations, in the case of interest to us the external perturbation in the interaction representation is of the form,

$$\boxed{\delta\mathcal{H}_I(t) = - \int d^3r A_i^0(\mathbf{r}, t) a_i(\mathbf{r}, t)} \quad (2.57)$$

where for short we wrote $A_i^0(\mathbf{r}, t)$ to represent a system's observable evolving in the system's Heisenberg representation,

$$A_i^0(\mathbf{r}, t) = e^{iH_0t/\hbar} A_i(\mathbf{r}) e^{-iH_0t/\hbar}. \quad (2.58)$$

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 at time t_0 , it suffices to evolve $B(\mathbf{r})$ with the full evolution operator, including the external perturbation.¹

$$\langle B(\mathbf{r}, t) \rangle = \langle U^\dagger(t, t_0) B(\mathbf{r}) U(t, t_0) \rangle \quad (2.59)$$

Using the interaction representation Eq.(2.42), the last equation becomes

$$\langle B(\mathbf{r}, t) \rangle = \left\langle U_I^\dagger(t, t_0) B^0(\mathbf{r}, t) U_I(t, t_0) \right\rangle. \quad (2.60)$$

In this last expression, $B^0(\mathbf{r}, t)$ is now in the system's Heisenberg representation of the system *without the external perturbation*. We also used the fact that $e^{-iH_0t_0/\hbar}$ commutes with the density matrix and that the trace has a cyclic property to cancel the extra $e^{-iH_0t_0/\hbar}$ and $e^{iH_0t_0/\hbar}$ appearing in the equation for the evolution operator in Eq.(2.42).

Using the explicit expression Eq.(2.57) for the external perturbation in the equation for the evolution operator in the interaction representation (2.55), we have that the term linear in applied field is then given by,

$$\delta \langle B(\mathbf{r}, t) \rangle = \frac{i}{\hbar} \int_{t_0}^t dt' \int d^3r' \langle [B^0(\mathbf{r}, t), A_i^0(\mathbf{r}', t')] \rangle a_i(\mathbf{r}', t'). \quad (2.61)$$

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

$$\boxed{\delta \langle B(\mathbf{r}, t) \rangle = \int_{-\infty}^{\infty} dt' \int d^3r' \chi_{BA_i}^R(\mathbf{r}, t; \mathbf{r}', t') a_i(\mathbf{r}', t')} \quad (2.62)$$

with,

$$\boxed{\chi_{BA_i}^R(\mathbf{r}, t; \mathbf{r}', t') = \frac{i}{\hbar} \langle [B^0(\mathbf{r}, t), A_i^0(\mathbf{r}', t')] \rangle \theta(t - t')}. \quad (2.63)$$

This response function 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. For the moment, recall that the superscript 0 here means to zeroth order in the external probe. In other words, the linear response is given by an equilibrium correlation function. One normally does not write the superscript 0 which is usually kept to mean non-interacting system. *From now on, we drop this superscript.*

¹We 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 2 *Translationally invariant case:* Since we compute equilibrium averages, the susceptibility $\chi_{BA_i}^R(\mathbf{r}, t; \mathbf{r}', t')$ 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 (2.62), we obtain from the convolution theorem in this case,

$$\boxed{\delta \langle B(\mathbf{q}, \omega) \rangle = \chi_{BA_i}^R(\mathbf{q}, \omega) a_i(\mathbf{q}, \omega).} \quad (2.64)$$

Remark 3 *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 4 *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’’.

Remark 5 *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 $k_B T$, the linearization should be correct. In other words, linear response theory should be valid for a time

$$t < \frac{k_B T}{e E v}. \quad (2.65)$$

This is unfortunately a ridiculously small time. Taking $v \approx \sqrt{k_B T/m}$ the condition becomes $t < \sqrt{m k_B T}/e E$ with $E = 1\text{V/cm}$, $\sqrt{m k_B T}/e E \approx \sqrt{10^{-30} 10^{-23} 10^2}/10^{-19} \approx 10^{-6}\text{s}$. Indeed, 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.[2] 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. In a Boltzmann picture, 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.[2]

Remark 6 *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.[3] We will see explicitly later that it is possible to compute irreversible absorption with this approach. We will also see how irreversibility comes in the infinite-volume limit.

2.3 General properties of correlation functions

It is useful to know 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 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!

2.3.1 Notations and definitions

To start with, recall the definition

$$\chi_{BA}^R(\mathbf{r}, t; \mathbf{r}', t') = \frac{i}{\hbar} \langle [B(\mathbf{r}, t), A(\mathbf{r}', t')] \rangle \theta(t - t'). \quad (2.66)$$

We have removed the superscript 0 which was only used as a crutch in the derivation of linear-response theory to indicate that the operators were evolving with the unperturbed Hamiltonian. Since the unperturbed Hamiltonian in the present context is the full Hamiltonian of the system, including interactions, we will drop the superscript 0 from now on. It will be used later in a context where the unperturbed Hamiltonian is that of non-interacting particles.

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

$$\boxed{\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \frac{1}{2\hbar} \langle [B(\mathbf{r}, t), A(\mathbf{r}', t')] \rangle}. \quad (2.67)$$

The two in the denominator looks strange, but it will allow χ'' to generally be the imaginary part of a response function without extra factors of 2. With this definition, we have

$$\chi_{BA}^R(\mathbf{r}, t; \mathbf{r}', t') = 2i\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t')\theta(t - t'). \quad (2.68)$$

To shorten the notation, we will also use the notation

$$\boxed{\chi_{A_i A_j}^R(t - t') = \frac{i}{\hbar} \langle [A_i(t), A_j(t')] \rangle \theta(t - t')}. \quad (2.69)$$

In this notation 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.

Exercise 2.3.1 *Check time-translational invariance explicitly by using Heisenberg's representation, the cyclic property of the trace and the fact that the density matrix ($Z^{-1}e^{-\beta H}$ in the canonical ensemble, or $\Xi^{-1}e^{-\beta(H-\mu N)}$ in the grand-canonical) commutes with the time-evolution operator $e^{-iHt/\hbar}$.*

Corresponding to the short-hand notation, we have

$$\boxed{\chi''_{A_i A_j}(t - t') \equiv \frac{1}{2\hbar} \langle [A_i(t), A_j(t')] \rangle}. \quad (2.70)$$

$$\boxed{\chi_{A_i A_j}^R(t - t') = 2i\chi''_{A_i A_j}(t - t')\theta(t - t')}. \quad (2.71)$$

2.3.2 Symmetry properties of the response functions

The quantity $\chi''_{A_i A_j}(t-t')$ 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. Let us consider them in turn.[1]

Properties that depend on the symmetry of the Hamiltonian

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

$$[H, S] = 0 \quad (2.72)$$

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

$$[\rho, S] = 0 \quad (2.73)$$

In other words, $S^{-1}\rho S = \rho$ 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, one first takes advantage of the fact that the trace can be computed in any complete basis set. This means that the thermal average of any operator \mathcal{O} is equal to its thermal average in a basis where the symmetry operation S has been applied to every basis function. Since the symmetry operation commutes with the density matrix by assumption, one can then let the symmetry operations act on the operators instead of on the basis functions. In other words, we have

$$\langle S^{-1}\mathcal{O}S \rangle = \langle \mathcal{O} \rangle \quad (2.74)$$

It is because S and \mathcal{O} in general do not commute that the above equation leads to non-trivial consequences.

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

- *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,

$$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} + \mathbf{R}, t; \mathbf{r}' + \mathbf{R}, t') \quad (2.75)$$

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

$$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} - \mathbf{r}'; t - t') \quad (2.76)$$

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).

- *Parity*: Under a parity transformation, operators transform as follows

$$P^{-1}\mathcal{O}(\mathbf{r})P = \varepsilon^P\mathcal{O}(-\mathbf{r}) \quad (2.77)$$

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, $\varepsilon_\rho^P = 1$ for density since performing the symmetry operation $\mathbf{r}_\alpha \rightarrow -\mathbf{r}_\alpha$ for every particle coordinate appearing in the density operator

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^N e_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \quad (2.78)$$

we find

$$P^{-1}\rho(\mathbf{r})P = \sum_{\alpha=1}^N e_\alpha \delta(\mathbf{r} + \mathbf{r}_\alpha) = \sum_{\alpha=1}^N e_\alpha \delta(-\mathbf{r} - \mathbf{r}_\alpha) = \rho(-\mathbf{r}) \quad (2.79)$$

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

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^N \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r} - \mathbf{r}_\alpha) \quad (2.80)$$

$$P^{-1}\mathbf{p}(\mathbf{r})P = \sum_{\alpha=1}^N -\frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r} + \mathbf{r}_\alpha) = -\sum_{\alpha=1}^N \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(-\mathbf{r} - \mathbf{r}_\alpha) = -\mathbf{p}(-\mathbf{r}) \quad (2.81)$$

In general then, this implies that

$$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{r}, t; -\mathbf{r}', t') \quad (2.82)$$

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

$$\boxed{\chi''_{BA}(\mathbf{q}; t - t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{q}; t - t')} \quad (2.83)$$

- *Time-reversal symmetry in the absence of spin*: From the Schrödinger equation in the absence of spin, one can see that when the Hamiltonian is real, then complex conjugation leads to an equation that evolves the complex conjugate wave function as if $t \rightarrow -t$. We thus take time-reversed states as just this operation of complex conjugation. 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 [4] and Sakurai [8]. We present an oversimplified 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 is 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

$$\langle \alpha | X | \beta \rangle = \langle \alpha | (X | \beta \rangle) = (\langle \alpha | X) | \beta \rangle \quad (2.84)$$

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 \underline{K} when we want to take the complex conjugate of a ket, and \overline{K} to take the complex conjugate of a bra.

Remark 7 *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*

$$T_t (a_1 |\psi_1\rangle + a_2 |\psi_2\rangle) = a_1^* T_t |\psi_1\rangle + a_2^* T_t |\psi_2\rangle \quad (2.85)$$

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 $\langle \psi_1 | \underline{K} \underline{K} | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle \neq \langle \psi_1 | \psi_2 \rangle$ 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[4] 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 $|\langle \psi_2 | \psi_1 \rangle| = |\langle \psi'_2 | \psi'_1 \rangle|$ (equality of “rays”) then both unitary and anti-unitary transformations are allowed.

Remark 8 *The adjoint is not the inverse. Note that $T_t^\dagger T_t = \underline{K} \underline{K}$, 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

$$\langle i | \underline{K} \underline{O} \underline{K} | j \rangle = \left(\langle i | \underline{K} \right) \left(\underline{K} \underline{O}^* | j \rangle \right) = (\langle i | \underline{O}^* | j \rangle)^* = \langle j | \underline{O}^{\dagger*} | i \rangle. \quad (2.86)$$

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 $\mathcal{A} : \langle k | \mathcal{A} | l \rangle^* = \langle l | \mathcal{A}^\dagger | k \rangle$. Applying this expression Eq.(2.86) for diagonal expectation values, and recalling that the density matrix is real, we find for equilibrium averages,

$$\left\langle \underline{K} \underline{O} \underline{K} \right\rangle = \langle \underline{O}^{\dagger*} \rangle = \epsilon^t \langle \underline{O}^\dagger \rangle \quad (2.87)$$

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... 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.(2.87) gives, when A and B are *self-adjoint* operators, and $\underline{K} H = H \underline{K}$

$$\begin{aligned} \left\langle \underline{K} A(t) B \underline{K} \right\rangle &= \left\langle B^* e^{-iHt/\hbar} A^* e^{iHt/\hbar} \right\rangle \\ &= \epsilon_A^t \epsilon_B^t \langle BA(-t) \rangle \end{aligned} \quad (2.88)$$

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

$$\chi''_{A_i A_j}(t-t') = \epsilon_i^t \epsilon_j^t \chi''_{A_j A_i}(-t' - (-t)) \quad (2.89)$$

and for the corresponding Fourier transform in frequency,

$$\boxed{\chi''_{A_i A_j}(\omega) = \epsilon_i^t \epsilon_j^t \chi''_{A_j A_i}(\omega)}. \quad (2.90)$$

Remark 9 *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.(2.74),*

$$\langle T_t^{-1} \mathcal{O} T_t \rangle = \langle \mathcal{O} \rangle. \quad (2.91)$$

Hence as expected, Eqs.(2.87) and (2.91) together imply that operators that have an odd signature with respect to time reversal symmetry have a vanishing expectation value in equilibrium.

- *Time-reversal symmetry in the presence of spin:* 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

$$T_t = \underline{K} U \quad (2.92)$$

where \underline{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

$$U^\dagger \underline{K} \quad (2.93)$$

Let us first repeat the steps of calculating expectation values in time-reversed states, as in Eq.(2.86), but for the more general case

$$\langle i | U^\dagger \underline{K} \mathcal{O} \underline{K} U | j \rangle = \left(\langle i | U^\dagger \underline{K} \right) \left(\underline{K} \mathcal{O}^* U | j \rangle \right) = \left(\langle i | U^\dagger \mathcal{O}^* U | j \rangle \right)^* = \langle j | U^\dagger \mathcal{O}^\dagger{}^* U | i \rangle \quad (2.94)$$

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

$$U^\dagger \boldsymbol{\sigma}^\dagger{}^* U = -\boldsymbol{\sigma} \quad (2.95)$$

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

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad ; \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad ; \quad \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (2.96)$$

we have $\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$, and $\sigma_x^* = \sigma_x$, $\sigma_y^* = -\sigma_y$, $\sigma_z^* = \sigma_z$ so that Eq.(2.95) for time reversal gives us the following set of equations for the unitary operator U

$$U^\dagger \sigma_x U = -\sigma_x \quad (2.97)$$

$$U^\dagger \sigma_y U = \sigma_y \quad (2.98)$$

$$U^\dagger \sigma_z U = -\sigma_z \quad (2.99)$$

Given the fundamental properties of Pauli matrices

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

$$\sigma_i^2 = 1 \quad (2.100)$$

$$\sigma_i \sigma_j = i \sigma_k \quad (2.101)$$

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

$$U = e^{i\delta} \sigma_y \quad (2.102)$$

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.

$$T_t = \underline{K} e^{i\delta} \sigma_y \quad (2.103)$$

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

$$T_t |\uparrow\rangle = -ie^{-i\delta} |\downarrow\rangle \quad (2.104)$$

$$T_t |\downarrow\rangle = ie^{-i\delta} |\uparrow\rangle \quad (2.105)$$

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 $T_t T_t |\uparrow\rangle = -|\uparrow\rangle$, 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.[4] 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 (2.107) and of Hermiticity (2.109) 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.

Properties that follow from the definition.

Let us thus write down the general symmetry properties of $\chi''_{A_i A_j}(t - t')$ that simply follow from its definition (2.70).

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

$$\chi''_{A_i A_j}(t - t') = -\chi''_{A_j A_i}(t' - t) \quad (2.106)$$

which in frequency space reads,

$$\boxed{\chi''_{A_i A_j}(\omega) = -\chi''_{A_j A_i}(-\omega)}. \quad (2.107)$$

- *Hermiticity*: Taking the observables as Hermitian, as is usually the case, one can use the cyclic property of the trace and the Hermiticity of the density matrix to show that

$$\chi''_{A_i A_j}(t-t') = \left[\chi''_{A_j A_i}(t'-t) \right]^*. \quad (2.108)$$

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

In Fourier space, this becomes,

$$\boxed{\chi''_{A_i A_j}(\omega) = \left[\chi''_{A_j A_i}(\omega) \right]^*}. \quad (2.109)$$

Remark 10 *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.

Remark 11 *Most useful property*: The most important consequence of this section that we will often use is that correlation functions such as $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega)$ are odd in frequency and real

$$\boxed{\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(-\omega) = \left[\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) \right]^*}. \quad (2.110)$$

To prove this, we first use Hermiticity Eq.(2.109) in the form

$$\chi''_{\rho_{\mathbf{r}} \rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'} \rho_{\mathbf{r}}}(\omega) \right]^* \quad (2.111)$$

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

$$\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) = \int d^3 \mathbf{r} \int d^3 \mathbf{r}' e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \chi''_{\rho_{\mathbf{r}} \rho_{\mathbf{r}'}}(\omega) \quad (2.112)$$

$$= \left[\int d^3 \mathbf{r} \int d^3 \mathbf{r}' e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \chi''_{\rho_{\mathbf{r}'} \rho_{\mathbf{r}}}(\omega) \right]^* \quad (2.113)$$

$$= \left[\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) \right]^* \quad (2.114)$$

The commutator property Eq.(2.107), $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{-\mathbf{q}} \rho_{\mathbf{q}}}(-\omega)$ and symmetry under parity transformation Eq.(2.83), $\chi''_{\rho_{-\mathbf{q}} \rho_{\mathbf{q}}}(-\omega) = \chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(-\omega)$ then suffice to show that $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega)$ is also odd in frequency $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(-\omega)$. Instead of parity, one could have invoked time-reversal symmetry Eq.(2.90) and the commutator property Eq.(2.107) to show that $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega)$ is odd since then $\chi''_{\rho_{\mathbf{r}} \rho_{\mathbf{r}'}}(\omega) = \chi''_{\rho_{\mathbf{r}'} \rho_{\mathbf{r}}}(\omega) = -\chi''_{\rho_{\mathbf{r}'} \rho_{\mathbf{r}}}(-\omega)$ immediately implies that $\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}} \rho_{-\mathbf{q}}}(-\omega)$.

2.3.3 Kramers-Kronig relations and causality

These Kramers-Kronig relations are by far the best known and most useful relations. They relate real and imaginary parts of response functions and they come simply from causality. Causality is insured by the presence of the θ function in the expression for the response functions Eq.(2.71). 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.(2.62). Kramers-Kronig relations are the same causality statement as above, seen from the perspective of Fourier transforms. To be more specific, in this section we will derive the following results:

$$\boxed{\operatorname{Re} \left[\chi_{A_i A_j}^R(\omega) \right] = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\operatorname{Im} \left[\chi_{A_i A_j}^R(\omega') \right]}{\omega' - \omega}} \quad (2.115)$$

$$\boxed{\operatorname{Im} \left[\chi_{A_i A_j}^R(\omega) \right] = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\operatorname{Re} \left[\chi_{A_i A_j}^R(\omega') \right]}{\omega' - \omega}} \quad (2.116)$$

They come from analytic properties of the response functions in the complex frequency plane. We give two derivations.

The straightforward manner:

Let us first derive the relations the easy way. Suppose that we know the Fourier transform in frequency $\chi_{A_i A_j}^R(\omega)$ of the response function. We call it the retarded function because the response comes after the perturbation. It is causal. One way to make sure that its real time version $\chi_{A_i A_j}^R(t - t')$ contains $\theta(t - t')$ is to have $\chi_{A_i A_j}^R(\omega)$ analytic in the upper half-plane. To see that analyticity in the upper half-plane is a sufficient condition to have $\theta(t - t')$, consider

$$\chi_{A_i A_j}^R(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \chi_{A_i A_j}^R(\omega). \quad (2.117)$$

If $t - t'$ is negative, then it is possible to close the contour in the upper half plane since the exponential will decrease at positive imaginary frequencies. Since $\chi_{A_i A_j}^R(\omega)$ is analytic in that half-plane, the result will be zero, which is just another way to say that $\chi_{A_i A_j}^R(t - t')$ is proportional to $\theta(t - t')$, as we had planned to show. In the next subsection, we will show that analyticity in the upper half plane is also a necessary condition to have $\theta(t - t')$.

Assuming that $\chi_{A_i A_j}^R(\omega)$ is analytic in the upper half plane, it is then easy to derive the Kramers-Kronig relations. It now suffices to use

$$\int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\eta} \chi_{A_i A_j}^R(\omega') = 2i \chi_{A_i A_j}^R(\omega + i\eta) \quad (2.118)$$

which is easy to prove by applying the residue theorem on a contour closed in the upper half plane where $\chi_{A_i A_j}^R(\omega)$ is analytic. This also assumes that $\chi_{A_i A_j}^R(\omega')$ falls off at least like a small power of $1/\omega'$ so that there is no contribution from the part at ∞ . We then need the following identity,

$$\lim_{\eta \rightarrow 0} \frac{1}{\omega \mp i\eta} = \lim_{\eta \rightarrow 0} \frac{\omega \pm i\eta}{\omega^2 + \eta^2} = \lim_{\eta \rightarrow 0} \left[\frac{\omega}{\omega^2 + \eta^2} \pm \frac{i\eta}{\omega^2 + \eta^2} \right] = \mathcal{P} \frac{1}{\omega} \pm i\pi\delta(\omega) \quad (2.119)$$

where δ is Dirac's delta function and \mathcal{P} means principal part integral. — Suppose the factor $1/(\omega + i\eta)$ on the left is in an integral that can be done by contour integration. Then, knowing the definition of the delta function, this can be used as the definition of principal part.— Using this identity and setting equal the real parts of our contour integral (2.118) we obtain, upon taking the $\lim \eta \rightarrow 0$,

$$\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\operatorname{Re} \left[\chi_{A_i A_j}^R(\omega') \right]}{\omega' - \omega} - \operatorname{Im} \left[\chi_{A_i A_j}^R(\omega) \right] = -2 \operatorname{Im} \left[\chi_{A_i A_j}^R(\omega) \right] \quad (2.120)$$

while from the imaginary part,

$$\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} \left[\chi_{A_i A_j}^R(\omega') \right]}{\omega' - \omega} + \text{Re} \left[\chi_{A_i A_j}^R(\omega) \right] = 2 \text{Re} \left[\chi_{A_i A_j}^R(\omega) \right]. \quad (2.121)$$

This is precisely what we mean by the Kramers-Kronig relations, namely we recover the results Eqs.(2.115)(2.116) at the beginning of this section. From the proof just given, Kramers-Kronig relations will apply if

- $\chi_{A_i A_j}^R(\omega)$ is analytic, as a function of complex frequency, in the upper half-plane.
- $\chi_{A_i A_j}^R(\omega)$ falls off at least as a small power of ω at infinity.

Spectral representation and alternate derivation.

It is instructive to perform a derivation which starts from what we found earlier. We will gain as a bonus an explicit expression for real and imaginary parts in terms of correlation functions, as well as a derivation of the analyticity properties from scratch. In fact this will also complete the proof that analyticity in the upper half-plane is both necessary and sufficient to have causality.

Using the convolution theorem, we would write for the frequency-space version of the response functions, (2.71)

$$\chi_{A_i A_j}^R(\omega) = 2i \int \frac{d\omega'}{2\pi} \chi_{A_i A_j}''(\omega') \theta(\omega - \omega'). \quad (2.122)$$

This looks nice, but it does not really mean anything yet because we encounter a serious problem when we try to evaluate the Fourier transform of the θ function. Indeed,

$$\int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) = \frac{e^{i\omega t}}{i\omega} \Big|_0^{\infty} \quad (2.123)$$

and we have no idea what $e^{i\omega\infty}$ means. To remedy this, we have to return to the expression for the linear response (2.62). Assuming that the external field a_i is turned-on adiabatically from $t = -\infty$, we multiply whatever we had before by $e^{\eta t}$, taking the limit of vanishing η at the end of the calculation. We also adiabatically turn off the *response* at $t \rightarrow \infty$ by using a factor $e^{-\eta t}$. The equation for the response in time (2.71) is then simply multiplied by $e^{\eta(t-t')}$, so that it still depends only on the time difference. Furthermore, when we take its Fourier transform, $\int_{-\infty}^{\infty} d(t-t') e^{i\omega(t-t')} e^{-\eta(t-t')}$, 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. To be more specific, the equation for the response (2.71) now reads,

$$\chi_{A_i A_j}^R(t-t') e^{-\eta(t-t')} = 2i \chi_{A_i A_j}''(t-t') \theta(t-t') e^{-\eta(t-t')} \quad (2.124)$$

so that in the calculation of the response (2.122) we have,

$$\int_{-\infty}^{\infty} d(t-t') e^{i(\omega+i\eta-\omega')(t-t')} \theta(t-t') = \frac{e^{i(\omega+i\eta-\omega')(t-t')}}{i(\omega+i\eta-\omega')} \Big|_0^{\infty} = \frac{1}{i(\omega'-\omega-i\eta)}. \quad (2.125)$$

Everything behaves as if we had computed the Fourier transform for $\omega+i\eta$ instead of ω ,

$$\chi_{A_i A_j}^R(\omega+i\eta) = 2i \int \frac{d\omega'}{2\pi} \chi_{A_i A_j}''(\omega') \theta(\omega+i\eta-\omega') \quad (2.126)$$

$$= \int \frac{d\omega'}{\pi} \frac{\chi''_{A_i A_j}(\omega')}{\omega' - (\omega + i\eta)}. \quad (2.127)$$

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

$$\chi_{A_i A_j}(z) = \int \frac{d\omega'}{\pi} \frac{\chi''_{A_i A_j}(\omega')}{\omega' - z} \quad (2.128)$$

we can write for the retarded response,

$$\chi_{A_i A_j}^R(\omega) = \lim_{\eta \rightarrow 0} \chi_{A_i A_j}(z)|_{z=\omega+i\eta} \quad (2.129)$$

and for the advanced one,

$$\chi_{A_i A_j}^A(\omega) = \lim_{\eta \rightarrow 0} \chi_{A_i A_j}(z)|_{z=\omega-i\eta}. \quad (2.130)$$

Using the above results, it is easy to see that $\chi_{A_i A_j}^R(\omega)$ is analytic in the upper half plane, while $\chi_{A_i A_j}^A(\omega)$ is analytic in the lower-half plane. One can even explicitly see from the equation (2.127) for the function which is analytic in the upper-half plane $\chi_{A_i A_j}^R(\omega)$ that the poles or the integrand in the lower-half frequency plane are just below the real axis, a distance η along the imaginary direction. The residue at a given pole will depend on the value of $\chi''_{A_i A_j}$ at the corresponding value of the real coordinate of the pole.

Remark 12 *If $\chi''_{A_i A_j}(\omega')$ is given by a sum of delta function, then $\chi_{A_i A_j}(z)$ has a series of poles just below the real axis. This is what occurs with the so-called Lehman representation that we will discuss later. On the other hand, if $\chi''_{A_i A_j}(\omega')$ is a continuous function, as occurs in an infinite system, then the poles of $\chi_{A_i A_j}(z)$ are below the real axis, but not necessarily close to it. The passage from a series of poles to a continuous function is what introduces irreversibility in many-body systems.*

Definition 3 *Equations such as (2.128) are called spectral representations.*

Remark 13 *Why spectral representation: The reason for this name is that, as we discuss in the next section below, $\chi''_{A_i A_j}(\omega')$ 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.*

$\chi_{A_i A_j}(z)$ is a function which is equal to $\chi_{A_i A_j}^R(\omega)$ for z infinitesimally above the real axis, and to $\chi_{A_i A_j}^A(\omega)$ for z infinitesimally below the real axis. On the real axis of the complex z plane $\chi_{A_i A_j}(z)$ has a cut whenever $\chi''_{A_i A_j}(\omega) \neq 0$ since

$$\left[\chi_{A_i A_j}(\omega + i\eta) - \chi_{A_i A_j}(\omega - i\eta) \right] = 2i\chi''_{A_i A_j}(\omega). \quad (2.131)$$

So much for taking the Fourier transform of a response which is so simple looking in its ordinary time version Eq.(2.71). Time-reversal invariance (2.90) and Hermiticity in Eq.(2.109) imply, for two operators with the same signature under time-reversal, that $\chi''_{A_i A_j}(\omega')$ is a real function. Hence, from the mathematical

identity for principal part Eq.(2.119) and from the spectral representation (2.128) we have, for two hermitian operators A_i, A_j with the same signature under time reversal, that

$$\boxed{\text{Im} \left[\chi_{A_i A_j}^R(\omega) \right] = \chi''_{A_i A_j}(\omega)} \quad (2.132)$$

so that from the spectral representation we recover the first of the Kramers-Krönig relation (2.115). The other one can be derived following the same route as in the simpler derivation, namely apply $\int \frac{d\omega}{\pi} \frac{1}{\omega - \omega' + i\eta}$ on both sides of the spectral representation. For two hermitian operators A_i, A_j with opposite signatures under time reversal Eqs.(2.90) and (2.109) imply that $\chi''_{A_i A_j}(\omega')$ is purely imaginary. In this case,

$$\boxed{\text{Re} \left[\chi_{A_i A_j}^R(\omega) \right] = i\chi''_{A_i A_j}(\omega)}. \quad (2.133)$$

Remark 14 *Kramers-Kronig and time reversal: The Kramers Krönig relations do not depend on these subtleties of signatures under time-reversal. However the relation between real and imaginary parts of the response and commutator Eq.(2.132) does. If we can compute either the real or imaginary part of the response, the Kramers Krönig relations give us the part we do not know. In any case, everything about the system is in $\chi''_{A_i A_j}(\omega)$.*

2.3.4 Positivity of $\omega\chi''(\omega)$ and dissipation

We want to show that the key function of the previous discussion, namely $\chi''_{A_i A_j}(\omega)$ 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 $\omega\chi''_{A_i A_j}(\omega)$ 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.(2.25), this means that the power dissipated by the external world is

$$\frac{dW}{dt} = \frac{d\delta\mathcal{H}(t)}{dt} = - \int d^3r A_i(\mathbf{r}) \frac{da_i(\mathbf{r}, t)}{dt} = -A_i \frac{da_i(t)}{dt}. \quad (2.134)$$

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

$$\frac{dW}{dt} = - [\langle A_i \rangle + \langle \delta A_i \rangle] \frac{da_i(t)}{dt} \quad (2.135)$$

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,

$$\overline{W} = - \int_{-T/2}^{T/2} dt \langle \delta A_i(t) \rangle \frac{da_i(t)}{dt} > 0. \quad (2.136)$$

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

$$- \int \frac{d\omega}{2\pi} \langle \delta A_i(\omega) \rangle i\omega a_i(-\omega) > 0. \quad (2.137)$$

Finally, linear response theory gives

$$- \int \frac{d\omega}{2\pi} a_i(-\omega) \chi_{A_i A_j}^R(\omega) i\omega a_j(\omega) > 0 \quad (2.138)$$

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

$$\overline{W} = -\frac{1}{2} \int \frac{d\omega}{2\pi} a_i(-\omega) \left[\chi_{A_i A_j}^R(\omega) - \chi_{A_j A_i}^R(-\omega) \right] i\omega a_j(\omega) > 0. \quad (2.139)$$

Calling the spectral representation (2.129) to the rescue, we can write

$$\left[\chi_{A_i A_j}^R(\omega) - \chi_{A_j A_i}^R(-\omega) \right] = \int \frac{d\omega'}{\pi} \frac{\chi_{A_i A_j}''(\omega')}{\omega' - (\omega + i\eta)} - \int \frac{d\omega'}{\pi} \frac{\chi_{A_j A_i}''(\omega')}{\omega' - (-\omega + i\eta)}. \quad (2.140)$$

We know from the fact that $\chi_{A_i A_j}''$ is a commutator that (2.107) $\chi_{A_i A_j}''(\omega) = -\chi_{A_j A_i}''(-\omega)$. Using this identity and the change of variables $\omega' \rightarrow -\omega'$ in the last integral, we immediately have that

$$\left[\chi_{A_i A_j}^R(\omega) - \chi_{A_j A_i}^R(-\omega) \right] = \int \frac{d\omega'}{\pi} \chi_{A_i A_j}''(\omega') \left[\frac{1}{\omega' - \omega - i\eta} + \frac{1}{-\omega' + \omega - i\eta} \right] \quad (2.141)$$

$$= 2i \chi_{A_i A_j}''(\omega). \quad (2.142)$$

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

$$\int \frac{d\omega}{2\pi} a_i^*(\omega) \left[\chi_{A_i A_j}''(\omega) \omega \right] a_j(\omega) > 0. \quad (2.143)$$

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

$$\boxed{a_i^*(\omega) \left[\chi_{A_i A_j}''(\omega) \omega \right] a_j(\omega) > 0} \quad (2.144)$$

for all frequencies. This is the definition of a positive-definite matrix. Going to the basis where $\chi_{A_i A_j}''$ is diagonal, we see that this implies that all the eigenvalues are positive. Also, when there is only one kind of external perturbation applied,

$$\boxed{\chi_{A_i A_i}''(\omega) \omega > 0.} \quad (2.145)$$

We have seen that for Hermitian operators with the same signature under time reversal, $\chi_{A_i A_i}''(\omega)$ is a real and odd function of frequency so the above equation is satisfied. The positive definiteness of $\chi_{A_i A_j}''(\omega) \omega$ by itself however does not suffice to prove that $\chi_{A_i A_i}''(\omega)$ is an odd function of frequency.

One can check explicitly that $\chi_{A_i A_i}''(\omega)$ contains spectral information about excited states by doing backwards the steps that lead us from Fermi's golden rule to correlation functions.

2.3.5 Fluctuation-dissipation theorem

This very useful theorem relates linear response to equilibrium fluctuations measured in scattering experiments. It takes the form,

$$\boxed{S_{A_i A_j}(\omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \chi_{A_i A_j}''(\omega) = 2\hbar(1 + n_B(\omega)) \chi_{A_i A_j}''(\omega)} \quad (2.146)$$

where $n_B(\omega) = 1/(e^{\beta\hbar\omega} - 1)$ is the Bose factor while the “structure factor” or correlation function is defined by,

$$S_{A_i A_j}(t) \equiv \langle A_i(t)A_j \rangle - \langle A_i \rangle \langle A_j \rangle = \langle (A_i(t) - \langle A_i \rangle)(A_j(0) - \langle A_j \rangle) \rangle \quad (2.147)$$

$$\equiv \langle \delta A_i(t) \delta A_j \rangle. \quad (2.148)$$

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.(2.146) is a correlation function for dissipation while the right-hand side contains the dissipation function χ'' just discussed. This is a key theorem of statistical physics.

To prove the theorem, it suffices to trivially relate the definitions,

$$\chi''_{A_i A_j}(t) = \frac{1}{2\hbar} \langle [A_i(t), A_j] \rangle = \frac{1}{2\hbar} \langle [\delta A_i(t), \delta A_j] \rangle = \frac{1}{2\hbar} (S_{A_i A_j}(t) - S_{A_j A_i}(-t)) \quad (2.149)$$

then to use the key identity,

$$\boxed{S_{A_j A_i}(-t) = S_{A_i A_j}(t - i\hbar\beta)}. \quad (2.150)$$

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, time-translation invariance follows, and

$$S_{A_j A_i}(-t) = Z^{-1} Tr [e^{-\beta H} \delta A_j(-t) \delta A_i] = Z^{-1} Tr [e^{-\beta H} \delta A_j \delta A_i(t)] \quad (2.151)$$

To reverse the order of δA_i and δA_j , it suffices to use the cyclic property, so that

$$S_{A_j A_i}(-t) = Z^{-1} Tr [\delta A_i(t) e^{-\beta H} \delta A_j]. \quad (2.152)$$

Simple manipulations and Heisenberg’s representation for the time-evolution of the operators gives,

$$S_{A_j A_i}(-t) = Z^{-1} Tr [e^{-\beta H} e^{\beta H} \delta A_i(t) e^{-\beta H} \delta A_j] \quad (2.153)$$

$$= Z^{-1} Tr [e^{-\beta H} \delta A_i(t - i\hbar\beta) \delta A_j] = S_{A_i A_j}(t - i\hbar\beta). \quad (2.154)$$

This is precisely what we wanted to prove. The rest is an exercise in Fourier transforms,

$$\int dt e^{i\omega t} S_{A_i A_j}(t - i\hbar\beta) = \int dt e^{i\omega(t+i\hbar\beta)} S_{A_i A_j}(t) = e^{-\beta\hbar\omega} S_{A_i A_j}(\omega). \quad (2.155)$$

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 $e^{iHt} A e^{-iHt}$ 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 $\chi''_{A_i A_j}(t)$ and susceptibility Eq.(2.149), one then recovers the fluctuation-dissipation theorem (2.146).

A few remarks before concluding.

Remark 15 *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,*

$$S_{A_i A_j}(t - i\hbar\beta) = e^{-i\hbar\beta \frac{\partial}{\partial t}} S_{A_i A_j}(t).$$

Remark 16 *Relation to detailed balance: The Fourier-space version of the periodicity condition (2.150) is a statement of detailed balance:*

$$\boxed{S_{A_j A_i}(-\omega) = e^{-\beta \hbar \omega} S_{A_i A_j}(\omega)}. \quad (2.156)$$

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). 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..

Remark 17 *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.*

2.3.6 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.

Thermodynamic sum-rules.

Suppose we compute the linear response to a time-independent perturbation. For example, compute the response of the magnetization to a time-independent magnetic field. This should give us the susceptibility. Naturally, we have to leave the adiabatic switching-on, i.e. the infinitesimal η . In general then,

$$\delta \langle A_i(\omega = 0) \rangle = \chi_{A_i A_j}^R(\omega = 0) a_j(\omega = 0). \quad (2.157)$$

Returning to the notation where \mathbf{q} is explicitly written,

$$\delta \langle A_i(\mathbf{q}, \omega = 0) \rangle = \chi_{A_i A_j}^R(\mathbf{q}, \omega = 0) a_j(\mathbf{q}, \omega = 0). \quad (2.158)$$

Using the spectral representation (2.128) and the usual relation between $i\eta$ and principal parts, Eq.(2.119), we also have,

$$\chi_{A_i A_j}^R(\mathbf{q}, \omega = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi_{A_i A_j}''(\mathbf{q}, \omega)}{\omega - i\eta} = \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi_{A_i A_j}''(\mathbf{q}, \omega)}{\omega}. \quad (2.159)$$

There is no contribution from the imaginary part on the grounds that there can be no dissipation zero-frequency dissipation in a stable system. In fact, as long as the thermodynamic derivatives involve operators that have the same symmetry under time reversal, then $\chi''_{A_i A_j}(\mathbf{q}, \omega)$ is odd, as proven at the end of the section on symmetry properties, so that $\chi''_{A_i A_j}(\mathbf{q}, \omega = 0) = 0$. Note that in practice, the principal part in the above equation is not necessary since $\chi''_{A_i A_j}(\mathbf{q}, \omega)$ usually vanishes linearly in ω for small ω . To be completely general however, it is preferable to keep the principal part.

Recalling that the thermodynamic derivatives are in general for uniform ($\mathbf{q} = 0$) applied probes, the above formula become,

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \chi_{A_i A_j}^R(\mathbf{q}, \omega = 0) = \frac{\partial A_i}{\partial a_j} \equiv \chi_{A_i A_j}. \quad (2.160)$$

$$\boxed{\chi_{A_i A_j} = \lim_{\mathbf{q} \rightarrow \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q}, \omega)}{\omega}}. \quad (2.161)$$

This is called a thermodynamic sum-rule. As an example, consider the density n response. It obeys the so-called compressibility sum rule,

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \chi_{nn}^R(\mathbf{q}, \omega = 0) = \lim_{\mathbf{q} \rightarrow \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} = \left(\frac{\partial n}{\partial \mu} \right)_{T, V}. \quad (2.162a)$$

As usual, a few remarks are in order:

Remark 18 *Order of limits: It is extremely important to note that for thermodynamic sum rules, the $\omega \rightarrow 0$ limit is taken first, before the $\mathbf{q} \rightarrow 0$ limit. The other limit describes transport properties as we shall see. Another important question is that of the principal part integral. As follows from a problem set, in the long wave length limit we have $\chi''_{nn}(\mathbf{q}, \omega) = \frac{2Dq^2\omega}{\omega^2 + (Dq^2)^2} \chi_{nn}$ where D is the diffusion constant. One can check explicitly with that form 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.(2.162a). If we take the limit $\mathbf{q} \rightarrow \mathbf{0}$ before doing the integral however, $\lim_{\mathbf{q} \rightarrow \mathbf{0}} \chi''_{nn}(\mathbf{q}, \omega)$ takes the form $\omega\delta(\omega)$ so it is important NOT to take the principal part integral to get the correct result (in other words, under the integral sign the $\eta \rightarrow 0$ limit must be taken before the $\mathbf{q} \rightarrow \mathbf{0}$ limit). We also see this as follows. If we return to the original form $\lim_{\eta \rightarrow 0} 1/(\omega - i\eta) = \lim_{\eta \rightarrow 0} \omega/(\omega^2 + \eta^2) + i\eta/(\omega^2 + \eta^2)$, and then do the integral of the first term (real part), we can check that we have to take the $\eta \rightarrow 0$ limit under the integral sign before the $\mathbf{q} \rightarrow \mathbf{0}$ limit to recover the result obtained by doing the integral at finite \mathbf{q} and then taking the $\mathbf{q} \rightarrow \mathbf{0}$ 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*

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} = \lim_{\mathbf{q} \rightarrow \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} \quad (2.162)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q} \rightarrow \mathbf{0}} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} \quad (2.162)$$

$$\neq \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q} \rightarrow \mathbf{0}} \frac{\chi''_{nn}(\mathbf{q}, \omega)}{\omega} \quad (2.162)$$

Remark 19 *Thermodynamic sum-rule and moments: Thermodynamic sum-rules are in a sense the inverse first moment over frequency of $\chi''_{A_i A_j}(\mathbf{q}, \omega)$ (the latter being analogous to the weight). Other sum-rules are over positive moments, as we now demonstrate.*

Alternate derivation. Here is another way to derive the thermodynamic sum rules. First note that thermodynamic variables involve conserved quantities, namely quantities that commute with the Hamiltonian. Take for example N , the total number of particles. Since N commutes with the Hamiltonian, in the grand-canonical ensemble we have the classical result

$$\langle NN \rangle - \langle N \rangle^2 = \frac{1}{\beta} \left(\frac{\partial n}{\partial \mu} \right)_{T,V}$$

By definition,

$$\langle NN \rangle - \langle N \rangle^2 = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{NN}(\omega) \quad (2.166)$$

Using the general fluctuation-dissipation theorem, we now relate this quantity to $\chi''_{NN}(\omega)$ as follows. 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. For such a conserved quantity, the fluctuation-dissipation theorem Eq.(2.146) then becomes

$$S_{NN}(\omega) = \lim_{\omega \rightarrow 0} \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \chi''_{NN}(\omega) = \frac{2}{\beta\omega} \chi''_{NN}(\omega) \quad (2.167)$$

from which we obtain what is basically the thermodynamic sum-rule Eq.(2.162a)

$$\langle NN \rangle - \langle N \rangle^2 = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{NN}(\omega) \quad (2.168a)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{NN}(\omega)}{\beta\omega} = \frac{1}{\beta} \left(\frac{\partial n}{\partial \mu} \right)_{T,V} \quad (2.168b)$$

This is then the classical form of the fluctuation-dissipation theorem. In this form, the density fluctuations are related to the response $(\partial n / \partial \mu)_{T,V}$ (itself related to the compressibility).

Moments, sum rules, and high-frequency expansions.

Odd derivatives of $\chi''_{A_i A_j}$ at equal-time are easy to compute and provide us with moments:

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \chi''_{A_i A_j}(\omega) &= \left(i \frac{\partial}{\partial t} \right)^n \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} 2\chi''_{A_i A_j}(\omega) \right]_{t=0} \\ &= \frac{1}{\hbar} \left\langle \left[\left(i \frac{\partial}{\partial t} \right)^n A_i(t), A_j(0) \right] \right\rangle_{t=0} = \frac{1}{\hbar} \left\langle \left[\left[\left[A_i(t), \frac{H}{\hbar} \right], \frac{H}{\hbar} \right], \dots, A_j(0) \right] \right\rangle_{t=0} \end{aligned} \quad (2.169)$$

(2.170)

which may all easily be computed through n equal-time commutations with the Hamiltonian.

Suppose the spectrum of excitations is bounded, as usually happens when the input momentum \mathbf{q} is finite. Then, $\chi''_{A_i A_j}(\omega') = 0$ for $\omega' > D$ where D is some large frequency. Then, for $\omega > D$, we can expand the denominator since the condition $\omega'/\omega \ll 1$ will always be satisfied. This gives us a high-frequency expansion,

$$\chi_{A_i A_j}^R(\mathbf{q}, \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q}, \omega')}{\omega' - \omega - i\eta} \quad (2.171)$$

$$\approx \sum_{n=1}^{\infty} \frac{-1}{\omega^{2n}} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} (\omega')^{2n-1} \chi''_{A_i A_j}(\mathbf{q}, \omega') \quad (2.172)$$

where we have explicitly taken into account the fact that only odd moments of $\chi''_{A_i A_j}$ do not vanish because it is an odd function. Clearly, in the $\omega \rightarrow \infty$ limit, the susceptibilities in general scale as $1/\omega^2$, a property we will use later in the context of analytic continuations.

The f sum-rule as an example.

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

$$\boxed{\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q}, \omega) = \frac{n\mathbf{q}^2}{m}.} \quad (2.173)$$

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. The proof is as follows. We first use the above results for moments

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q}, \omega) = \frac{i}{\hbar\mathcal{V}} \left\langle \left[\frac{\partial n_{\mathbf{q}}(t)}{\partial t}, n_{-\mathbf{q}}(t) \right] \right\rangle \quad (2.174)$$

$$= -\frac{1}{\hbar^2\mathcal{V}} \langle [[H, n_{\mathbf{q}}(t)], n_{-\mathbf{q}}(t)] \rangle \quad (2.175)$$

In the first equality, we have also used translational invariance to write,

$$\int d(\mathbf{r} - \mathbf{r}') e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} f(\mathbf{r} - \mathbf{r}') = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \int d\mathbf{r}' e^{-i\mathbf{q}\cdot\mathbf{r}'} f(\mathbf{r} - \mathbf{r}') \quad (2.176)$$

where \mathcal{V} is the integration volume. The computation of the equal-time commutator is self-explanatory,

$$n_{\mathbf{q}} = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}) = \sum_{\alpha} e^{-i\mathbf{q}\cdot\mathbf{r}_{\alpha}} \quad (2.177)$$

$$[p_{\beta}^x, n_{\mathbf{q}}] = \frac{\hbar}{i} \left[\frac{\partial}{\partial x_{\beta}}, \sum_{\alpha} e^{-i\mathbf{q}\cdot\mathbf{r}_{\alpha}} \right] = -\hbar q^x e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}. \quad (2.178)$$

Assuming that the interactions commute with the density operator, and using $[\mathbf{p} \cdot \mathbf{p}, n] = \mathbf{p} [\mathbf{p}, n] + [\mathbf{p}, n] \mathbf{p}$ we have

$$[H, n_{\mathbf{q}}(t)] = \sum_{\beta} \left[\frac{p_{\beta}^2}{2m}, n_{\mathbf{q}} \right] = \frac{1}{2m} \sum_{\beta} (\mathbf{p}_{\beta} \cdot (-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}) + (-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}) \cdot \mathbf{p}_{\beta}) \quad (2.179)$$

$$[[H, n_{\mathbf{q}}(t)], n_{-\mathbf{q}}(t)] = -\frac{1}{m} \sum_{\beta=1}^N \hbar^2 \mathbf{q}^2 e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}} e^{i\mathbf{q}\cdot\mathbf{r}_{\beta}} = -\frac{\hbar^2 \mathbf{q}^2 N}{m} \quad (2.180)$$

which proves the result (2.173) when substituted in the expression in terms of commutator (2.175) 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.)

2.4 Kubo formula 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. It is 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, we discuss in turn longitudinal and transverse response, exposing the consequences of gauge invariance. After a brief application to the definition of superconductors, metals and insulators, we make the connection between conductivity and dielectric constant.

2.4.1 Response of the current to external vector and scalar potentials

Our discussion follows that of Baym [5]. In the presence of an electromagnetic field, observable quantities must be invariant under the gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda \quad (2.181)$$

$$\phi \rightarrow \phi - \frac{1}{c} \frac{\partial\Lambda}{\partial t} \quad (2.182)$$

$$\Psi \rightarrow e^{ie\Lambda/\hbar c} \Psi \quad (2.183)$$

where the last transformation is the transformation for a one-body Schrodinger wave function. The coupling of a particle of charge e is obtained then by the substitution

$$\mathbf{p}_\alpha = \frac{\hbar}{i} \nabla_\alpha \rightarrow \frac{\hbar}{i} \nabla_\alpha - \frac{e}{c} \mathbf{A}(\mathbf{r}_\alpha). \quad (2.184)$$

The kinetic-energy operator is also modified by the addition of the vector potential. In a general gauge,

$$-\frac{\hbar^2}{2m} \nabla_\alpha^2 \rightarrow -\frac{\hbar^2}{2m} \nabla_\alpha^2 - \frac{e\hbar}{2mci} (\mathbf{A}(\mathbf{r}_\alpha) \cdot \nabla_\alpha + \nabla_\alpha \cdot \mathbf{A}(\mathbf{r}_\alpha)) + \frac{e^2}{2mc^2} \mathbf{A}^2(\mathbf{r}_\alpha). \quad (2.185)$$

This means that to linear order in the vector potential, the change in the Hamiltonian is

$$\delta\mathcal{H}(t) = - \sum_\alpha \frac{e\hbar}{2mci} (\mathbf{A}(\mathbf{r}_\alpha) \cdot \nabla_\alpha + \nabla_\alpha \cdot \mathbf{A}(\mathbf{r}_\alpha)) = -\frac{1}{c} \int d\mathbf{r} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{j}(\mathbf{r}). \quad (2.186)$$

where, continuing with our first-quantization point of view, the current so-called *paramagnetic current* for particles of charge e was defined by,

$$\mathbf{j}(\mathbf{r}) = \frac{e}{2m} \sum_\alpha (\delta(\mathbf{r} - \mathbf{r}_\alpha) \mathbf{p}_\alpha + \mathbf{p}_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha)). \quad (2.187)$$

Given the fact that $[\mathbf{r}_\beta, \mathbf{p}_\alpha] = i\hbar\delta_{\alpha,\beta}$ there is an ambiguity in 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.

Given Eq.(2.184) for the momentum and the effect of gauge transformations on observables, as in Eq.(2.181), the gauge-invariant (observable) current operator $\mathbf{j}^A(\mathbf{r})$ to linear order in the vector potential is

$$\mathbf{j}^A(\mathbf{r}) = \mathbf{j}(\mathbf{r}) - \frac{e^2}{mc} \sum_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}) \delta(\mathbf{r} - \mathbf{r}_{\alpha}) = \mathbf{j}(\mathbf{r}) - \frac{e}{mc} \mathbf{A}(\mathbf{r}) \rho(\mathbf{r}) \quad (2.188)$$

where we have defined the charge density as before $\rho(\mathbf{r}) = en(\mathbf{r})$.

Remark 20 Remark 21 Our definition of the current-density operator Eq.(2.187) automatically takes care of the relative position of the vector potential and of the gradients in the above equation.

Remark 22 * The gauge invariant current $\mathbf{j}^A(\mathbf{r})$ operator may also be obtained from a functional derivative of the second order in \mathbf{A} Hamiltonian with respect to vector potential.

It is easier to add an ordinary scalar potential! The modification is then only in the Hamiltonian:

$$\delta\mathcal{H}(t) = \int d\mathbf{r} \phi(\mathbf{r}, t) \rho(\mathbf{r}). \quad (2.189)$$

Using the explicit expression for the current Eq.(2.188) and our linear-response formulae, we have that the general expression for the response is

$$\delta \langle j_{\mu}^A(\mathbf{q}, \omega) \rangle = \left[\chi_{j_{\mu} j_{\nu}}^R(\mathbf{q}, \omega) - \frac{ne^2}{m} \delta_{\mu\nu} \right] \frac{A_{\nu}(\mathbf{q}, \omega)}{c} - \chi_{j_{\mu} \rho}^R(\mathbf{q}, \omega) \phi(\mathbf{q}, \omega). \quad (2.190)$$

There is a sum over the repeated indices ν . The term proportional to $-\frac{ne^2}{m} \delta_{\mu\nu}$ in this expression, called the diamagnetic term, comes from the last term in the expression for the gauge invariant current Eq.(2.188). 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 formula Eq.(2.190) may be used to compute the response to an arbitrary external electromagnetic field since as usual,

$$\mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - \nabla \phi \quad (2.191)$$

$$\mathbf{B} = \nabla \times \mathbf{A}. \quad (2.192)$$

2.4.2 Kubo formula for the transverse response

When we study the response to applied fields whose direction is perpendicular to the direction of \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 field is always transverse since $\nabla \cdot \mathbf{B} = \nabla \cdot \nabla \times \mathbf{A} = 0$. Let us decompose the vector potential into a transverse and a longitudinal part. This is easily done by using the unit vector $\hat{\mathbf{q}} = \mathbf{q}/|\mathbf{q}|$

$$\mathbf{A}^L \equiv \hat{\mathbf{q}} \hat{\mathbf{q}} \cdot \mathbf{A} \equiv \hat{\mathbf{q}} (\hat{\mathbf{q}} \cdot \mathbf{A}) \quad (2.193)$$

$$\mathbf{A}^T \equiv \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}} \right) \cdot \mathbf{A}. \quad (2.194)$$

In the last equation, $\overleftrightarrow{\mathbf{I}}$ is the vector notation for $\delta_{\mu\nu}$. We introduced the following notation for the multiplication of tensors with vectors,

$$\left(\overleftrightarrow{\sigma} \cdot \mathbf{A} \right)_\mu = \sum_\nu \sigma_{\mu\nu} A_\nu. \quad (2.195)$$

The transverse and longitudinal parts of a tensor are obtained as follows,

$$\overleftrightarrow{\sigma}^T(\mathbf{q}, \omega) = \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}} \right) \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}} \right) \quad (2.196)$$

$$\overleftrightarrow{\sigma}^L(\mathbf{q}, \omega) = \widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q}, \omega) \cdot \widehat{\mathbf{q}}\widehat{\mathbf{q}} \quad (2.197)$$

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 usually in a wire made of homogeneous and isotropic material in the presence of the skin effect. This is illustrated in Fig.(2-2).

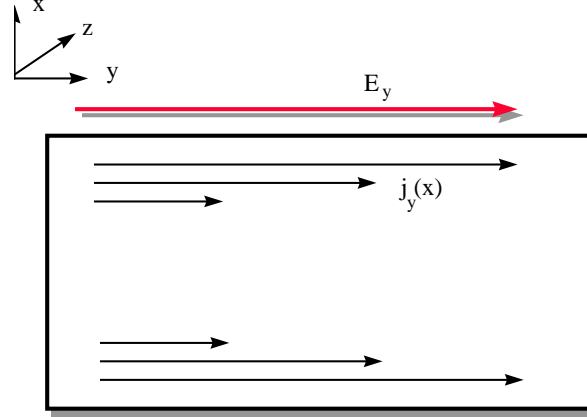


Figure 2-2 Application of a transverse electric field: skin effect.

Then the conductivity defined by $\delta \langle j_y(q_x, \omega) \rangle \equiv \sigma_{yy}(q_x, \omega) E_y(q_x, \omega)$ follows from the relation between current and vector potential Eq.(2.190) and the relation $E_y(q_x, \omega) = i(\omega + i\eta)A_y(q_x, \omega)/c$ between vector potential and electric field.

$$\sigma_{yy}(q_x, \omega) = \frac{1}{i(\omega + i\eta)} \left[\chi_{j_y j_y}^R(q_x, \omega) - \frac{ne^2}{m} \right] \quad (2.198)$$

In writing the relation between transverse electric field and vector potential, 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.

2.4.3 Kubo formula for the longitudinal response

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.(2.190) in a way that makes the response look explicitly invariant under gauge transformations. As usual current conservation and gauge invariance are intimately related!

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = -\nabla \cdot \mathbf{j}(\mathbf{r}, t) \quad (2.199)$$

$$\frac{\partial \rho(\mathbf{q}, t)}{\partial t} = -i\mathbf{q} \cdot \mathbf{j}(\mathbf{q}, t) \quad (2.200)$$

Take \mathbf{q} in the x direction to be specific. Some gymnastics on the susceptibility in terms of commutator gives,

$$\frac{\partial \chi_{j_x \rho}^R(q_x, t)}{\partial t} = \delta(t) \frac{i}{\hbar \mathcal{V}} \langle [j_x(q_x, 0), \rho(-q_x, 0)] \rangle + \theta(t) \frac{i}{\hbar \mathcal{V}} (-iq_x) \langle [j_x(q_x, 0), j_x(-q_x, -t)] \rangle. \quad (2.201)$$

The equal-time commutator is calculated from the f sum rule. First use the definition of $\chi_{j_x \rho}''(q_x, \omega)$

$$\frac{i}{\hbar \mathcal{V}} \langle [j_x(q_x, 0), \rho(-q_x, 0)] \rangle = i \int \frac{d\omega}{\pi} \chi_{j_x \rho}''(q_x, \omega) \quad (2.202)$$

then current conservation

$$= i \int \frac{d\omega}{\pi} \frac{\omega}{q_x} \chi_{\rho \rho}''(q_x, \omega) \quad (2.203)$$

and finally the f sum rule Eq.(2.173) to rewrite the last expression as

$$= iq_x \frac{ne^2}{m} \quad (2.204)$$

Substituting back in the expression for the time derivative of the current-charge susceptibility Eq.(2.201) and Fourier transforming in frequency, we have

$$\boxed{-i(\omega + i\eta) \chi_{j_x \rho}^R(q_x, \omega) = iq_x \frac{ne^2}{m} - iq_x \chi_{j_x j_x}^R(q_x, \omega).} \quad (2.205)$$

Using this in the general formula for the response of the current Eq.(2.190) the longitudinal linear response function can be written in terms of the gauge invariant electric field in two different ways:

$$\delta \langle j_x(q_x, \omega) \rangle = \frac{1}{i(\omega + i\eta)} \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right] \left(\frac{i(\omega + i\eta) A_x(q_x, \omega)}{c} - iq_x \phi(q_x, \omega) \right) \quad (2.206)$$

$$= \left[\frac{1}{iq_x} \chi_{j_x \rho}^R(q_x, \omega) \right] \left(\frac{i(\omega + i\eta) A_x(q_x, \omega)}{c} - iq_x \phi(q_x, \omega) \right). \quad (2.207)$$

Hence, replacing the gauge-invariant combination of potentials by the field,

$$E_x(q_x, \omega) = \frac{i(\omega + i\eta) A_x(q_x, \omega)}{c} - iq_x \phi(q_x, \omega) \quad (2.208)$$

we find the following Kubo formulae for the longitudinal conductivity $\delta \langle j_x(q_x, \omega) \rangle \equiv \sigma_{xx}(q_x, \omega) E_x(q_x, \omega)$

$$\boxed{\sigma_{xx}(q_x, \omega) = \frac{1}{i(\omega + i\eta)} \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right] = \left[\frac{1}{iq_x} \chi_{j_x \rho}^R(q_x, \omega) \right].} \quad (2.209)$$

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.

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,

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda \quad (2.210)$$

$$\phi \rightarrow \phi - \frac{1}{c} \frac{\partial\Lambda}{\partial t} \quad (2.211)$$

Let $\phi = 0$. Then

$$\delta \langle j_x(q_x, \omega) \rangle = \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right] \frac{A_x(q_x, \omega)}{c} \quad (2.212)$$

Doing a gauge transformation with $\Lambda(x, t)$ 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 should be zero since it corresponds to zero electric field. This will be the case if

$$\boxed{\left[\chi_{j_x j_x}^R(q_x, 0) - \frac{ne^2}{m} \right] = 0} \quad (2.213)$$

This can be proven explicitly by using the spectral representation and $\chi_{j_x j_x}''(q_x, 0) = 0$,

$$\chi_{j_x j_x}^R(q_x, 0) = \int \frac{d\omega'}{\pi} \frac{\chi_{j_x j_x}''(q_x, \omega')}{\omega'} \quad (2.214)$$

as well as the conservation of charge,

$$= \int \frac{d\omega'}{\pi} \frac{\chi_{j_x j_x}''(q_x, \omega')}{\omega'} = \int \frac{d\omega'}{\pi} \frac{\omega' \chi_{\rho\rho}''(q_x, \omega')}{q_x^2} \quad (2.215)$$

and the f -sum rule (2.173)

$$= \frac{1}{q_x^2} \int \frac{d\omega'}{\pi} \omega' \chi_{\rho\rho}''(q_x, \omega') = \frac{ne^2}{m} = \chi_{j_x j_x}^R(q_x, 0). \quad (2.216)$$

The form

$$\boxed{\int \frac{d\omega'}{\pi} \frac{\chi_{j_x j_x}''(q_x, \omega')}{\omega'} = \frac{ne^2}{m}} \quad (2.217)$$

of the above result, obtained by combining Eqs.(2.213) and (2.214) will be used quite often below.

Another possibility is to let $\mathbf{A} = 0$. Then, the general Kubo formula (2.190) gives

$$\delta \langle j_x(\mathbf{q}, \omega) \rangle = -\chi_{j_x \rho}^R(\mathbf{q}, \omega) \phi(\mathbf{q}, \omega). \quad (2.218)$$

If we let $\Lambda(x, t)$ 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 must be zero, hence

$$\boxed{\chi_{j_x \rho}^R(0, \omega) = 0} \quad (2.219)$$

That this is true, again follows from current conservation since

$$\chi_{j_x \rho}^R(0, \omega) = \int \frac{d\omega'}{\pi} \frac{\chi_{j_x \rho}''(0, \omega')}{\omega' - \omega - i\eta} \quad (2.220)$$

and

$$\chi''_{j_x\rho}(0, \omega') = \int dt e^{i\omega t} \frac{1}{2\hbar\mathcal{V}} \left\langle \left[\int d\mathbf{r} j_\mu(\mathbf{r}, \mathbf{t}), \int d\mathbf{r}' \rho(\mathbf{r}') \right] \right\rangle = 0 \quad (2.221)$$

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 23 Both results Eq.(2.213) and Eq.(2.219) are consistent with the general relation found between both types of correlation functions Eq.(2.205). It suffices to take the $\mathbf{q} \rightarrow 0$ limit assuming that $\chi_{j_x j_x}^R(q_x, \omega)$ is finite or diverges less slowly than $1/q_x$ to prove Eq.(2.219) and to take $\omega \rightarrow 0$ assuming that $\chi_{j_\mu\rho}^R(q_x, \omega)$ is finite or diverges less slowly than $1/\omega$ to prove Eq.(2.213).

Longitudinal conductivity sum-rule and an alternate expression for the longitudinal conductivity.

The expression for the longitudinal conductivity

$$\sigma_{xx}(q_x, \omega) = \frac{1}{i(\omega + i\eta)} \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right] \quad (2.222)$$

can be written in an even more convenient manner by using our previous results Eq.(2.217) obtained from the f -sum rule and the spectral representation for the current-current correlation function

$$\sigma_{xx}(q_x, \omega) = \frac{1}{i(\omega + i\eta)} \left[\int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x, \omega')}{\omega' - \omega - i\eta} - \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x, \omega')}{\omega'} \right] \quad (2.223)$$

$$= \frac{1}{i(\omega + i\eta)} \left[\int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x, \omega')(\omega + i\eta)}{\omega'(\omega' - \omega - i\eta)} \right] \quad (2.224)$$

$$\boxed{\sigma_{xx}(q_x, \omega) = \frac{1}{i} \left[\int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x, \omega')}{\omega'(\omega' - \omega - i\eta)} \right]} \quad (2.225)$$

From this formula, we easily obtain with the usual identity for principal parts, Eq.(2.119)

$$\boxed{\text{Re } \sigma_{xx}(q_x, \omega) = \frac{\chi''_{j_x j_x}(q_x, \omega)}{\omega}} \quad (2.226)$$

from which we obtain the conductivity sum rule valid for arbitrary q_x

$$\boxed{\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \text{Re} [\sigma_{xx}(q_x, \omega)] = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\chi''_{j_x j_x}(q_x, \omega)}{\omega} = \frac{ne^2}{2m} = \frac{\omega_p^2}{8\pi}} \quad (2.227)$$

directly from the f -sum rule Eq.(2.217). In the above expression, ω_p^2 is the plasma frequency. 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 24 *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,*

$$\boxed{\sigma_{xx}(q_x, \omega) = \mathcal{P} \frac{1}{i\omega} \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right] - \pi\delta(\omega) \left[\chi_{j_x j_x}^R(q_x, \omega) - \frac{ne^2}{m} \right]} \quad (2.228)$$

is obtained from Eq.(2.222) 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,

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \operatorname{Re} [\sigma_{xx}(q_x, \omega)] &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\chi''_{j_x j_x}(q_x, \omega)}{\omega} - \frac{\operatorname{Re} \chi_{j_x j_x}^R(q_x, 0)}{2} + \frac{ne^2}{2m} \\ &= \frac{ne^2}{2m}. \end{aligned}$$

Remark 25 *Practical use of sum rule: The n that appears in the conductivity sum rule is the full electronic density. In practical 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 26 *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 27 *If we need to consider the $q_x \rightarrow 0$ 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.*

Drude weight and zero frequency conductivity

In everything that preceded, the magnitude of \mathbf{q} was arbitrary. Let us now look at the response for a uniform, or very long wavelength field, i.e. $q_x \rightarrow 0$. It is important to notice that this is the proper way to compute the *DC* conductivity: Take the $\mathbf{q} \rightarrow 0$ limit, before the $\omega \rightarrow 0$ limit. In the opposite limit the response vanishes as we saw from gauge invariance (2.213). 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 $\mathbf{q} \rightarrow \mathbf{0}$ limit first, we ensure that we are looking at an infinite volume, where energy levels can be arbitrarily 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.

In the correct limit, the above formulas (2.226) and (2.228) for conductivity give us either the simple formula,

$$\operatorname{Re} [\sigma_{xx}(0, \omega)] = \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} \quad (2.229)$$

or the more complicated-looking formula

$$\operatorname{Re} [\sigma_{xx}(0, \omega)] = \mathcal{P} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} - \pi \delta(\omega) \left[\operatorname{Re} [\chi_{j_x j_x}^R(0, \omega)] - \frac{ne^2}{m} \right] \quad (2.230)$$

Note that since the conductivity sum rule is satisfied for arbitrary q_x , it is also satisfied here. It is also easy to prove by directly integrating the last equation as we have just done in one of last remarks of the last section. The coefficient of the delta function at zero frequency $\delta(\omega)$ is called the Drude weight D :

$$D = \pi \lim_{\omega \rightarrow 0} \left[\frac{ne^2}{m} - \operatorname{Re} [\chi_{j_x j_x}^R(0, \omega)] \right]. \quad (2.231)$$

Remark 28 *Alternate derivation:* To be reassured that the Drude weight would also come out from the first expression for the conductivity Eq.(2.229), it suffices to show that both expressions are equal, namely that

$$\frac{\chi''_{j_x j_x}(0, \omega)}{\omega} - \mathcal{P} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} = -\pi \delta(\omega) \left[\text{Re} [\chi_{j_x j_x}^R(0, \omega)] - \frac{ne^2}{m} \right] \quad (2.232)$$

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

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} - \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{j_x j_x}(0, \omega)}{\omega} \quad (2.233)$$

$$= \lim_{\omega \rightarrow 0} \lim_{q_x \rightarrow 0} \left[\frac{ne^2}{m} - \text{Re} [\chi_{j_x j_x}^R(q_x, \omega)] \right] \quad (2.234)$$

an expression that is clearly correct, as can be shown by using the spectral representation (or Kramers-Kronig representation) of the current-current correlation function and the f -sum rule Eq.(2.217).

Remark 29 *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.(2.222), that it can also be extracted from the imaginary part,

$$D = \pi \lim_{\omega \rightarrow 0} \omega \text{Im} [\sigma_{xx}(0, \omega)] \quad (2.235)$$

2.4.4 Metals, insulators and superconductors

For free electrons, the $q_x \rightarrow 0$ conductivity is a delta function at zero-frequency whose Drude weight is $D = \pi ne^2/m$.

Proof: Write Newton's equation of motion for the current,

$$\frac{\partial \mathbf{j}(\mathbf{q} = \mathbf{0}, t)}{\partial t} = \frac{ne^2}{m} \mathbf{E}(\mathbf{q} = \mathbf{0}, t) \quad (2.236)$$

$$\mathbf{j}(\mathbf{q} = \mathbf{0}, \omega) = -\frac{1}{i(\omega + i\eta)} \frac{ne^2}{m} \mathbf{E}(\mathbf{q} = \mathbf{0}, \omega) \quad (2.237)$$

then the conductivity has only a Drude contribution (free acceleration).

$$\text{Re} \frac{\mathbf{j}(\mathbf{q} = \mathbf{0}, \omega)}{\mathbf{E}(\mathbf{q} = \mathbf{0}, \omega)} = \text{Re} \sigma(\mathbf{q} = \mathbf{0}, \omega) = \pi \frac{ne^2}{m} \delta(\omega) \quad (2.238)$$

For interacting electrons, the current of a single particle is no longer a conserved quantity and there is a contribution from $\pi \lim_{\omega \rightarrow 0} \text{Re} [\chi_{j_x j_x}^R(0, \omega)]$. The rest of the weight is at finite frequency. Hence, the criterion given by Kohn [6] for a system to be a *metal* is that it has a non-zero Drude weight Eq.(2.231), or in other words a finite *DC* conductivity. In a realistic situation where impurities or inelastic processes outside the electronic system are present, the situation becomes more complicated because the δ function is broadened.

Kohn's criterion [6] to have an *insulator* is that it has a vanishing *DC* conductivity (or equivalently $D = 0$). This is the case whenever

$$\lim_{\omega \rightarrow 0} \text{Re} [\chi_{j_x j_x}^R(0, \omega)] = \lim_{\omega \rightarrow 0} \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\chi_{j_x j_x}''(0, \omega')}{\omega' - \omega} = \frac{ne^2}{m} \quad (2.239)$$

Recalling the result obtained from the f -sum rule (or equivalently from gauge invariance), (2.217)

$$\chi_{j_x j_x}^R(q_x, 0) = \int \frac{d\omega'}{\pi} \frac{\chi_{j_x j_x}''(q_x, \omega')}{\omega'} = \frac{ne^2}{m} \quad (2.240)$$

this means that a system is an insulator only when the order of limits can be inverted:

$$\lim_{\omega \rightarrow 0} \lim_{q_x \rightarrow 0} \text{Re} [\chi_{j_x j_x}^R(q_x, \omega)] = \lim_{q_x \rightarrow 0} \lim_{\omega \rightarrow 0} \text{Re} [\chi_{j_x j_x}^R(q_x, \omega)]. \quad (2.241)$$

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 30 *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. [7]*

Finally, *superconductors* are an interesting case. While gauge invariance (or f -sum rule) implies (2.213) that

$$\left[\chi_{j_x j_x}^R(q_x, 0) - \frac{ne^2}{m} \right] = 0. \quad (2.242)$$

there is no such principle that forces the *transverse* response to vanish. Indeed, gauge transformations (2.181) are always longitudinal. Hence, it is possible to have,

$$\left[\chi_{j_y j_y}^R(q_x, 0) - \frac{ne^2}{m} \right] = -\frac{n_s e^2}{m} \quad (2.243)$$

where n_s is any density less than n . A superconductor will indeed have such a non-vanishing “transverse Drude weight”. We will show in Eq.(2.258) below that positivity of the dissipation implies that n_s cannot be larger than n .

Definition 4 n_s is called the *superfluid density*.

Remark 31 *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.*

Proof: Assume this is the case. Then we will show that the system exhibits perfect screening of magnetic fields (the Meissner effect). This is done by starting from the general formula for the response to a transverse electromagnetic field (2.190)

$$\delta \langle j_\mu^T(\mathbf{q}, \omega) \rangle = \left[\left(\chi_{j_\mu j_\nu}^R(\mathbf{q}, \omega) \right)^T - \frac{ne^2}{m} \delta_{\mu\nu} \right] \frac{A_\nu^T(\mathbf{q}, \omega)}{c}.$$

To simplify the discussion, we take a simple case where the \mathbf{q} dependence of the prefactor can be neglected in the zero-frequency limit, (we keep the zeroth order term in the power series in \mathbf{q}),

$$\delta \langle j_{\mu}^T(\mathbf{q}, 0) \rangle = -\frac{n_s e^2}{m} \frac{A_{\mu}^T(\mathbf{q}, 0)}{c}. \quad (2.244)$$

We have written n_s to emphasize that this quantity is in general different from n . This quantity, n_s is called the superfluid density. The above equation is the so-called London equation. Taking the curl on both sides of the Fourier transformed expression,

$$\nabla \times \delta \langle \mathbf{j}(\mathbf{r}, \omega=0) \rangle = -\frac{n_s e^2}{m} \frac{\mathbf{B}(\mathbf{r}, \omega=0)}{c} \quad (2.245)$$

and then employing Maxwell's equation $\nabla \times \mathbf{B}(\mathbf{r}, \omega=0) = 4\pi \mathbf{j}(\mathbf{r}, \omega=0)/c$ 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,

$$\nabla^2(\mathbf{B}) = \frac{4\pi n_s e^2}{mc^2} \mathbf{B} \quad (2.246)$$

whose solution in the half-plane geometry shown in figure (2-3) is,

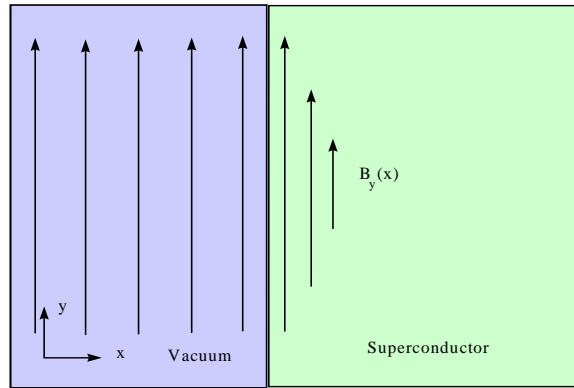


Figure 2-3 Penetration depth in a superconductor.

$$B_y(x) = B_y(0)e^{-x/\lambda_L}$$

with the London penetration depth

$$\lambda_L^{-2} = \frac{4\pi n_s e^2}{mc^2}. \quad (2.247)$$

In the case where $n_s = n$, which often occurs at zero temperature, then

$$c^2 = \omega_p^2 \lambda_L^2. \quad (2.248)$$

The magnetic field is completely expelled from a superconductor. This is perfect diamagnetism.

Why are the transverse and longitudinal zero-frequency responses different in a superconductor? This can happen only if

$$\lim_{q_x \rightarrow 0} \chi_{j_x j_x}^R(q_x, 0, \omega = 0) \neq \lim_{q_y \rightarrow 0} \chi_{j_x j_x}^R(0, q_y, \omega = 0) \quad (2.249)$$

	D	D_S
Metal	D	0
Insulator	0	0
Superconductor	D	D_S

Table 2.1 Difference between metal, insulator and superconductor, as seen from the limiting value of correlation functions

or in other words

$$\lim_{q_x \rightarrow 0} \int dt \int d\mathbf{r} e^{-iq_x x} \chi_{j_x j_x}^R(\mathbf{r}, \omega = 0) \neq \lim_{q_y \rightarrow 0} \int dt \int d\mathbf{r} e^{-iq_y y} \chi_{j_x j_x}^R(\mathbf{r}, \omega = 0). \quad (2.250)$$

This occurs in a superconductor because long-range order leads to $\chi_{j_x j_x}^R(\mathbf{r}, \omega = 0)$ which does not decay fast enough for the integral to be uniformly convergent. 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 all cases

$$\left[\chi_{j_x j_x}^R(q_x, 0) - \frac{ne^2}{m} \right] = 0 \quad (2.251)$$

by gauge invariance (f -sum rule) Eq.(2.213). 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 (2.231)

$$D = \pi \lim_{\omega \rightarrow 0} \left[\frac{ne^2}{m} - \text{Re} [\chi_{j_x j_x}^R(0, \omega)] \right] \quad (2.252)$$

and the transverse analog of the f -sum rule,

$$\boxed{D_S = \pi \lim_{q_x \rightarrow 0} \left[\frac{ne^2}{m} - \chi_{j_y j_y}^R(q_x, 0) \right]} \quad (2.253)$$

As we just saw, contrary to its longitudinal analog, D_S is not constrained to vanish by gauge invariance. It is instead related to the inverse penetration depth in a superconductor. The table summarizes the results.

Remark 32 *Definition of superconductor:* 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, neither metal nor insulators have a non-zero D_S .

Remark 33 *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.

2.4.5 Conductivity sum rules at finite wave vector, transverse and longitudinal

Let us first establish the transverse conductivity sum rule for finite wave vector probes, such as microwaves, or electromagnetic radiation in general. Following the last paragraph of the previous section, a superconductor exhibits a zero-frequency

delta function response at finite wave-vector in the transverse response. Indeed, starting from the Kubo formula Eq.(2.198)

$$\text{Re } \sigma_{yy}(q_x, \omega) = \mathcal{P} \frac{1}{\omega} \left[\chi''_{j_y j_y}(q_x, \omega) \right] - \pi \delta(\omega) \left[\text{Re } \chi_{j_y j_y}^R(q_x, 0) - \frac{ne^2}{m} \right] \quad (2.254)$$

$$= \mathcal{P} \frac{\chi''_{j_y j_y}(q_x, \omega)}{\omega} + D_S(q_x) \delta(\omega) \quad (2.255)$$

In this last expression, D_S can in principle now depend on q_x . Normally the penetration depth is large ($q_x \rightarrow 0$) and that dependence can be neglected. The sum-rule for the conductivity is established by starting from the first from of the above equations, Eq.(2.254)

$$\begin{aligned} \lim_{q_x \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \text{Re}[\sigma_{yy}(q_x, \omega)] &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega} \left[\chi''_{j_y j_y}(q_x, \omega) \right] - \frac{1}{2} \left[\text{Re } \chi_{j_y j_y}^R(q_x, 0) - \frac{ne^2}{m} \right] \\ &= \frac{ne^2}{2m}. \end{aligned} \quad (2.256)$$

Although written for the transverse case, clearly the last value $ne^2/(2m)$ would be obtained for the longitudinal response as well. And it is valid for a superconductor as well as for a normal metal.

However, in the case of a superconductor, if we do not include the delta function for the transverse response Eq.(2.255), then we have

$$\begin{aligned} \lim_{q_x \rightarrow 0} \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \text{Re}[\sigma_{yy}(q_x, \omega)] &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega} \left[\chi''_{j_y j_y}(q_x, \omega) \right] \\ &= \frac{1}{2} \text{Re } \chi_{j_y j_y}^R(q_x, 0) \end{aligned} \quad (2.257)$$

$$= \frac{(n - n_s) e^2}{2m} \quad (2.258)$$

where we used the result Eq.(2.243) for $\text{Re } \chi_{j_y j_y}^R(q_x, 0)$. This last expression would be equal to $ne^2/(2m)$ only for the longitudinal response. The missing weight for the transverse response is in the delta function at the origin. The weight of that delta function is $D_S/(2\pi) = n_s e^2/2m$. It is necessarily less than $ne^2/(2m)$ so that $n_s < n$ as we had promised to prove.

In a conductivity experiment with electromagnetic radiation, the piece proportional to $\delta(\omega)$ is not accessible, so the above result prevails.

Remark 34 *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 35 *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,*

$$\text{Im } \sigma_{yy}(q_x, \omega) = \frac{1}{\omega} \left[\frac{ne^2}{m} - \text{Re } \chi_{j_y j_y}^R(q_x, \omega) \right] - \pi \delta(\omega) \chi''_{j_y j_y}(q_x, 0) \quad (2.259)$$

$$\lim_{\omega \rightarrow 0} \omega \text{Im } \sigma_{yy}(q_x, \omega) = \frac{D_S}{\pi} \quad (2.260)$$

since $\chi''_{j_y j_y}(q_x, 0) = 0$.

2.4.6 Relation between conductivity and dielectric constant

The relation between dielectric constant and conductivity is a matter of macroscopic electromagnetism. The dielectric constant is basic to optical measurements, hence it will be useful to relate it to correlation functions that we can compute later.

Let us consider a translationally invariant system, so that it suffices to consider the Fourier-space version of Maxwell's equations

$$i\mathbf{q} \cdot \mathbf{E} = 4\pi\rho \quad (2.261)$$

$$i\mathbf{q} \times \mathbf{E} = \frac{i(\omega + i\eta)}{c} \mathbf{B} \quad (2.262)$$

$$i\mathbf{q} \cdot \mathbf{B} = 0 \quad (2.263)$$

$$i\mathbf{q} \times \mathbf{B} = \frac{4\pi}{c} \mathbf{j} - \frac{i(\omega + i\eta)}{c} \mathbf{E}. \quad (2.264)$$

Transverse dielectric constant.

Using the definition of transverse conductivity, the last of Maxwell's equations reads,

$$i\mathbf{q} \times \mathbf{B} = \frac{4\pi}{c} \overset{\leftarrow}{\sigma}^T \cdot \mathbf{E} - \frac{i(\omega + i\eta)}{c} \mathbf{E}. \quad (2.265)$$

Using the second Maxwell equation on the left-hand side, as well as $i\mathbf{q} \cdot \mathbf{E} = 0$ for transverse response and $\mathbf{q} \times (\mathbf{q} \times \mathbf{E}) = \mathbf{q}(\mathbf{q} \cdot \mathbf{E}) - q^2 \mathbf{E}$, we have

$$q^2 \mathbf{E} = \frac{4\pi i(\omega + i\eta)}{c^2} \overset{\leftarrow}{\sigma}^T \cdot \mathbf{E} + \frac{(\omega + i\eta)^2}{c^2} \mathbf{E} \equiv \frac{(\omega + i\eta)^2}{c^2} \overset{\leftarrow}{\epsilon}^T \mathbf{E} \quad (2.266)$$

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,

$$\overset{\leftarrow}{\epsilon}^T(\mathbf{q}, \omega) = 1 + \frac{4\pi i}{(\omega + i\eta)} \overset{\leftarrow}{\sigma}^T \quad (2.267)$$

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 expression for the conductivity in terms of response function, we have that

$$\boxed{\overset{\leftarrow}{\epsilon}^T(\mathbf{q}, \omega) = \left(1 - \frac{\omega_p^2}{(\omega + i\eta)^2}\right) \overset{\leftarrow}{I} + \frac{4\pi}{(\omega + i\eta)^2} \left(\overset{\leftarrow}{\chi}_{\mathbf{jj}}^R(\mathbf{q}, \omega)\right)^T}. \quad (2.268)}$$

Remark 36 *Bound charges:* When one can separate the charges into bound and free in the calculation of $\overset{\leftarrow}{\chi}_{\mathbf{jj}}^R(\mathbf{q}, \omega)$, the contribution of the bound charges to $\frac{4\pi}{(\omega + i\eta)^2} \overset{\leftarrow}{\chi}_{\mathbf{jj}}^R(\mathbf{q}, \omega)$ is usually included with the 1 and called, $\overset{\leftarrow}{\epsilon}_{\text{bound}}^T$.

Remark 37 *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 38 *Electromagnetic field and plasmon:* One can see from the equation for the electric field (2.266) that in general the electromagnetic field does see the plasmon (negative dielectric constant for $\omega < \omega_p$ in Eq.(2.268) means no propagation below the plasma frequency).

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

$$i\mathbf{q} \cdot \mathbf{E} = 4\pi (\rho_e + \delta \langle \rho \rangle). \quad (2.269)$$

The longitudinal dielectric constant is defined by

$$i\mathbf{q} \cdot \overleftrightarrow{\epsilon}^L \cdot \mathbf{E} = 4\pi \rho_e. \quad (2.270)$$

With a longitudinal applied field, this means that

$$(\epsilon^L)^{-1} = \frac{\rho_e + \delta \langle \rho \rangle}{\rho_e}. \quad (2.271)$$

The linear response to an external charge can be computed from the response to the scalar potential it induces

$$\phi_e(\mathbf{q}, \omega) = \frac{4\pi}{q^2} \rho_e(\mathbf{q}, \omega). \quad (2.272)$$

As above, linear response to

$$\delta \mathcal{H}(t) = \int d\mathbf{r} \rho(\mathbf{r}) \phi_e(\mathbf{r}, t) \quad (2.273)$$

is given by

$$\delta \langle \rho(\mathbf{q}, \omega) \rangle = -\chi_{\rho\rho}^R(\mathbf{q}, \omega) \phi_e(\mathbf{q}, \omega) \quad (2.274)$$

so that simple substitution in the equation for $(\epsilon^L)^{-1}$ gives,

$$\boxed{\frac{1}{\epsilon^L(\mathbf{q}, \omega)} = 1 - \frac{4\pi}{q^2} \chi_{\rho\rho}^R(\mathbf{q}, \omega)}. \quad (2.275)$$

Remark 39 *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 at the beginning of this Chapter. Indeed, the fluctuation-dissipation theorem gives us

$$S_{\rho\rho}(\mathbf{q}, \omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \text{Im} [\chi_{\rho\rho}^R(\mathbf{q}, \omega)] = -\frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \frac{q^2}{4\pi} \text{Im} \left[\frac{1}{\epsilon^L(\mathbf{q}, \omega)} \right]. \quad (2.276)$$

The following properties of the dielectric constants are worthy of interest

Remark 40 *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 41 $\epsilon^L(\mathbf{q}, \omega) \neq \epsilon^T(\mathbf{q}, \omega)$ in general

Looking in what follows at the case $\omega \ll cq$, we assume that $\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \approx 0$. Then there are simple things to say about the significance of the poles and zeros of the dielectric constant.

Remark 42 *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 guaranteed by the fact the excitation is transverse, while $\nabla \times \mathbf{E} = 0$ implies zero electric field in a transverse mode. Nevertheless, $\mathbf{D}^T \neq 0$ can occur even if the electric field is zero when $\epsilon^T = \infty$. The corresponding poles are those of the transverse part of $\chi_{\mathbf{jj}}^R(\mathbf{q}, \omega)$.*

Remark 43 *Collective longitudinal excitations: The zeros of ϵ^L locate the longitudinal collective modes since $(\epsilon^L)^{-1} = \frac{\rho_e + \delta \langle \rho \rangle}{\rho_e} = \infty$ 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 $\chi_{\rho\rho}^R(\mathbf{q}, \omega)$.*

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3. 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 field $\Psi(\mathbf{r}, t)$. What about correlation functions of the field $\Psi(\mathbf{r}, t)$ itself? First of all, they are certainly necessary from a theoretical point of view to get a full description of the system. But more than that, they are related to experiment, more specifically to photoemission 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 field. These correlation functions are called Green's functions, or propagators. They 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[1][2] [3][4]. Here we introduce Green's functions in the simple context 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 we discuss definitions and general properties.

From now on, we work in units where $\hbar = 1$.

3.1 Definition of the propagator, or Green's function

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 $\Psi(\mathbf{r}, t)$. Let us then show that the evolution of $\Psi(\mathbf{r}, t)$ is governed by a propagator, then, later in this chapter, we develop perturbation theory for the propagator.

Let $t = 0$ be the time at which the Schrödinger and Heisenberg pictures coincide. Then

$$\Psi(\mathbf{r}, t) = \langle \mathbf{r} | e^{-iHt} | \Psi_H \rangle. \quad (3.1)$$

If instead of knowing the Heisenberg wave function $|\Psi_H\rangle$ we know the initial value of the Schrödinger wave function

$$|\Psi_0(t')\rangle = e^{-iHt'} |\Psi_H\rangle \quad (3.2)$$

we can write the wave function $\Psi(\mathbf{r}, t)$ in terms of the initial state in the Schrödinger picture

$$\Psi(\mathbf{r}, t) = \langle \mathbf{r} | e^{-iH(t-t')} |\Psi_0(t')\rangle. \quad (3.3)$$

To rewrite the same thing in terms of the initial wave function,

$$\Psi_0(\mathbf{r}', t') = \langle \mathbf{r}' | \Psi_0(t') \rangle \quad (3.4)$$

it suffices to use a complete set of states

$$\Psi(\mathbf{r}, t)\theta(t-t') = \int d\mathbf{r}' \langle \mathbf{r} | e^{-iH(t-t')} | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi_0(t') \rangle \theta(t-t') \quad (3.5)$$

where the $\theta(t-t')$ is added to make causality explicit. This last equation may be rewritten as

$$\Psi(\mathbf{r}, t)\theta(t-t') = i \int d\mathbf{r}' G^R(\mathbf{r}, t; \mathbf{r}', t') \Psi_0(\mathbf{r}', t') \quad (3.6)$$

if we introduce the following definition of the retarded Green's function in the position representation

$$\boxed{G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle \mathbf{r} | e^{-iH(t-t')} | \mathbf{r}' \rangle \theta(t-t')} \quad (3.7)$$

This may look like a useless exercise in definitions, but in fact there are many reasons to work with the retarded Green's function $G^R(\mathbf{r}, t; \mathbf{r}', t')$.

- $G^R(\mathbf{r}, t; \mathbf{r}', t')$ does not depend on the initial condition $\Psi_0(\mathbf{r}', t')$.
- $G^R(\mathbf{r}, t; \mathbf{r}', t')$ 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. These functions provide an alternate formulation of quantum mechanics.
- $G^R(\mathbf{r}, t; \mathbf{r}', t')$ is the analog of the Green's function used in the general context of differential equations (electromagnetism for example).
- Perturbation theory for $G^R(\mathbf{r}, t; \mathbf{r}', t')$ can be developed in a natural manner.
- $G^R(\mathbf{r}, t; \mathbf{r}', t')$ is generalizable to the many-body context where it keeps the same Physical interpretation (but not exactly the same mathematical definition).

Definition 5 $G^R(\mathbf{r}, t; \mathbf{r}', t')$ 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.

3.2 Information contained in the one-body propagator

It is very useful to work with the Fourier transform in time of $G^R(\mathbf{r}, t; \mathbf{r}', t')$ because it contains information about the energy spectrum

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = -i \int_0^\infty d(t-t') e^{i\omega(t-t')} \langle \mathbf{r} | e^{-iH(t-t')} | \mathbf{r}' \rangle e^{-\eta(t-t')}. \quad (3.8)$$

In this expression, we have used the $\theta(t-t')$ and the usual trick of adiabatic turning on to be able to define the Fourier transform of the θ function. Insert in this equation a complete set of energy eigenstates

$$H|n\rangle = E_n|n\rangle \quad (3.9)$$

$$\langle n|e^{-iH(t-t')}|m\rangle = e^{-iE_n(t-t')}\delta_{n,m} \quad (3.10)$$

to obtain for the Green's function

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = -i \sum_n \langle \mathbf{r}|n\rangle \int_0^\infty dt e^{i(\omega+i\eta-E_n)t} \langle n|\mathbf{r}'\rangle \quad (3.11)$$

or using $\Psi_n(\mathbf{r}) = \langle \mathbf{r}|n\rangle$

$$\boxed{G^R(\mathbf{r}, \mathbf{r}'; \omega) = \sum_n \frac{\langle \mathbf{r}|n\rangle \langle n|\mathbf{r}'\rangle}{\omega+i\eta-E_n} = \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')}{\omega+i\eta-E_n}} \quad (3.12)$$

$$\boxed{= \sum_n \langle \mathbf{r}|n\rangle \langle n|\frac{1}{\omega+i\eta-H}|n\rangle \langle n|\mathbf{r}'\rangle = \langle \mathbf{r}|\frac{1}{\omega+i\eta-H}|\mathbf{r}'\rangle}.$$

From this form, 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 what will be called later a Lehmann representation.

3.2.1 Operator representation.

The last equation may be seen as the position representation of the general operator

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega+i\eta-H}} \quad (3.13)$$

which is also called the *resolvent* operator. In other words,

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \langle \mathbf{r}|\widehat{G}^R(\omega)|\mathbf{r}'\rangle.$$

In real time, the corresponding expression is

$$\boxed{\widehat{G}^R(t) = -ie^{-iHt}\theta(t)} \quad (3.14)$$

The advanced propagator is

$$\boxed{\widehat{G}^A(t) = ie^{-iHt}\theta(-t)} \quad (3.15)$$

$$\boxed{\widehat{G}^A(\omega) = \frac{1}{\omega-i\eta-H}} \quad (3.16)$$

3.2.2 Relation to the density of states

The density of states is an observable which may be found directly from the Green's function. The one-particle density of states is defined by

$$\boxed{\rho(E) = \sum_n \delta(E - E_n)} = \sum_n \int d\mathbf{r} \langle n | \mathbf{r} \rangle \langle \mathbf{r} | n \rangle \delta(E - E_n) \quad (3.17)$$

$$\boxed{= -\frac{1}{\pi} \int d\mathbf{r} \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}; E)} \quad (3.18)$$

which can be rewritten in a manner which does not refer to the explicit representation (such as $|\mathbf{r}\rangle$ above)

$$\boxed{\rho(E) = -\frac{1}{\pi} \operatorname{Tr} \left[\operatorname{Im} \widehat{G}^R(E) \right]}. \quad (3.19)$$

The quantity

$$\rho(\mathbf{r}, E) = -\frac{1}{\pi} \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}; E) \quad (3.20)$$

is called the local density of states, a quantity relevant in particular when there is no translational invariance.

3.2.3 Spectral representation, sum rules and high frequency expansion

Green's functions have many formal properties that are analogous to those of response functions. We discuss some of them here.

Spectral representation and Kramers-Kronig relations.

Returning to the explicit representation in energy eigenstates, (3.12), it can be written in a manner which reminds us of the spectral representation

$$\boxed{G^R(\mathbf{r}, \mathbf{r}'; \omega)} = \sum_n \frac{\Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} = \int \frac{d\omega'}{2\pi} \frac{\sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') 2\pi\delta(\omega' - E_n)}{\omega + i\eta - \omega'} \quad (3.21)$$

$$\boxed{= \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'}} = \int \frac{d\omega'}{2\pi} \frac{-2 \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} = \int d\omega' \frac{\rho(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} \quad (3.22)$$

which defines the spectral weight

$$A(\mathbf{r}, \mathbf{r}'; \omega') = \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') 2\pi\delta(\omega' - E_n) \quad (3.23)$$

for the one-particle Green's functions. Note that in momentum space we would have, for a translationally invariant system,

$$\boxed{G^R(\mathbf{k}; \omega)} = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}; \omega')}{\omega + i\eta - \omega'} \quad (3.24)$$

with

$$\boxed{A(\mathbf{k}; \omega') = -2 \operatorname{Im} G^R(\mathbf{k}; \omega')} \quad (3.25)$$

$$A(\mathbf{k}; \omega') = \sum_n \Psi_n(\mathbf{k}) \Psi_n^*(\mathbf{k}) 2\pi\delta(\omega' - E_n) \quad (3.26)$$

$$= \sum_n \langle \mathbf{k} | n \rangle \langle n | \mathbf{k} \rangle 2\pi\delta(\omega' - E_n). \quad (3.27)$$

Remark 44 *Assumptions in relating A to $\text{Im } G^R$: 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 $A(\mathbf{r}, \mathbf{r}'; \omega') = -2 \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega')$ as we did in Eq.(3.22).*

Remark 45 *Analogies with ordinary correlation functions. Contrary to the spectral representation for correlation functions introduced earlier, there is $\frac{d\omega'}{2\pi}$ instead of $\frac{d\omega'}{\pi}$. Furthermore, the denominator involves $\omega + i\eta - \omega'$ instead of $\omega' - \omega - i\eta$. 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

$$\text{Re} [G^R(\mathbf{r}, \mathbf{r}'; \omega)] = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} [G^R(\mathbf{r}, \mathbf{r}'; \omega')]}{\omega' - \omega}. \quad (3.28)$$

The other reciprocal Kramers-Kronig relation follows as before.

$$\text{Im} [G^R(\mathbf{r}, \mathbf{r}'; \omega)] = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Re} [G^R(\mathbf{r}, \mathbf{r}'; \omega')]}{\omega' - \omega} \quad (3.29)$$

Sum rules

As before, the imaginary part, here equal to the local density of states, obeys sum rules

$$\int \frac{d\omega'}{2\pi} (-2 \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega')) = \int \frac{d\omega'}{2\pi} \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') 2\pi \delta(\omega' - E_n) \quad (3.30)$$

$$= \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (3.31)$$

so that

$$\int d(\mathbf{r} - \mathbf{r}') \int \frac{d\omega'}{2\pi} (-2 \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega')) = 1. \quad (3.32)$$

More sum rules are trivially derived. For example,

$$\boxed{\int d\mathbf{r} \int \frac{d\omega'}{2\pi} \omega' (-2 \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega'))} = \int d\mathbf{r} \int d\omega' \omega' \rho(\mathbf{r}, \omega') = \int d\mathbf{r} \sum_n E_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}) \quad (3.33)$$

$$= \int d\mathbf{r} \langle \mathbf{r} | H | \mathbf{r} \rangle. \quad (3.34)$$

In operator form, all of the above results are trivial

$$\boxed{\int \frac{d\omega'}{2\pi} \omega^n \text{Tr} [-2 \text{Im} (\widehat{G}^R)]} = \int \frac{d\omega}{2\pi} \omega^n \text{Tr} \left[-2 \text{Im} \left(\frac{1}{\omega + i\eta - H} \right) \right] \quad (3.35)$$

$$\boxed{= \int d\omega \omega^n \text{Tr} \delta(\omega - H) = \text{Tr}(H^n)}$$

Evaluating the trace in the position representation, we recover previous results. Special cases include

$$\int d\mathbf{r} \int \frac{d\omega'}{2\pi} (\omega')^n (-2 \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega')) = \int d\mathbf{r} \langle \mathbf{r} | H^n | \mathbf{r} \rangle \quad (3.36)$$

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\omega'}{2\pi} (\omega')^n (-2 \text{Im } G^R(\mathbf{k}, \mathbf{k}; \omega')) = \int \frac{d\mathbf{k}}{(2\pi)^3} \langle \mathbf{k} | H^n | \mathbf{k} \rangle$$

Remark 46 *Recall that in the case of sum rules for χ'' , there was also an implicit trace since we were computing equilibrium expectation values.*

High frequency expansion.

Once we have established sum rules, we can use them for high frequency expansions. Consider the spectral representation in the form

$$G^R(\mathbf{k}, \mathbf{k}; \omega) = \int \frac{d\omega'}{2\pi} \frac{-2 \operatorname{Im} G^R(\mathbf{k}, \mathbf{k}; \omega')}{\omega + i\eta - \omega'}. \quad (3.37)$$

Then for ω sufficiently large that $\operatorname{Im} G^R(\mathbf{k}, \mathbf{k}; \omega) = 0$ (see remark below), the Green's function becomes purely real and one can expand the denominator so that at asymptotically large frequencies,

$$G^R(\mathbf{k}, \mathbf{k}; \omega) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\omega'}{2\pi} (\omega')^n (-2 \operatorname{Im} G^R(\mathbf{k}, \mathbf{k}; \omega')) \quad (3.38)$$

Integrating on both sides and using sum rules, we obtain,

$$\int \frac{d\mathbf{k}}{(2\pi)^3} G^R(\mathbf{k}, \mathbf{k}; \omega) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\mathbf{k}}{(2\pi)^3} \langle \mathbf{k} | H^n | \mathbf{k} \rangle \quad (3.39)$$

or in more general terms,

$$\operatorname{Tr} [\hat{G}^R(\omega)] \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \operatorname{Tr} (H^n) \quad (3.40)$$

which is an obvious consequence of the high-frequency expansion of (3.13)

$$\hat{G}^R(\omega) = \frac{1}{\omega + i\eta - H} \quad (3.41)$$

Remark 47 $\operatorname{Im} G^R(\mathbf{k}, \mathbf{k}; \omega) = 0$ at high frequency. Indeed consider the relation of this quantity to the spectral weight Eq.(3.25) and the explicit representation of the spectral weight Eq.(3.27). 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 48 The leading high-frequency behavior is in $1/\omega$, contrary to that of correlation functions which was in $1/\omega^2$.

3.2.4 Relation to transport and fluctuations

The true many-body case is much more complicated, but for the single-particle Schrödinger equation, life is easy. We 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.[1].

Let $S_{\rho\rho}(\mathbf{k}, \omega)$ be the charge structure factor for example.

$$S_{\rho\rho}(\mathbf{k}, \omega) = \frac{1}{\mathcal{V}} \int dt e^{i\omega t} \langle \rho_{\mathbf{k}}(t) \rho_{-\mathbf{k}} \rangle = \frac{1}{\mathcal{V}} \int dt e^{i\omega t} \langle e^{iHt} \rho_{\mathbf{k}} e^{-iHt} \rho_{-\mathbf{k}} \rangle. \quad (3.42)$$

The real-time retarded propagator was

$$\hat{G}^R(t) = -ie^{-iHt} \theta(t) \quad (3.43)$$

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

$$S_{\rho\rho}(\mathbf{k}, \omega) = \frac{-1}{\mathcal{V}} \int dt e^{i\omega t} \left\langle \left(\widehat{G}^R(-t) - \widehat{G}^A(-t) \right) \rho_{\mathbf{k}} \left(\widehat{G}^R(t) - \widehat{G}^A(t) \right) \rho_{-\mathbf{k}} \right\rangle. \quad (3.44)$$

Because of the θ functions, $\widehat{G}^R(-t)\widehat{G}^R(t) = 0$.

Remark 49 *Alternate proof: We can also see this in the Fourier transform version*

$$S_{\rho\rho}(\mathbf{k}, \omega) = \frac{-1}{\mathcal{V}} \int \frac{d\omega'}{2\pi} \left\langle \left(\widehat{G}^R(\omega') - \widehat{G}^A(\omega') \right) \rho_{\mathbf{k}} \left(\widehat{G}^R(\omega' + \omega) - \widehat{G}^A(\omega' + \omega) \right) \rho_{-\mathbf{k}} \right\rangle. \quad (3.45)$$

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

$$\boxed{S_{\rho\rho}(\mathbf{k}, \omega) = \frac{1}{\mathcal{V}} \int \frac{d\omega'}{2\pi} \left\langle \widehat{G}^R(\omega') \rho_{\mathbf{k}} \widehat{G}^A(\omega' + \omega) \rho_{-\mathbf{k}} + \widehat{G}^A(\omega') \rho_{\mathbf{k}} \widehat{G}^R(\omega' + \omega) \rho_{-\mathbf{k}} \right\rangle} \quad (3.46)$$

In a specific case, to compute matrix elements in the energy representation, one recalls that

$$G^R(n, n'; E) = \langle n | \frac{1}{E - H + i\eta} | n' \rangle = \delta_{nn'} \frac{1}{E - E_n + i\eta} \quad (3.47)$$

$$G^A(n, n'; E) = \langle n | \frac{1}{E - H - i\eta} | n' \rangle \quad (3.48)$$

3.2.5 Green's functions for differential equations

The expression for the propagator (3.6)

$$\Psi(\mathbf{r}, t)\theta(t - t') = i \int d\mathbf{r}' G^R(\mathbf{r}, t; \mathbf{r}', t') \Psi_0(\mathbf{r}', t') \quad (3.49)$$

clearly shows that it is the integral version of the differential equation which evolves the wave function. In other words, it is the inverse of the differential operator for $\Psi(\mathbf{r}, t)$. That may be seen as follows

$$i \frac{\partial}{\partial t} [\Psi(\mathbf{r}, t)\theta(t - t')] = i\delta(t - t') \Psi(\mathbf{r}, t) + i\theta(t - t') \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) \quad (3.50)$$

$$= i\delta(t - t') \Psi(\mathbf{r}, t) + H(\mathbf{r})\theta(t - t') \Psi(\mathbf{r}, t). \quad (3.51)$$

where we have used the Schrödinger equation in position space (that is why $H(\mathbf{r})$ appears). Replacing $\Psi(\mathbf{r}, t)\theta(t - t')$ in by its expression in terms of propagator, and using $\delta(t - t') \Psi(\mathbf{r}, t) = \Psi_0(\mathbf{r}, t')$ we obtain

$$i \frac{\partial}{\partial t} \left[i \int d\mathbf{r}' G^R(\mathbf{r}, t; \mathbf{r}', t') \Psi_0(\mathbf{r}', t') \right] = \quad (3.52)$$

$$\delta(t-t') i \int d\mathbf{r}' \delta^3(\mathbf{r}-\mathbf{r}') \Psi_0(\mathbf{r}', t') + H(\mathbf{r}) \left[i \int d\mathbf{r}' G^R(\mathbf{r}, t; \mathbf{r}', t') \Psi_0(\mathbf{r}', t') \right] \quad (3.53)$$

and since the equation is valid for arbitrary initial condition $\Psi_0(\mathbf{r}', t')$, then

$$\boxed{\left[i \frac{\partial}{\partial t} - H(\mathbf{r}) \right] G^R(\mathbf{r}, t; \mathbf{r}', t') = \delta(t-t') \delta^3(\mathbf{r}-\mathbf{r}')}. \quad (3.54)$$

This is indeed the definition of the Green's function for the Schrödinger equation seen as a differential equation.

Remark 50 *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.*

We can do the same manipulations in operator form. Recalling that

$$\widehat{G}^R(t) = -ie^{-iHt}\theta(t) \quad (3.55)$$

with H the Hamiltonian operator for the Hilbert space, then the differential equation which is obeyed is

$$\left[i \frac{\partial}{\partial t} - H \right] \widehat{G}^R(t) = \delta(t) \quad (3.56)$$

which takes exactly the form above, (3.54) if we write the equation in the position representation and use the completeness relation $\int d\mathbf{r} |\mathbf{r}\rangle \langle \mathbf{r}| = 1$ a few times. Formally, we can invert the last equation,

$$\boxed{\widehat{G}^R(t) = \left[i \frac{\partial}{\partial t} - H \right]^{-1} \delta(t)} \quad (3.57)$$

which is meaningless unless we specify that the boundary condition is that $G^R(-\infty) = 0$. This should be compared with Eq.(3.13).

Remark 51 *Boundary condition in time vs pole location in frequency space: From the equation for the propagator (3.54) it appears that one can add to $G^R(\mathbf{r}, t; \mathbf{r}', t')$ any solution of the homogeneous form of the differential equation (right-hand side equal to zero). The boundary condition that $G^R(\mathbf{r}, t; \mathbf{r}', t')$ vanishes for all $t-t' < 0$ (the in) and is equal to $-i$ at $t = 0$ makes the solution unique. For a first-order differential equation, one boundary condition at $t-t' = 0^+$ suffices to know the function at $t-t' > 0$. We will not know then the value before $t-t' = 0$ but we specify that it is equal to zero as long as $t-t' < 0$. 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 $\widehat{G}(t) = -ie^{-iHt}\theta(t) - iCe^{-iHt}$, 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 $G^A(\mathbf{r}, t; \mathbf{r}', t')$ we need to specify the vanishing of the function at $t-t' > 0$ and we can find its value at all times prior to $t-t' = 0^-$ by stating that it is equal to $+i$ at that time. Indeed, in that case $C = -1$ in $\widehat{G}(t) = -ie^{-iHt}\theta(t) - iCe^{-iHt}$ so that $\widehat{G}^A(t) = -ie^{-iHt}\theta(t) + ie^{-iHt} = ie^{-iHt}\theta(-t)$, as in the earlier definition Eq.(3.15).*

3.3 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 notions such as self-energy and Dyson equation. As an example, we will treat in more details the propagation of an electron in a random potential.

3.3.1 General starting point for perturbation theory.

If we can diagonalize H , then we know the propagator

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega - H + i\eta}} \quad (3.58)$$

from the identities we developed above,

$$G^R(n, n'; E) = \langle n | \frac{1}{E - H + i\eta} | n' \rangle = \delta_{nn'} \frac{1}{E - E_n + i\eta} \quad (3.59)$$

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \sum_n \frac{\Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} \quad (3.60)$$

We want to develop perturbation methods to evaluate the propagator in the case where one part of the Hamiltonian, say H_0 can be diagonalized while the other part, say V , cannot be diagonalized in the same basis. The easiest manner to proceed (when V is independent of time) is using the operator methods that follow. First, write

$$(\omega + i\eta - H_0 - V) \widehat{G}^R(\omega) = 1. \quad (3.61)$$

Putting the perturbation V on the right-hand side, and using

$$\widehat{G}_0^R(\omega) = \frac{1}{\omega + i\eta - H_0} \quad (3.62)$$

we have

$$\left(\widehat{G}_0^R(\omega)\right)^{-1} \widehat{G}^R(\omega) = 1 + V \widehat{G}^R(\omega). \quad (3.63)$$

Multiplying by $\widehat{G}_0^R(\omega)$ on both sides, we write the equation in the form

$$\boxed{\widehat{G}^R(\omega) = \widehat{G}_0^R(\omega) + \widehat{G}_0^R(\omega) V \widehat{G}^R(\omega)}. \quad (3.64)$$

In scattering theory, this is the propagator version of the Lippmann-Schwinger equation. Perturbation theory is obtained by iterating the above equation. Stopping the iteration at an arbitrary point may however lead to misleading results, as we shall discuss in the following section.

But before this, we point out that perturbation theory here can be seen as resulting from the following matrix identity,

$$\boxed{\frac{1}{X+Y} = \frac{1}{X} - \frac{1}{X} Y \frac{1}{X+Y}} \quad (3.65)$$

To prove this identity, multiply by $X + Y$ either from the left or from the right. For example

$$\frac{1}{X+Y} (X+Y) = \frac{1}{X} X + \frac{1}{X} Y - \frac{1}{X} Y \frac{1}{X+Y} (X+Y) = 1 \quad (3.66)$$

3.3.2 Feynman diagrams for a one-body potential and their physical interpretation.

The Lippmann Schwinger equation Eq.(3.64) may be represented by diagrams. The thick line stands for $\hat{G}^R(\omega)$ while the thin line stands for $\hat{G}_0^R(\omega)$ and the dotted line with a cross represents the action of V .

Iterating the basic equation (3.64), one obtains the series

$$\hat{G}^R(\omega) = \hat{G}_0^R(\omega) + \hat{G}_0^R(\omega) V \hat{G}_0^R(\omega) + \hat{G}_0^R(\omega) V \hat{G}_0^R(\omega) V \hat{G}_0^R(\omega) + \dots \quad (3.67)$$

which we represent diagrammatically by Fig.(3-1). Physically, one sees that the full propagator is obtained by free propagation between scatterings off the potential.

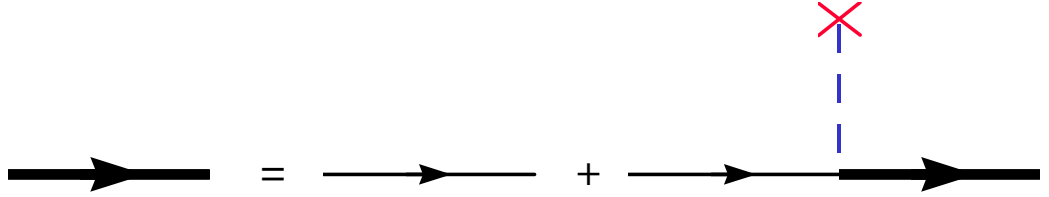


Figure 3-1 Diagrammatic representation of the Lippmann-Schwinger equation for scattering.

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, $\langle \mathbf{r}_1 | V | \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle \mathbf{r}_1 | V | \mathbf{r}_1 \rangle$, we have that

$$\langle \mathbf{r} | \hat{G}^R(\omega) | \mathbf{r}' \rangle = \langle \mathbf{r} | \hat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{r} | \hat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | V | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | \hat{G}_0^R(\omega) | \mathbf{r}' \rangle + \dots \quad (3.68)$$

$$= \langle \mathbf{r} | \hat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \langle \mathbf{r} | \hat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | V | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | \hat{G}_0^R(\omega) | \mathbf{r}' \rangle + \dots \quad (3.69)$$

Remark 52 *Physical interpretation and path integral: Given that $\langle \mathbf{r} | \hat{G}^R(\omega) | \mathbf{r}' \rangle$ 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.*

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 (3-2).

- Let each thin line with an arrow stand for $\langle \mathbf{r} | \hat{G}_0^R(\omega) | \mathbf{r}' \rangle$. 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.

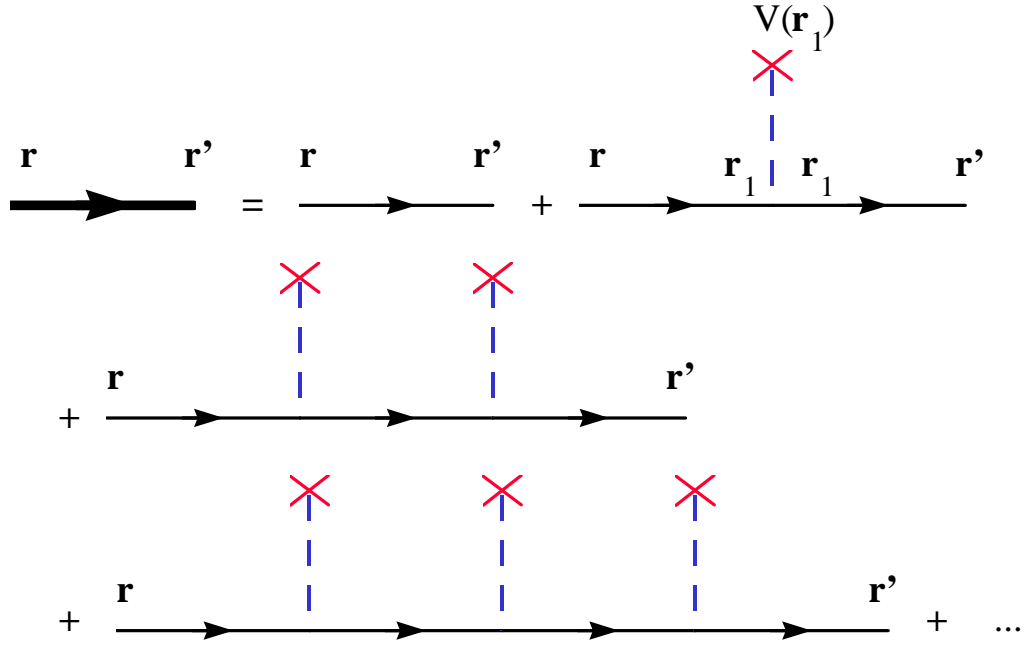


Figure 3-2 Iteration of the propagator for scattering off impurities.

- The X at the end of a dotted line stands for a potential $\langle \mathbf{r}_1 | V | \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle \mathbf{r}_1 | V | \mathbf{r}_1 \rangle$.
- 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. All topologically distinct possibilities must be considered in the sum. One scattering is distinct from two etc...

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 (3.67). Using complete sets of states again, as well as the definition $\langle \mathbf{k} | \hat{G}_0^R(\omega) | \mathbf{k}' \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k}' \rangle = G_0^R(\mathbf{k}, \omega) (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')$ we have that for a particle with a quadratic dispersion law, or a Hamiltonian $H_0 = p^2/2m$

$$G_0^R(\mathbf{k}, \omega) = \frac{1}{\omega + i\eta - \frac{k^2}{2m}}. \quad (3.70)$$

In this basis, the perturbation series becomes

$$\langle \mathbf{k} | \hat{G}^R(\omega) | \mathbf{k}' \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k}' \rangle + \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k}_1 \rangle \langle \mathbf{k}_1 | \hat{G}^R(\omega) | \mathbf{k}' \rangle. \quad (3.71)$$

Solving by iteration to second order, we obtain,

$$\langle \mathbf{k} | \hat{G}^R(\omega) | \mathbf{k}' \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k}' \rangle + G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k}' \rangle G_0^R(\mathbf{k}', \omega) \quad (3.72)$$

$$+ \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k}_1 \rangle G_0^R(\mathbf{k}_1, \omega) \langle \mathbf{k}_1 | V | \mathbf{k}' \rangle G_0^R(\mathbf{k}', \omega) + \dots \quad (3.73)$$

The diagrams shown in the following figure Fig.(3-3) are now labeled differently. The drawing is exactly the same as well as the rule of summing over all topologically distinct diagrams.

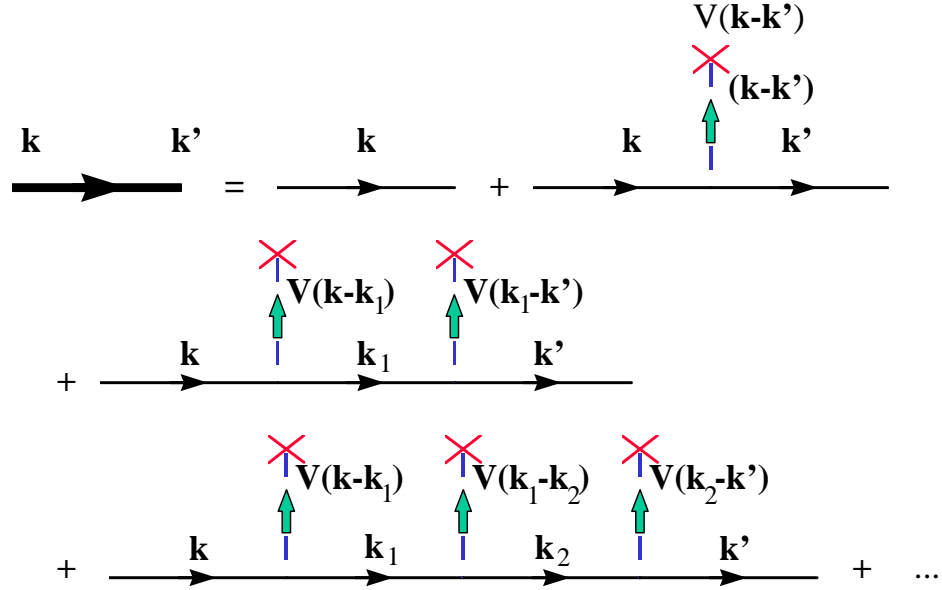


Figure 3-3 Feynman diagrams for scattering off impurities in momentum space (before impurity averaging).

However,

- Each free propagator has a label \mathbf{k}, ω . One can think of momentum \mathbf{k} flowing along the arrow.
- 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 $\langle \mathbf{k} | V | \mathbf{k}'' \rangle$. One can think of momentum $\mathbf{k} - \mathbf{k}''$ flowing along the dotted line, and being lost into the X .
- One must integrate $\int \frac{d\mathbf{k}''}{(2\pi)^3}$ over momenta not determined by momentum conservation. If there are n potential scatterings, there are $n - 1$ momenta to be integrated over.

3.3.3 Dyson's equation, irreducible self-energy

Suppose we truncate the perturbation expansion to some finite order. For example, consider the truncated series for the diagonal element $\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle$

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle + G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k} \rangle G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle \quad (3.74)$$

Stopping this 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.(3.25) and (3.27) 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

$$\text{Im} \frac{1}{(\omega + i\eta - \frac{k^2}{2m})^2} = -\frac{\partial}{\partial \omega} \text{Im} \frac{1}{\omega + i\eta - \frac{k^2}{2m}} \quad (3.75)$$

$$= \pi \frac{\partial}{\partial \omega} \delta\left(\omega - \frac{k^2}{2m}\right) \quad (3.76)$$

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

$$\langle \mathbf{k} | V | \mathbf{k} \rangle G_0^R(\mathbf{k}, \omega) = \frac{\langle \mathbf{k} | V | \mathbf{k} \rangle}{\omega + i\eta - \frac{k^2}{2m}} \quad (3.77)$$

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

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle + G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k} \rangle G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle \quad (3.78)$$

$$+ G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k} \rangle G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k} \rangle G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle + \dots \quad (3.79)$$

which may be generated by

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle + G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | V | \mathbf{k} \rangle \langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle \quad (3.80)$$

then things start to make more sense since the solution

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = \frac{\langle \mathbf{k} | \mathbf{k} \rangle}{(G_0^R(\mathbf{k}, \omega))^{-1} - \langle \mathbf{k} | V | \mathbf{k} \rangle} \quad (3.81)$$

has simple poles corresponding to eigenenergies shifted from $\frac{k^2}{2m}$ to $\frac{k^2}{2m} + \langle \mathbf{k} | V | \mathbf{k} \rangle$ 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. However, the simple procedure above gave $\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle$ that even satisfies the first sum rule $\int \frac{d\omega}{2\pi} \text{Tr} \left[-2 \text{Im} \left(\widehat{G}^R(\omega) \right) \right] = \text{Tr} [H^0] = 1$ as well as the second $\int \frac{d\omega}{2\pi} \omega \text{Tr} \left[-2 \text{Im} \left(\widehat{G}^R \right) \right] = \text{Tr} [H]$.

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.

This is done by defining the *irreducible self-energy* $\Sigma(\mathbf{k}, \omega)$ by the equation

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = G_0^R(\mathbf{k}, \omega) \langle \mathbf{k} | \mathbf{k} \rangle + G_0^R(\mathbf{k}, \omega) \Sigma^R(\mathbf{k}, \omega) \langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle. \quad (3.82)$$

This is the so-called *Dyson equation* whose diagrammatic representation is given in Fig.(3-4) and whose solution can be found algebraically

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k} \rangle = \frac{\langle \mathbf{k} | \mathbf{k} \rangle}{(G_0^R(\mathbf{k}, \omega))^{-1} - \Sigma^R(\mathbf{k}, \omega)}. \quad (3.83)$$

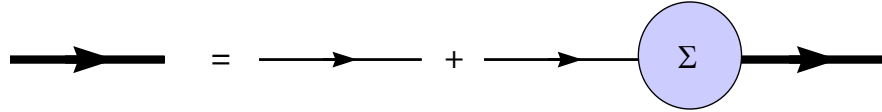


Figure 3-4 Dyson's equation and irreducible self-energy.

The definition of the self-energy is found in principle by comparing with the exact result Eq.(3.71) 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 $\Sigma(\mathbf{k}, \omega)$ should contain all possible diagrams which 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 one-self that this is the correct definition by noting that iteration of the Dyson equation (3.82) will give back all missing $G_0^R(\mathbf{k}, \omega)$ in intermediate states.

$\Sigma(\mathbf{k}, \omega)$ 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 does not have much interest from the point of view of calculations.

To first order then, $\Sigma(\mathbf{k}, \omega)$ is given by the diagram in Fig.(3-5) whose algebraic expression can be read off

$$\Sigma^R(\mathbf{k}, \omega) = \langle \mathbf{k} | V | \mathbf{k} \rangle. \quad (3.84)$$

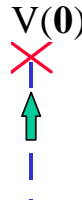


Figure 3-5 First-order irreducible self-energy.

This is the first-order shift to the energies we had found above. To second order, the diagram is given in Fig.(3-6) and its algebraic expression is

$$\Sigma^R(\mathbf{k}, \omega) = \int_{\mathbf{k}_1 \neq \mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3} \langle \mathbf{k} | V | \mathbf{k}_1 \rangle G_0^R(\mathbf{k}_1, \omega) \langle \mathbf{k}_1 | V | \mathbf{k} \rangle. \quad (3.85)$$

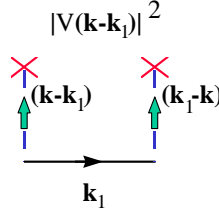


Figure 3-6 Second order irreducible self-energy (before impurity averaging).

Remark 53 *Locator expansion:* The choice of H_0 is dictated by the problem. One could take V as the unperturbed Hamiltonian and the hopping as a perturbation. One then has the “locator expansion”.

3.4 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.(3.83), 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 (3.82), 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,

$$\text{Re} [\Sigma^R(\mathbf{r}, \mathbf{r}'; \omega) - \Sigma^R(\mathbf{r}, \mathbf{r}'; \infty)] = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} [\Sigma^R(\mathbf{r}, \mathbf{r}'; \omega')]}{\omega' - \omega}. \quad (3.86)$$

$$\text{Im} [\Sigma^R(\mathbf{r}, \mathbf{r}'; \omega)] = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Re} [\Sigma^R(\mathbf{r}, \mathbf{r}'; \omega') - \Sigma^R(\mathbf{r}, \mathbf{r}'; \infty)]}{\omega' - \omega} \quad (3.87)$$

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:

$$\mathcal{P} = |\mathbf{k}\rangle \langle \mathbf{k}| \quad ; \quad \mathcal{Q} = 1 - \mathcal{P} = \int \frac{d\mathbf{k}'}{(2\pi)^3} |\mathbf{k}'\rangle \langle \mathbf{k}'| - |\mathbf{k}\rangle \langle \mathbf{k}| \quad (3.88)$$

with the usual properties for projection operators

$$\mathcal{P}^2 = \mathcal{P} \quad ; \quad \mathcal{Q}^2 = \mathcal{Q} \quad ; \quad \mathcal{P} + \mathcal{Q} = 1 \quad (3.89)$$

The following manipulations will illustrate methods widely used in projection operator techniques.[5]

Since H_0 is diagonal in this representation, we have that

$$\mathcal{P} G_0^R(\mathbf{k}, \omega) \mathcal{Q} = \mathcal{Q} G_0^R(\mathbf{k}, \omega) \mathcal{P} = 0 \quad (3.90)$$

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

$$\mathcal{P}\hat{G}^R\mathcal{P} = \mathcal{P}\hat{G}_0^R\mathcal{P} + \mathcal{P}\hat{G}_0^RV\hat{G}^R\mathcal{P} = \mathcal{P}\hat{G}_0^R\mathcal{P} + \mathcal{P}\hat{G}_0^RV\mathcal{P}\hat{G}^R\mathcal{P} + \mathcal{P}\hat{G}_0^RV\mathcal{Q}\hat{G}^R\mathcal{P}. \quad (3.91)$$

To close the equation, we need $\mathcal{Q}\hat{G}^R\mathcal{P}$, which can also be evaluated,

$$\mathcal{Q}\hat{G}^R\mathcal{P} = \mathcal{Q}\hat{G}_0^RV\hat{G}^R\mathcal{P} = \mathcal{Q}\hat{G}_0^RV\mathcal{P}\hat{G}^R\mathcal{P} + \mathcal{Q}\hat{G}_0^RV\mathcal{Q}\hat{G}^R\mathcal{P} \quad (3.92)$$

$$\mathcal{Q}\hat{G}^R\mathcal{P} = \frac{1}{1 - \mathcal{Q}\hat{G}_0^RV\mathcal{Q}}\mathcal{Q}\hat{G}_0^RV\mathcal{P}\hat{G}^R\mathcal{P}. \quad (3.93)$$

Substituting in the previous result, we find

$$\mathcal{P}\hat{G}^R\mathcal{P} = \mathcal{P}\hat{G}_0^R\mathcal{P} + \mathcal{P}\hat{G}_0^RV \left[1 + \frac{1}{1 - \mathcal{Q}\hat{G}_0^RV\mathcal{Q}}\mathcal{Q}\hat{G}_0^RV \right] \mathcal{P}\hat{G}^R\mathcal{P} \quad (3.94)$$

$$\mathcal{P}\hat{G}^R\mathcal{P} = \mathcal{P}\hat{G}_0^R\mathcal{P} + \mathcal{P}\hat{G}_0^R\mathcal{P}V \left[1 + \frac{1}{1 - \mathcal{Q}\hat{G}_0^RV\mathcal{Q}}\mathcal{Q}\hat{G}_0^RV\mathcal{P} \right] \mathcal{P}\hat{G}^R\mathcal{P} \quad (3.95)$$

This means that the self-energy operator is defined algebraically by

$$\boxed{\hat{\Sigma}^R = \mathcal{P}V\mathcal{P} + \mathcal{P}V\mathcal{Q}\frac{1}{1 - \mathcal{Q}\hat{G}_0^RV\mathcal{Q}}\mathcal{Q}\hat{G}_0^RV\mathcal{P}}. \quad (3.96)$$

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 54 *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.[5]*

Remark 55 *High-frequency behavior of self-energy and sum rules: Given the $1/\omega$ high-frequency behavior of \hat{G}_0^R , one can see that the infinite frequency limit of the self-energy is a constant given by $\mathcal{P}V\mathcal{P} = |\mathbf{k}\rangle\langle\mathbf{k}|V|\mathbf{k}\rangle\langle\mathbf{k}|$ and that the next term in the high-frequency expansion is $\mathcal{P}V\mathcal{Q}\frac{1}{\omega}\mathcal{Q}V\mathcal{P}$ as follows from the high-frequency behavior of \hat{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 56 *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 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.*

3.5 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.

3.5.1 Impurity averaging

Assume that electrons scatter from the potential produced by uniformly distributed impurities

$$V_C(\mathbf{r}) = \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) \quad (3.97)$$

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.

$$V_C(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) = \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \int d\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_i)} v(\mathbf{r} - \mathbf{R}_i) \quad (3.98)$$

$$= v(\mathbf{q}) \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \quad (3.99)$$

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,

$$\overline{V_C(\mathbf{q})} = v(\mathbf{q}) \sum_{i=1}^{N_i} \overline{(e^{-i\mathbf{q}\cdot\mathbf{R}_i})} = v(\mathbf{q}) \sum_{i=1}^{N_i} \frac{1}{\mathcal{V}} \int d\mathbf{R}_i e^{-i\mathbf{q}\cdot\mathbf{R}_i} = v(\mathbf{q}) \frac{N_i}{\mathcal{V}} (2\pi)^3 \delta(\mathbf{q}) \quad (3.100)$$

$$= n_i v(\mathbf{0}) (2\pi)^3 \delta(\mathbf{q}) \quad (3.101)$$

where n_i is the impurity concentration. We will also need to consider averages of products of impurity potentials,

$$\overline{V_C(\mathbf{q}) V_C(\mathbf{q}')} = v(\mathbf{q}) v(\mathbf{q}') \overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \sum_{j=1}^{N_i} e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}. \quad (3.102)$$

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

$$\overline{\sum_{i=1}^{N_i} \sum_{j \neq i}^{N_i} e^{-i\mathbf{q} \cdot \mathbf{R}_i} e^{-i\mathbf{q}' \cdot \mathbf{R}_j}} = \sum_{i=1}^{N_i} \sum_{j \neq i}^{N_i} \left(\overline{e^{-i\mathbf{q} \cdot \mathbf{R}_i}} \overline{e^{-i\mathbf{q}' \cdot \mathbf{R}_j}} \right) = \frac{(N_i^2 - N_i)}{\mathcal{V}^2} (2\pi)^3 \delta(\mathbf{q}) (2\pi)^3 \delta(\mathbf{q}'). \quad (3.103)$$

When $i = j$ however, we are considering only one impurity so that

$$\overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q} \cdot \mathbf{R}_i} e^{-i\mathbf{q}' \cdot \mathbf{R}_i}} = n_i (2\pi)^3 \delta(\mathbf{q} + \mathbf{q}'). \quad (3.104)$$

Gathering the results, and using the result that for a real potential $|v(\mathbf{q})|^2 = v(\mathbf{q})v(-\mathbf{q})$ we find

$$\overline{V_C(\mathbf{q})V_C(\mathbf{q}')} = \frac{(N_i^2 - N_i)}{\mathcal{V}^2} \left(v(\mathbf{0}) (2\pi)^3 \delta(\mathbf{q}) \right) \left(v(\mathbf{0}) (2\pi)^3 \delta(\mathbf{q}') \right) + n_i |v(\mathbf{q})|^2 (2\pi)^3 \delta(\mathbf{q} + \mathbf{q}'). \quad (3.105)$$

3.5.2 Averaging of the perturbation expansion for the propagator

Let us return to the perturbation expansion in momentum space to second order Eq.(3.73).Using

$$\langle \mathbf{k} | V_C | \mathbf{k}' \rangle = \int d\mathbf{r} \langle \mathbf{k} | \mathbf{r} \rangle V_C(\mathbf{r}) \langle \mathbf{r} | \mathbf{k}' \rangle = V_C(\mathbf{k} - \mathbf{k}') \quad (3.106)$$

and $\langle \mathbf{k} | \mathbf{k}' \rangle = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')$, we rewrite the perturbation expansion and average it,

$$\overline{\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k}' \rangle} = G_0^R(\mathbf{k}, \omega) (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') + G_0^R(\mathbf{k}, \omega) \overline{V_C(\mathbf{k} - \mathbf{k}')} G_0^R(\mathbf{k}', \omega) \quad (3.107)$$

$$+ \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k}, \omega) \overline{V_C(\mathbf{k} - \mathbf{k}_1) G_0^R(\mathbf{k}_1, \omega) V_C(\mathbf{k}_1 - \mathbf{k}')} G_0^R(\mathbf{k}', \omega) + \dots \quad (3.108)$$

Using what we have learned about impurity averaging, this is rewritten as,

$$\begin{aligned} \langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k}' \rangle = & \{ G_0^R(\mathbf{k}, \omega) + G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) \\ & + G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) \\ & - G_0^R(\mathbf{k}, \omega) \left[n_i |v(\mathbf{0})|^2 \frac{1}{\mathcal{V}} \right] G_0^R(\mathbf{k}, \omega) G_0^R(\mathbf{k}, \omega) \\ & + G_0^R(\mathbf{k}, \omega) \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k}_1, \omega) \left[n_i |v(\mathbf{k} - \mathbf{k}_1)|^2 \right] G_0^R(\mathbf{k}, \omega) + \dots \} (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') \end{aligned} \quad (3.109)$$

Recalling the relation between discrete sums and integrals,

$$\int \frac{d\mathbf{k}_1}{(2\pi)^3} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} \quad (3.110)$$

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

$$\begin{aligned}
 \langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k}' \rangle = & \{ G_0^R(\mathbf{k}, \omega) + G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) \\
 & + G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) [n_i v(\mathbf{0})] G_0^R(\mathbf{k}, \omega) \\
 & + G_0^R(\mathbf{k}, \omega) \left(\int_{\mathbf{k}_1 \neq \mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k}_1, \omega) [n_i |v(\mathbf{k} - \mathbf{k}_1)|^2] \right) G_0^R(\mathbf{k}, \omega) + \dots \} (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')
 \end{aligned}
 \tag{3.111}$$

The diagrams corresponding to this expansion are illustrated in Fig.(3-7)

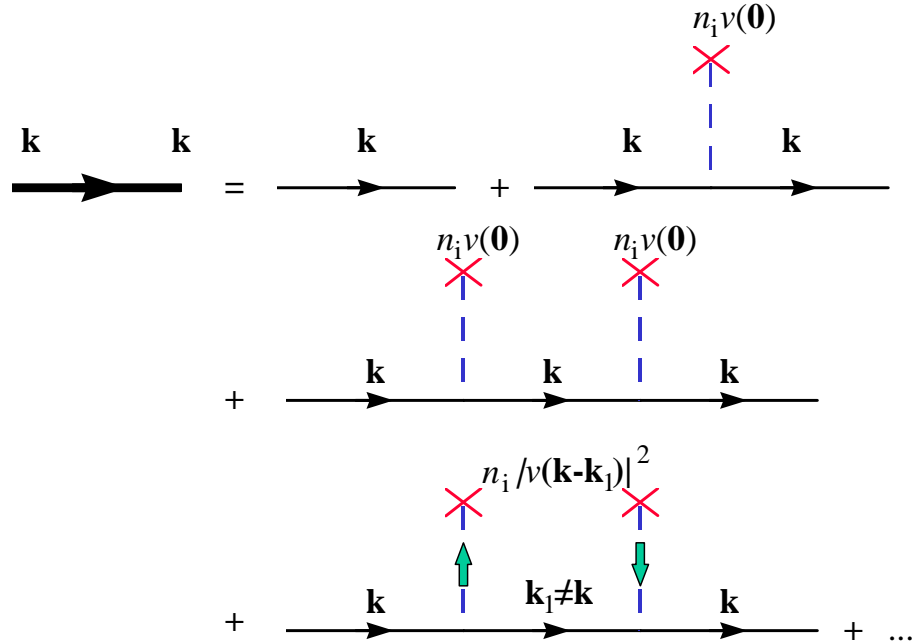


Figure 3-7 Direct iterated solution to the Lippmann-Schwinger equation after impurity averaging.

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

$$\langle \mathbf{k} | \widehat{G}^R(\omega) | \mathbf{k}' \rangle = \frac{\langle \mathbf{k} | \mathbf{k}' \rangle}{(G_0^R(\mathbf{k}, \omega))^{-1} - \Sigma^R(\mathbf{k}, \omega)}. \quad (3.112)$$

If we take the diagrams in Fig.(3-8) for the self-energy, expansion of the last equation for the Green's function, or iteration of Dyson's equation in diagrammatic Fig.(3-4), regive the terms discussed above in the straightforward expansion since the algebraic expression for the self-energy we just defined is

$$\Sigma^R(\mathbf{k}, \omega) = [n_i v(\mathbf{0})] + \int_{\mathbf{k}_1 \neq \mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3} \left[n_i |v(\mathbf{k} - \mathbf{k}_1)|^2 \right] G_0^R(\mathbf{k}_1, \omega). \quad (3.113)$$

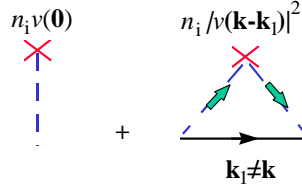


Figure 3-8 Second-order irreducible self-energy in the impurity averaging technique.

Remark 57 *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

$$E = \frac{k^2}{2m} + \text{Re} [\Sigma^R(\mathbf{k}, E)]. \quad (3.114)$$

Remark 58 *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 Lorentzian and the corresponding propagator in time is $G^R(\mathbf{k}, \omega) = -ie^{-i(k^2/2m - a)t} e^{-t/\tau}$. 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.(3.113) is

$$\text{Im} \Sigma^R(\mathbf{k}, \omega) = -\pi \int_{\mathbf{k}_1 \neq \mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3} \left[n_i |v(\mathbf{k} - \mathbf{k}_1)|^2 \right] \delta\left(\omega - \frac{k_1^2}{2m}\right) \quad (3.115)$$

$$= -\pi \int d\epsilon N(\epsilon) \frac{d\Omega}{4\pi} \left[n_i |v(\mathbf{k} - \mathbf{k}_1)|^2 \right] \delta(\omega - \epsilon) \quad (3.116)$$

where in the last expression, $N(\epsilon)$ 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 $-\text{Im} \Sigma^R(\mathbf{k}, \omega)$ 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 59 *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 $\int \frac{d\omega}{2\pi} \text{Tr} \left[-2 \text{Im} \left(\widehat{G}^R(\omega) \right) \right] = \text{Tr} [H^0] = 1$ as well as the second $\int \frac{d\omega}{2\pi} \omega \text{Tr} \left[-2 \text{Im} \left(\widehat{G}^R \right) \right] = \text{Tr} [H]$. 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 60 *Average self-energy and self-averaging:* We could have obtained precisely the same result by directly averaging the self-energies (3.84)(3.85) defined in the previous subsection (3.82). 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 (3.85) would have given only the correlated contribution $\int_{\mathbf{k}_1 \neq \mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3} \left[n_i |v(\mathbf{k} - \mathbf{k}_1)|^2 \right] G_0^R(\mathbf{k}_1, \omega)$. A $G_0^R(\mathbf{k}, \omega)$ in the intermediate state would be necessary to obtain a contribution $[n_i v(\mathbf{0})]^2$. It is possible to average directly the self-energy in the Dyson equation Eq.(3.82) 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 61 *Correlations in the impurity distribution:* If we had taken into account impurity-impurity correlations in the joint average (3.103),

$$\overline{\sum_{i=1}^{N_i} \sum_{j \neq i}^{N_i} e^{-i\mathbf{q} \cdot \mathbf{R}_i} e^{-i\mathbf{q}' \cdot \mathbf{R}_j}}, \quad (3.117)$$

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 62 *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.(3-9) 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.

Remark 63 *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

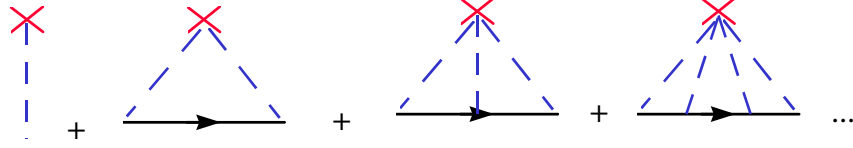


Figure 3-9 Taking into account multiple scattering from a single impurity.

function will be given by Eq.(3.12)

$$G^R(\mathbf{k}, \mathbf{k}; \omega) = \sum_n \frac{\langle \mathbf{k} | n \rangle \langle n | \mathbf{k} \rangle}{\omega + i\eta - E_n} \quad (3.118)$$

$$-\frac{1}{\pi} \text{Im} [G^R(\mathbf{k}, \mathbf{k}; \omega)] = \sum_n \langle \mathbf{k} | n \rangle \langle n | \mathbf{k} \rangle \delta(\omega - E_n). \quad (3.119)$$

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 $-\frac{1}{\pi} \text{Im} [G^R(\mathbf{k}, \mathbf{k}; \omega)]$ 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 $\eta \rightarrow 0$ limit.

Remark 64 Origin of poles far from the real axis: 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

$$-\frac{1}{\pi} \text{Im} [G^R(\mathbf{k}, \mathbf{k}; \omega)] = \frac{1}{\pi} \frac{-\text{Im} [\Sigma^R(\mathbf{k}, \omega)]}{\left(\omega - \frac{k^2}{2m} - \text{Re}[\Sigma^R(\mathbf{k}, \omega)]\right)^2 + (\text{Im}[\Sigma^R(\mathbf{k}, \omega)])^2} \quad (3.120)$$

then there are many cases, such as the one of degenerate electrons scattering off impurities, where for small ω we can approximate $\text{Im}(\Sigma^R(\mathbf{k}, \omega))$ by a constant and $\text{Re}[\Sigma^R(\mathbf{k}, \omega)]$ 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.(3.24) 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.(3.27) 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 $\eta \rightarrow 0$.

3.6 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.(3-10). The density operators act at the far left and far right of these diagrams.

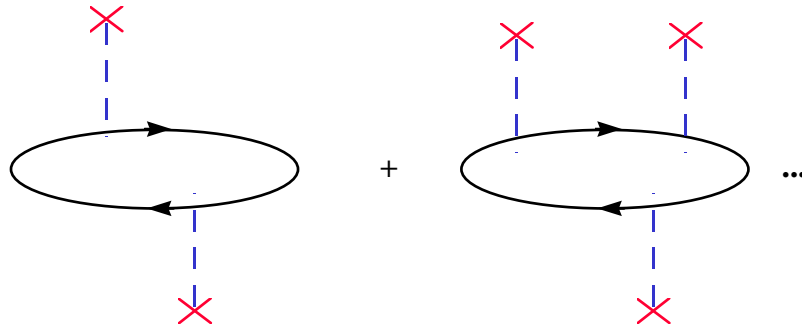


Figure 3-10 Some diagrams contributing to the density-density correlation function before impurity averaging.

After impurity averaging, we obtain for example diagrams of the form illustrated in Fig.(3-11)

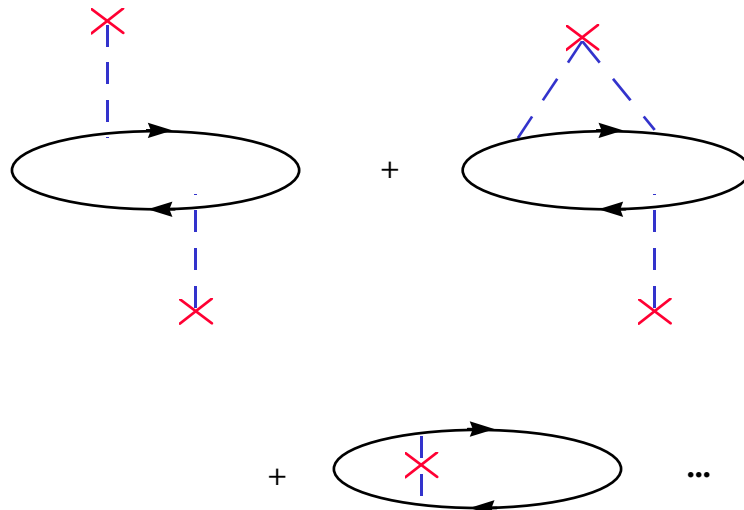


Figure 3-11 Some of the density-density diagrams after impurity averaging.

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.(3-11) 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 one in Fig.(3-11), are so-called vertex corrections.

Subsets of vertex corrections that can be resummed correspond to ladders or bubbles. Ladder diagrams, illustrated in Fig.(3-12) correspond to the so-called Bethe-Salpeter equation, or T-matrix equation. They occur in the problem of superconductivity and of localization.

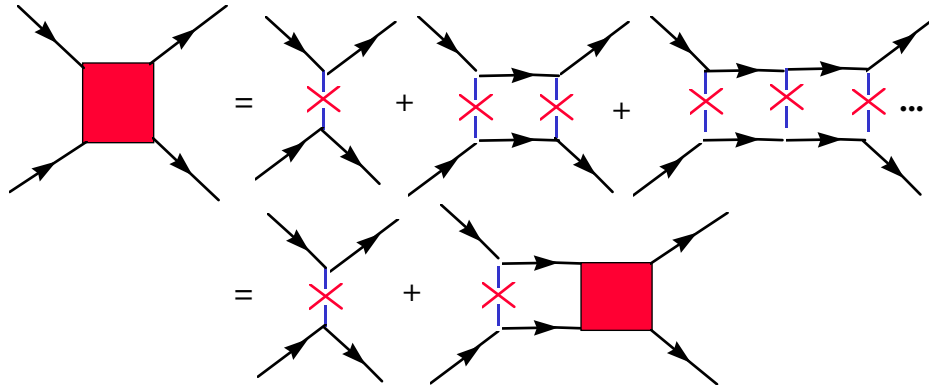


Figure 3-12 Ladder diagrams for T-matrix or Bethe-Salpeter equation.

The bubbles illustrated in Fig.(3-13) 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.

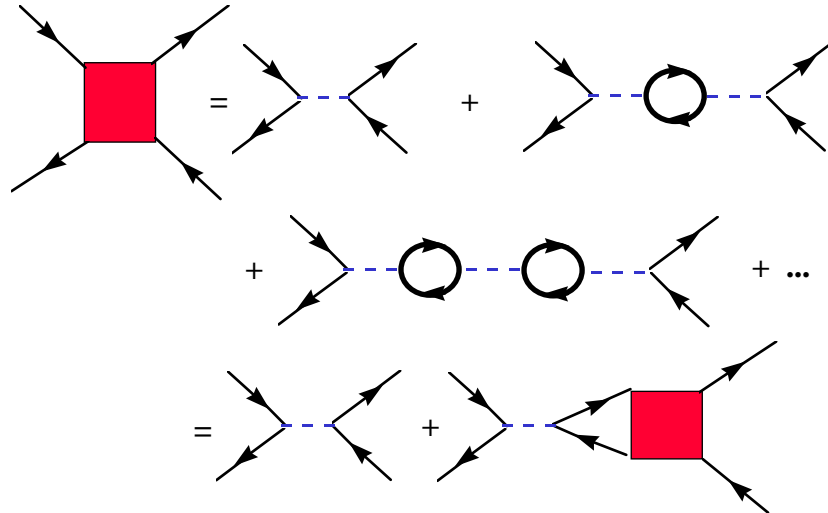


Figure 3-13 Bubble diagrams for particle-hole excitations.

Finally, self-consistent Hartree-Fock theory can be formulated using skeleton diagrams, as illustrated in Fig.(3-14). 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.

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.

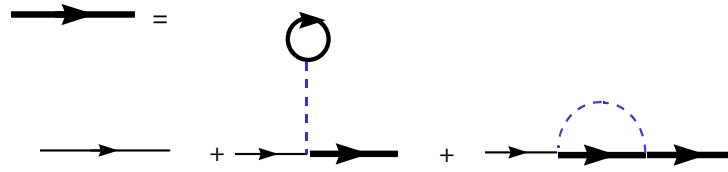


Figure 3-14 Diagrammatic representation of the Hartree-Fock approximation.

We come back on all these notions as in the context of the “real” many-body problem that we now begin to discuss.

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Part II

Traditional approaches to
the normal state $d \geq 3$.

4. FINITE TEMPERATURE FORMALISM

We are now ready to start working with the real many-body problem. This chapter will be rather formal but we will make the link with the previous chapter and also we will try to do applications as soon as possible in the following chapter.

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.

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 $\sqrt{2}^{-1} \langle \mathbf{r}_1 | \otimes \langle \mathbf{r}_2 | [|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle]$. 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

$$\psi(x, y) = (x - y) N e^{-|x-y|/a} \quad (4.1)$$

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.

The plan then is as follows. Starting with a short summary of important results of second quantization, we will then motivate the definition of the Green's function in the many-body context by analogy with what we just saw. Then, we return to perturbation theory to show that it is most natural to work in imaginary time. This leads us to the Matsubara Green's function. We show that if we know this Green's function, we also happen to know the retarded one, as well as all the one-body quantities of physical interest. 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.

4.1 Main results from second quantization

We want to write one- and two-body operators in a way which is independent of the number of particles present in the system.

Choose a complete set of normalized one-body wave functions. Following Negele and Orland[1] we introduce the antisymmetrized (symmetrized) many-body state

$$|\alpha_1\alpha_2\dots\alpha_N\rangle \quad (4.2)$$

In this state, one particle is put in the one-body state whose label is α_1 , another one in the one-body state whose label is α_2 , until the N 'th particle. The resulting state is symmetrized if we have bosons, and antisymmetrized if we have fermions. A normalized basis may be obtained from

$$|\alpha_1\alpha_2\dots\alpha_N\rangle = \frac{1}{\sqrt{\prod_{\alpha} n_{\alpha}!}} |\alpha_1\alpha_2\dots\alpha_N\rangle$$

With N -particles, the quantity

$$\langle \mathbf{r}_1\mathbf{r}_2\dots\mathbf{r}_N | \alpha_1\alpha_2\dots\alpha_N \rangle \quad (4.3)$$

is proportional to a Slater determinant if we have fermions, and to a permanent if we have bosons.

Creation operators a_{α}^{\dagger} add a particle in the one-body state α and antisymmetrize (symmetrize) the resulting many-body state. The adjoints remove a particle and antisymmetrize (symmetrize). They are destruction, or annihilation, operators. A normalized many-body state made up of single-particle states can then be written in the form

$$|\alpha_1\alpha_2\dots\alpha_N\rangle = \frac{1}{\sqrt{\prod_{\alpha} n_{\alpha}!}} a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \dots a_{\alpha_N}^{\dagger} |0\rangle \quad (4.4)$$

where $a_{\alpha} |0\rangle = 0$. Given their definition, the creation-annihilation operators obey the following algebra

for fermions

$$\{a_{\alpha}, a_{\beta}^{\dagger}\} \equiv a_{\alpha} a_{\beta}^{\dagger} + a_{\beta}^{\dagger} a_{\alpha} = \delta_{\alpha,\beta} \quad (4.5)$$

$$\{a_{\alpha}, a_{\beta}\} \equiv a_{\alpha} a_{\beta} + a_{\beta} a_{\alpha} = 0 \quad (4.6)$$

$$\{a_{\alpha}^{\dagger}, a_{\beta}^{\dagger}\} \equiv a_{\alpha}^{\dagger} a_{\beta}^{\dagger} + a_{\beta}^{\dagger} a_{\alpha}^{\dagger} = 0 \quad (4.7)$$

for bosons

$$[a_{\alpha}, a_{\beta}^{\dagger}] \equiv a_{\alpha} a_{\beta}^{\dagger} - a_{\beta}^{\dagger} a_{\alpha} = \delta_{\alpha,\beta} \quad (4.8)$$

$$[a_{\alpha}, a_{\beta}] \equiv a_{\alpha} a_{\beta} - a_{\beta} a_{\alpha} = 0 \quad (4.9)$$

$$[a_{\alpha}^{\dagger}, a_{\beta}^{\dagger}] \equiv a_{\alpha}^{\dagger} a_{\beta}^{\dagger} - a_{\beta}^{\dagger} a_{\alpha}^{\dagger} = 0 \quad (4.10)$$

Given a unitary transformation from a basis labeled by α and one labeled by μ , the operators transform as follows,

$$a_{\alpha} = \sum_{\mu} \langle \alpha | \mu \rangle c_{\mu} \quad (4.11)$$

$$a_{\alpha}^{\dagger} = \sum_{\mu} c_{\mu}^{\dagger} \langle \mu | \alpha \rangle. \quad (4.12)$$

as can be seen from the fact that creating a particle in a state $|\alpha\rangle = \sum_{\mu} |\mu\rangle \langle\mu|\alpha\rangle$ and antisymmetrizing is like creating a particle in the proper linear combination of states $|\mu\rangle$ and antisymmetrizing. The inverse transformations are easy to derive using the completeness and orthogonality relations. It is easy to check that the new operators obey the above commutation or anticommutation relations. When this is the case, it is said that one is dealing with a canonical transformation.

For either fermions or bosons, the operator which gives the number of particles in state α is

$$\hat{n}_{\alpha} = a_{\alpha}^{\dagger} a_{\alpha}$$

$$\hat{n}_{\alpha} |\alpha_1 \alpha_2 \dots \alpha_N\rangle = n_{\alpha} |\alpha_1 \alpha_2 \dots \alpha_N\rangle \quad (4.13)$$

where n_{α} is the number of particles in state α .

4.1.1 One-body operators

The matrix elements of an arbitrary one-body operator \hat{U} (in the N -particle case) may thus be computed in the many-body basis made of one-body states where \hat{U} is diagonal

$$\hat{U} |\alpha\rangle = U_{\alpha} |\alpha\rangle = \langle\alpha| U |\alpha\rangle |\alpha\rangle \quad (4.14)$$

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. This allows us to rewrite,

$$\hat{U} |\alpha_1 \alpha_2 \dots \alpha_N\rangle = \left(\sum_{i=1}^N U_{\alpha_i} \right) |\alpha_1 \alpha_2 \dots \alpha_N\rangle = \sum_{\alpha} U_{\alpha} \hat{n}_{\alpha} |\alpha_1 \alpha_2 \dots \alpha_N\rangle \quad (4.15)$$

where now the sum in $\sum_{\alpha} U_{\alpha} \hat{n}_{\alpha}$ extends over the complete set of one-body states and 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 it extends over *states*. Using the change of basis formula explained above, we have that

$$\hat{U} = \sum_{\alpha} U_{\alpha} \hat{n}_{\alpha} = \sum_{\alpha} \langle\alpha| U |\alpha\rangle a_{\alpha}^{\dagger} a_{\alpha} = \sum_{\lambda\mu} \langle\lambda| U |\mu\rangle a_{\lambda}^{\dagger} a_{\mu} \quad (4.16)$$

Let us give examples in the position and momentum representation. But first a definition of states and normalization.

Definition 6 *In this strange, but commonly used, basis where we take continuum notation for space and discrete notation for momentum, we have the conventions*

$$\sum_{\mathbf{k}} |\mathbf{k}\rangle \langle\mathbf{k}| = 1 = \int d\mathbf{r} |\mathbf{r}\rangle \langle\mathbf{r}|$$

$$\langle\mathbf{r}|\mathbf{k}\rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{r}} \quad (4.17)$$

$$\langle\mathbf{k}|\mathbf{r}\rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (4.18)$$

From these definitions, we have 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

$$\langle\mathbf{r}|\mathbf{r}'\rangle = \sum_{\mathbf{k}} \langle\mathbf{r}|\mathbf{k}\rangle \langle\mathbf{k}|\mathbf{r}'\rangle = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}') \quad (4.19)$$

$$\langle \mathbf{k} | \mathbf{k}' \rangle = \int d\mathbf{r} \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k}' \rangle = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{r} \cdot (\mathbf{k} - \mathbf{k}')} = \delta_{\mathbf{k}, \mathbf{k}'} \quad (4.20)$$

Example 7 *Example of one-body operator: Taking discrete values of momentum, as on a lattice, we have*

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle c_{\mathbf{k}} \quad (4.21)$$

$$\psi^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger \langle \mathbf{k} | \mathbf{r} \rangle \quad (4.22)$$

The momentum operators obey the algebra of a discrete set of creation operators. Taking fermions as an example,

$$\boxed{\{c_{\mathbf{k}}, c_{\mathbf{k}'}^\dagger\} = \delta_{\mathbf{k}, \mathbf{k}'} \quad ; \quad \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = \{c_{\mathbf{k}}^\dagger, c_{\mathbf{k}'}^\dagger\} = 0} \quad (4.23)$$

while the position space creation-annihilation operators obey

$$\boxed{\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\} = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle \mathbf{r} | \mathbf{k} \rangle \{c_{\mathbf{k}}, c_{\mathbf{k}'}^\dagger\} \langle \mathbf{k}' | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')} \quad (4.24)$$

$$\boxed{\{\psi(\mathbf{r}), \psi(\mathbf{r}')\} = \{\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\} = 0} \quad (4.25a)$$

A one-body scattering potential in the continuum would be represented by

$$\boxed{\hat{U} = \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})} \quad (4.26)$$

which looks similar to the usual Schrödinger average. Similarly, the kinetic energy operator in the momentum representation becomes

$$\hat{T} = \sum_{\mathbf{k}} \langle \mathbf{k} | \frac{k^2}{2m} | \mathbf{k} \rangle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} = \sum_{\mathbf{k}} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \frac{k^2}{2m} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle \psi(\mathbf{r}') \quad (4.27)$$

$$= \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \frac{k^2}{2m} \psi(\mathbf{r}') \quad (4.28)$$

$$= \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int d\mathbf{r} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}) \left(-\frac{1}{2m} \nabla^2 \right) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \psi(\mathbf{r}'). \quad (4.29)$$

Performing the \mathbf{k} summation and using partial integration assuming that everything vanishes at infinity or is periodic, we obtain,

$$\boxed{\hat{T} = \left(-\frac{1}{2m} \right) \int d\mathbf{r} \psi^\dagger(\mathbf{r}) (\nabla^2 \psi(\mathbf{r})) = \frac{1}{2m} \int d\mathbf{r} \nabla \psi^\dagger(\mathbf{r}) \cdot \nabla \psi(\mathbf{r})}. \quad (4.30)$$

4.1.2 Two-body operators.

A two-body operator involves the coordinates of two particles. An example is the Coulomb potential. In the basis where a two-body operator is diagonal, we have that

$$\hat{V} |\alpha\rangle \otimes |\beta\rangle = V_{\alpha\beta} |\alpha\rangle \otimes |\beta\rangle \quad (4.31)$$

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

$$\widehat{V} |\alpha_1 \alpha_2 \dots \alpha_N\rangle = \left(\frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N V_{\alpha_i \alpha_j} \right) |\alpha_1 \alpha_2 \dots \alpha_N\rangle \quad (4.32)$$

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 case $j = i$ in the sum. In general then,

$$\frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N V_{\alpha_i \alpha_j} \rightarrow \frac{1}{2} \sum_{\alpha} \sum_{\beta} V_{\alpha\beta} (\widehat{n}_{\alpha} \widehat{n}_{\beta} - \delta_{\alpha\beta} \widehat{n}_{\alpha}) \quad (4.33)$$

Defining

$$\boxed{\zeta = -1 \quad \text{for fermions}} \quad (4.34)$$

$$\boxed{\zeta = 1 \quad \text{for bosons}} \quad (4.35)$$

we can rewrite $\widehat{n}_{\alpha} \widehat{n}_{\beta} - \delta_{\alpha\beta} \widehat{n}_{\alpha}$ in terms of creation and annihilation operators in such a way that the form is valid for both fermions and bosons

$$\widehat{n}_{\alpha} \widehat{n}_{\beta} - \delta_{\alpha\beta} \widehat{n}_{\alpha} = a_{\alpha}^{\dagger} a_{\alpha} a_{\beta}^{\dagger} a_{\beta} - \delta_{\alpha\beta} a_{\alpha}^{\dagger} a_{\alpha} = a_{\alpha}^{\dagger} \zeta a_{\beta}^{\dagger} a_{\alpha} a_{\beta} = a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta} a_{\alpha} \quad (4.36)$$

Second quantized operators are thus written in the simple form

$$\widehat{V} = \frac{1}{2} \sum_{\alpha} \sum_{\beta} V_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta} a_{\alpha} \equiv \frac{1}{2} \sum_{\alpha} \sum_{\beta} (\alpha\beta | V | \alpha\beta) a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta} a_{\alpha} \quad (4.37)$$

where

$$|\alpha\beta\rangle \equiv |\alpha\rangle \otimes |\beta\rangle. \quad (4.38)$$

Under unitary transformation to an arbitrary basis we have

$$\boxed{\widehat{V} = \frac{1}{2} \sum_{\lambda} \sum_{\mu} \sum_{\nu} \sum_{\rho} (\lambda\mu | V | \nu\rho) a_{\lambda}^{\dagger} a_{\mu}^{\dagger} a_{\rho} a_{\nu}} \quad (4.39)$$

Remark 65 Note the inversion in the order of ρ and ν in the annihilation operators compared with the order in the matrix elements (This could have been for the creation operator instead).

Remark 66 The notation $(\lambda\mu | V | \nu\rho)$ for the two-body matrix element means, in the coordinate representation for example,

$$\int d\mathbf{r}_1 d\mathbf{r}_2 \phi_{\lambda}^*(\mathbf{r}_1) \phi_{\mu}^*(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \phi_{\nu}(\mathbf{r}_1) \phi_{\rho}(\mathbf{r}_2). \quad (4.40)$$

Definition 8 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”.

Example 9 In the case of a potential, such as the Coulomb potential, which acts on the densities, we have

$$\boxed{\widehat{V} = \frac{1}{2} \int d\mathbf{x} \int d\mathbf{y} v(\mathbf{x} - \mathbf{y}) \psi^{\dagger}(\mathbf{x}) \psi^{\dagger}(\mathbf{y}) \psi(\mathbf{y}) \psi(\mathbf{x})}. \quad (4.41)$$

4.1.3 Second quantized operators in the Heisenberg picture

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

$$\boxed{c_{\mathbf{k}}(t) = e^{i\hat{H}t} c_{\mathbf{k}} e^{-i\hat{H}t} \quad ; \quad c_{\mathbf{k}}^{\dagger}(t) = e^{i\hat{H}t} c_{\mathbf{k}}^{\dagger} e^{-i\hat{H}t}} \quad (4.42)$$

It is easy to compute the time evolution in the case where the Hamiltonian is quadratic in creation and annihilation operators. Take for example

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \quad (4.43)$$

The time evolution may be found from the Heisenberg equation of motion, which follows from differentiating the definition of the Heisenberg operators

$$i \frac{\partial c_{\mathbf{k}}(t)}{\partial t} = [c_{\mathbf{k}}(t), \hat{H}]. \quad (4.44)$$

To evaluate the commutator, we note that since \hat{H} commutes with itself,

$$[c_{\mathbf{k}}(t), \hat{H}] = [c_{\mathbf{k}}(t), e^{i\hat{H}t} \hat{H} e^{-i\hat{H}t}] = [c_{\mathbf{k}}(t), e^{i\hat{H}t} \left(\sum_{\mathbf{k}'} \epsilon_{\mathbf{k}'} c_{\mathbf{k}'}^{\dagger} c_{\mathbf{k}'} \right) e^{-i\hat{H}t}] \quad (4.45)$$

$$= \left[c_{\mathbf{k}}(t), \left(\sum_{\mathbf{k}'} \epsilon_{\mathbf{k}'} c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t) \right) \right] = \sum_{\mathbf{k}'} \epsilon_{\mathbf{k}'} [c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)]. \quad (4.46)$$

Commutator identities: The following are very useful identities to get equations of motions, and in general equal-time commutators.

$$[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA \quad (4.47)$$

$$\boxed{[A, BC] = [A, B]C + B[A, C]} \quad (4.48)$$

$$\boxed{[A, BC] = \{A, B\}C - B\{A, C\}} \quad (4.49)$$

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 anticommutated with the A .

The above identities can then be used to evaluate the needed commutator either for fermions

$$[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)] = \{c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\} c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}}(t) \quad (4.50)$$

or for bosons

$$[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t) c_{\mathbf{k}'}(t)] = [c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)] c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}}(t) \quad (4.51)$$

in either case then, the equation of motion becomes

$$i \frac{\partial c_{\mathbf{k}}(t)}{\partial t} = [c_{\mathbf{k}}(t), \hat{H}] = \epsilon_{\mathbf{k}} c_{\mathbf{k}}(t) \quad (4.52)$$

whose solution is

$$\boxed{c_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}}t} c_{\mathbf{k}}} \quad (4.53)$$

Taking the adjoint,

$$\boxed{c_{\mathbf{k}}^{\dagger}(t) = c_{\mathbf{k}}^{\dagger} e^{i\epsilon_{\mathbf{k}}t}}. \quad (4.54)$$

If we had been working in a basis where \widehat{H} was not diagonal, then repeating the steps above,

$$i \frac{\partial a_{\alpha}(t)}{\partial t} = [a_{\alpha}(t), \widehat{H}] = \sum_{\beta, \gamma} \langle \beta | \widehat{H} | \gamma \rangle [a_{\alpha}(t), a_{\beta}^{\dagger}(t) a_{\gamma}(t)] = \sum_{\gamma} \langle \alpha | \widehat{H} | \gamma \rangle a_{\gamma}(t) \quad (4.55)$$

whose solution is found by diagonalizing, integrating, and changing back the basis.

4.2 Motivation of the definition of the second quantized Green's function G^R

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.

Consider the definition we had before

$$G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle \mathbf{r} | e^{-iH(t-t')} | \mathbf{r}' \rangle \theta(t - t'). \quad (4.56)$$

Since in second-quantization the operator $\psi^{\dagger}(\mathbf{r})$ creates a particle at point \mathbf{r} , the following definition seems natural

$$G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle GS | \psi(\mathbf{r}) e^{-iH(t-t')} \psi^{\dagger}(\mathbf{r}') | GS \rangle \theta(t - t') \quad (4.57)$$

In this expression, $|GS\rangle$ is a many-body vacuum (ground-state). Choosing appropriately the zero of energy, $H|GS\rangle = 0|GS\rangle = 0$ so that the above result could be written

$$G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle GS | \psi(\mathbf{r}, t) \psi^{\dagger}(\mathbf{r}', t') | GS \rangle \theta(t - t'). \quad (4.58)$$

This is not quite what we want except in the case where there is a single particle propagating. Indeed, to keep the physical definition of the propagator, it is convenient to have at time $t = t' + 0^+$

$$G^R(\mathbf{r}, t + 0^+; \mathbf{r}', t) = -i \delta(\mathbf{r} - \mathbf{r}') \quad (4.59)$$

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,

$$|GS\rangle = \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N \Psi(\mathbf{r}_1 \dots \mathbf{r}_N) \psi^{\dagger}(\mathbf{r}_1) \dots \psi^{\dagger}(\mathbf{r}_N) |0\rangle \quad (4.60)$$

where $\Psi(\mathbf{r}_1 \dots \mathbf{r}_N)$ reduces to the Schrödinger wave function and $|0\rangle$ is a real vacuum. This means that $\langle GS | \psi(\mathbf{r}, t) \psi^{\dagger}(\mathbf{r}', t) | GS \rangle$ is not in general a delta function.

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.(4.59) 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:

$$G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle GS | \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right\} | GS \rangle \theta(t - t') \quad ; \quad \text{for fermions} \quad (4.61)$$

$$G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \langle GS | \left[\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right] | GS \rangle \theta(t - t') \quad ; \quad \text{for bosons} \quad (4.62)$$

This is the zero-temperature definition. At finite temperature, the ground-state expectation value is replaced by a thermodynamic average. Hence we shall in general work with

Definition 10

$$\boxed{G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right\} \right\rangle \theta(t - t') \quad ; \quad \text{for fermions}} \quad (4.63)$$

$$\boxed{G^R(\mathbf{r}, t; \mathbf{r}', t') = -i \left\langle \left[\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right] \right\rangle \theta(t - t') \quad ; \quad \text{for bosons}} \quad (4.64)$$

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

Remark 67 *Analogies: This definition is now analogous to $\chi^R = 2i\chi''\theta(t - t')$ which we had in linear response. The imaginary part of the Green's function will again be a commutator or an anticommutator and hence will obey sum-rules.*

Remark 68 *Green's function as a response function: Physically, this definition makes obvious that the Green's function is the response to an external probe which 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).*

4.2.1 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

$$\langle \mathbf{r} | H | \mathbf{r}_1 \rangle = -\frac{\nabla^2}{2m} \langle \mathbf{r} | \mathbf{r}_1 \rangle = -\frac{\nabla^2}{2m} \delta(\mathbf{r} - \mathbf{r}_1). \quad (4.65)$$

In the general second quantized case, we write

$$\hat{H} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi^\dagger(\mathbf{r}_2, t) \langle \mathbf{r}_2 | H | \mathbf{r}_1 \rangle \psi(\mathbf{r}_1, t) \quad (4.66)$$

We give two calculations of the Green's function, one directly from the definition and one from the equations of motion (Schrödinger's equation).

Calculation from the definition. For a *quadratic Hamiltonian*, one can also compute directly the Green's function from its definition since, if $|n\rangle$ is an eigenbasis, $\phi_n(\mathbf{r}) = \langle \mathbf{r} | n \rangle$, $\langle n' | H | n \rangle = E_n \delta_{n,n'}$

$$\psi(\mathbf{r}, t) = \sum_n \langle \mathbf{r} | n \rangle a_n(t) = \sum_n e^{-iE_n t} \langle \mathbf{r} | n \rangle a_n = \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) a_n \quad (4.67)$$

$$\left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \right\} = \sum_n \sum_m e^{-iE_n t} \phi_n(\mathbf{r}) \{a_n, a_m^\dagger\} \phi_m^*(\mathbf{r}') = \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \quad (4.68)$$

$$G^R(\mathbf{r}, t; \mathbf{r}', 0) = -i \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \right\} \right\rangle \theta(t) = -i \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \theta(t) \quad (4.69)$$

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \int dt e^{i(\omega + i\eta)t} (-i) \sum_n e^{-iE_n t} \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \theta(t) = \sum_n \frac{\phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} \quad (4.70)$$

Calculation from the equations of motion In general, the equation of motion can be obtained as follows

$$i \frac{\partial}{\partial t} G^R(\mathbf{r}, t; \mathbf{r}', t') = i \frac{\partial}{\partial t} \left[-i \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right\} \right\rangle \theta(t - t') \right] \quad (4.71)$$

$$= \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right\} \right\rangle \delta(t - t') + i \left\langle \left[\widehat{H}, \psi(\mathbf{r}, t) \right], \psi^\dagger(\mathbf{r}', t') \right\rangle \theta(t - t') \quad (4.72)$$

Following the steps analogous to those in Eq.(4.50) above, using the anti-commutation relations Eqs.(4.24)(4.25a) it is clear that

$$\left[\widehat{H}, \psi(\mathbf{r}, t) \right] = - \int d\mathbf{r}_1 \langle \mathbf{r} | H | \mathbf{r}_1 \rangle \psi(\mathbf{r}_1, t) \quad (4.73)$$

so that

$$i \frac{\partial}{\partial t} G^R(\mathbf{r}, t; \mathbf{r}', t') \quad (4.74)$$

$$= \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') - i \int d\mathbf{r}_1 \langle \mathbf{r} | H | \mathbf{r}_1 \rangle \left\langle \left\{ \psi(\mathbf{r}_1, t), \psi^\dagger(\mathbf{r}', t') \right\} \right\rangle \theta(t - t')$$

$$= \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') + \int d\mathbf{r}_1 \langle \mathbf{r} | H | \mathbf{r}_1 \rangle G^R(\mathbf{r}_1, t; \mathbf{r}', t') \quad (4.75)$$

This last expression may be rewritten as

$$\int d\mathbf{r}_1 \langle \mathbf{r} | i \frac{\partial}{\partial t} - \widehat{H} | \mathbf{r}_1 \rangle G^R(\mathbf{r}_1, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \quad (4.76)$$

$$= \langle \mathbf{r} | \mathbf{r}' \rangle \delta(t - t') \quad (4.77)$$

where we recognize the equation (3.54) found in the previous Chapter. Formally then

$$\langle \mathbf{r} | \left(i \frac{\partial}{\partial t} - \widehat{H} \right) G^R(t - t') | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbf{r}' \rangle \delta(t - t') \quad (4.78)$$

so that the operator form of the Green's function is the same as that found before, namely

$$\widehat{G}^R(t - t') = \left(i \frac{\partial}{\partial t} - \widehat{H} \right)^{-1} \delta(t - t') \quad (4.79)$$

It is convenient to rewrite the result for the equation of motion Eq.(4.76) in the following form that is more symmetrical in space and time.

$$\int d\mathbf{r}_1 \int dt_1 \langle \mathbf{r} | i \frac{\partial}{\partial t} - \widehat{H} | \mathbf{r}_1 \rangle \delta(t - t_1) G^R(\mathbf{r}_1, t_1; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}') \delta(t - t')$$
(4.80)

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,

$$G^R(\mathbf{r}, t; \mathbf{r}_1, t_1)^{-1} = \langle \mathbf{r} | i \frac{\partial}{\partial t} - \widehat{H} | \mathbf{r}_1 \rangle \delta(t - t_1).$$
(4.81)

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.

Definition 11 *The following short-hand notation is often used*

$$\boxed{G^R(1, 1') \equiv G^R(\mathbf{r}, t; \mathbf{r}', t')}$$
(4.82)

$$\boxed{G^R(1, \bar{1})^{-1} G^R(\bar{1}, 1') = \delta(1 - 1')}$$
(4.83)

where the index with the overbar stands for an integral.

4.3 Interaction representation and time-ordered product

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 2. 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.

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

$$H = H_0 + V$$
(4.84)

where

$$[H_0, V] \neq 0$$
(4.85)

Let us begin. We assume that H is time independent. Typical matrix elements we want to compute at finite temperature are of the form

$$\langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle$$
(4.86)

We do not write explicitly indices other than time to keep the notation simple. Recall the Heisenberg and Schrödinger picture

$$\psi_H(t) = e^{iHt} \psi_S e^{-iHt}$$
(4.87)

We define the time evolution operator

$$U(t, 0) = e^{-iHt} \quad (4.88)$$

so that

$$\psi_H(t) = U(0, t) \psi_S U(t, 0) \quad (4.89)$$

Because from now on we assume time-reversal symmetry, we will always make the replacement

$$U^\dagger(t, 0) = U(0, t) \quad (4.90)$$

as we just did. The differential equation for the time-evolution operator is

$$i \frac{\partial U(t, 0)}{\partial t} = H U(t, 0) \quad (4.91)$$

With the initial condition $U(0, 0) = 1$ it has $U(t, 0) = e^{-iHt}$ as its solution. It obeys the semi-group property

$$U(t, t') = U(t, 0) U(0, t') = e^{-iH(t-t')} \quad (4.92)$$

$$U^{-1}(t, 0) = U(0, t) \quad (4.93)$$

$$U(t_0, t_0) = 1 \quad (4.94)$$

for arbitrary t_0

We are now ready to introduce the interaction representation. In this representation, the fields evolve with the unperturbed Hamiltonian

$$\boxed{\hat{\psi}(t) = e^{iH_0 t} \psi_S e^{-iH_0 t}} \quad (4.95)$$

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,

$$\langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle = \langle i | e^{-\beta H} U(0, t) \psi_S U(t, 0) U(0, t') \psi_S^\dagger U(t', 0) | i \rangle \quad (4.96)$$

it suffices to notice that it is easy to remove the extra $e^{iH_0 t}$ coming from the replacement of ψ_S by $e^{-iH_0 t} \hat{\psi}(t) e^{iH_0 t}$ simply by including them in the definition of the evolution operator in the interaction representation

$$\hat{U}(t, 0) = e^{iH_0 t} U(t, 0) \quad (4.97)$$

$$\hat{U}(0, t) = U(0, t) e^{-iH_0 t} \quad (4.98)$$

$$\hat{U}(t, 0) \hat{U}(0, t) = \hat{U}(0, t) \hat{U}(t, 0) = 1 \quad (4.99)$$

With these definitions, we have that our general matrix element takes the form

$$\langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle = \langle i | e^{-\beta H} \hat{U}(0, t) \hat{\psi}(t) \hat{U}(t, 0) \hat{U}(0, t') \hat{\psi}^\dagger(t') \hat{U}(t', 0) | i \rangle \quad (4.100)$$

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

$$i \frac{\partial \hat{U}(t, 0)}{\partial t} = e^{iH_0 t} (-H_0 + H) U(t, 0) = e^{iH_0 t} V (e^{-iH_0 t} e^{iH_0 t}) U(t, 0) \quad (4.101)$$

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 $\widehat{U}(t, 0)$ is then

$$i \frac{\partial \widehat{U}(t, 0)}{\partial t} = \widehat{V}(t) \widehat{U}(t, 0)$$

Multiplying on the right by $\widehat{U}(0, t_0)$ we have a more general equation

$$\boxed{i \frac{\partial \widehat{U}(t, t_0)}{\partial t} = \widehat{V}(t) \widehat{U}(t, t_0)} \quad (4.102)$$

Remark 69 *Difficulties associated with the fact that we have non-commuting operators: The solution of this equation is not $e^{-i \int \widehat{V}(t) dt}$. 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 $\widehat{U}(t, t_0)$ as if it was a number. In reality it is an operator so that $\frac{\partial \widehat{U}(t, t_0)}{\partial t} \widehat{U}(t, t_0)^{-1} \neq \frac{\partial}{\partial t} \ln \widehat{U}(t, t_0)$. Indeed, note the ambiguity in writing the definition of this derivative: Should we write*

$$\frac{\partial}{\partial t} \ln \widehat{U}(t, t_0) = \lim_{\Delta t \rightarrow 0} \widehat{U}(t, t_0)^{-1} \left[\widehat{U}(t + \Delta t, t_0) - \widehat{U}(t, t_0) \right] / \Delta t$$

or

$$\lim_{\Delta t \rightarrow 0} \left[\widehat{U}(t + \Delta t, t_0) - \widehat{U}(t, t_0) \right] \widehat{U}(t, t_0)^{-1} / \Delta t ? \quad (4.103)$$

The two limits cannot be identical since in general

$$\lim_{\Delta t \rightarrow 0} \left[\widehat{U}(t + \Delta t, t_0), \widehat{U}(t, t_0)^{-1} \right] \neq 0. \quad (4.104)$$

because $\widehat{U}(t, t_0)$ is made up of operators such as V and $e^{-iH_0 t}$ that do not commute with each other.

To solve the equation for the evolution operator Eq.(4.102), 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.(4.94) gives immediately

$$\int_{t_0}^t \frac{\partial \widehat{U}(t', t_0)}{\partial t'} dt' = -i \int_{t_0}^t dt' \widehat{V}(t') \widehat{U}(t', t_0) \quad (4.105)$$

$$\widehat{U}(t, t_0) = 1 - i \int_{t_0}^t dt' \widehat{V}(t') \widehat{U}(t', t_0) \quad (4.106)$$

Solving by iteration, we find

$$\widehat{U}(t, t_0) = 1 - i \int_{t_0}^t dt' \widehat{V}(t') \widehat{U}(t', t_0) = \quad (4.107)$$

$$= 1 - i \int_{t_0}^t dt' \widehat{V}(t') + (-i)^2 \int_{t_0}^t dt' \widehat{V}(t') \int_{t_0}^{t'} dt'' \widehat{V}(t'') \quad (4.108)$$

$$+ (-i)^3 \int_{t_0}^t dt' \widehat{V}(t') \int_{t_0}^{t'} dt'' \widehat{V}(t'') \int_{t_0}^{t''} dt''' \widehat{V}(t''') + \dots \quad (4.109)$$

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

$$(-i)^3 \int_{t_0}^t dt' \widehat{V}(t') \int_{t_0}^{t'} dt'' \widehat{V}(t'') \int_{t_0}^{t''} dt''' \widehat{V}(t''') \quad (4.110)$$

$$= (-i)^3 \frac{1}{3!} T_c \left[\int_C dt_1 \widehat{V}(t_1) \int_C dt_2 \widehat{V}(t_2) \int_C dt_3 \widehat{V}(t_3) \right] \quad (4.111)$$

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”. Assuming $t > t_0$, it 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 left-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 $\widehat{V}(t_1) \widehat{V}(t_2) \widehat{V}(t_3)$ 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 $\widehat{U}(0, t)$. 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

$$\widehat{U}(t, t_0) = \sum_{k=0}^{\infty} (-i)^k \frac{1}{k!} T_c \left[\left(\int_C dt_1 \widehat{V}(t_1) \right)^k \right] \quad (4.112)$$

which we can in turn write in the convenient notation

$$\boxed{\widehat{U}(t, t_0) = T_c \left[\exp \left(-i \int_C dt_1 \widehat{V}(t_1) \right) \right]} \quad (4.113)$$

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 .

We can check the limiting case $[H_0, V] = 0$. Then \widehat{V} 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 $\widehat{U}(t, t_0)$ is the so-called S matrix. The time-ordering concept is due to Feynman and Dyson.

Remark 70 *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,[2] 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 $e^{-iH_0 t}$. 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 71 *The general case of time-dependent Hamiltonians: The problem we just solved for the time evolution in the interaction picture Eq.(4.102) is a much more general problem that poses itself whenever the Hamiltonian is time-dependent.*

4.4 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 $t \rightarrow -i\tau$. 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

$$e^{-\beta H} = U(-i\beta, 0) = e^{-iH_0(-i\beta)}\widehat{U}(-i\beta, 0) = e^{-\beta H_0}\widehat{U}(-i\beta, 0) \quad (4.114)$$

The solution of the imaginary time evolution equation

$$i\frac{\partial \widehat{U}(it'', 0)}{\partial (it'')} = \widehat{V}(it'')\widehat{U}(it'', 0)$$

is then

$$\widehat{U}(-i\beta, 0) = T_c \left[\exp \left(-i \int_C d(it'') \widehat{V}(it'') \right) \right] \quad (4.115)$$

where

$$\boxed{t'' \equiv \text{Im}(t)} \quad (4.116)$$

$$\widehat{V}(it'') = e^{-t'' H_0} V e^{t'' H_0} \quad (4.117)$$

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

$$\langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle = \langle i | e^{-\beta H_0} \widehat{U}(-i\beta, 0) \widehat{U}(0, t) \widehat{\psi}(t) \widehat{U}(t, 0) \widehat{U}(0, t') \widehat{\psi}^\dagger(t') \widehat{U}(t', 0) | i \rangle \quad (4.118)$$

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

$$|i\rangle = \widehat{U}(0, t_0) |i(t_0)\rangle \quad (4.119)$$

then we have

$$\langle i | e^{-\beta H} = \langle i(t_0) | \widehat{U}(t_0, 0) e^{-\beta H} = \langle i(t_0) | (e^{-\beta H_0} e^{\beta H_0}) (e^{iH_0 t_0} e^{-iH t_0}) e^{-\beta H} \quad (4.120)$$

$$= \langle i(t_0) | e^{-\beta H_0} e^{iH_0(t_0-i\beta)} e^{-iH(t_0-i\beta)} = \langle i(t_0) | e^{-\beta H_0} \widehat{U}(t_0-i\beta, 0) \quad (4.121)$$

This allows us to write an arbitrary matrix element entering the thermodynamic trace as the evolution along a contour in complex time

$$\begin{aligned} \langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle &= \langle i(t_0) | e^{-\beta H_0} \widehat{U}(t_0-i\beta, 0) \widehat{U}(0, t) \widehat{\psi}(t) \widehat{U}(t, 0) \widehat{U}(0, t') \widehat{\psi}^\dagger(t') \widehat{U}(t', 0) | i \rangle \\ &= \langle i(t_0) | e^{-\beta H_0} \widehat{U}(t_0-i\beta, t_0) \widehat{U}(t_0, t) \widehat{\psi}(t) \widehat{U}(t, t') \widehat{\psi}^\dagger(t') \widehat{U}(t', t_0) | i(t_0) \rangle \end{aligned} \quad (4.122)$$

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

$$\boxed{G^>(t-t') = -i \langle \psi_H(t) \psi_H^\dagger(t') \rangle} \quad (4.123)$$

$$\boxed{G^<(t-t') = i \langle \psi_H^\dagger(t') \psi_H(t) \rangle} \quad (4.124)$$

in such a way that

$$G^R(t-t') = -i \langle \{ \psi_H(t), \psi_H^\dagger(t') \} \rangle \theta(t-t') \equiv [G^>(t-t') - G^<(t-t')] \theta(t-t') \quad (4.125)$$

To evaluate $G^>(t-t')$ for example, we would expand the evolution operators such as $\widehat{U}(t', t_0)$ as a power series in \widehat{V} , each power of \widehat{V} being associated with an integral of a time ordered product that would start from t_0 to go to the creation operator $\widehat{\psi}^\dagger(t')$, then go to the destruction operator $\widehat{\psi}(t)$ until it returns to $t_0-i\beta$. This contour is illustrated in Fig.(4-1). 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 $\widehat{\psi}(t)$ always occur after $\widehat{\psi}^\dagger(t')$ on the contour, *i.e.* $\widehat{\psi}(t)$ is on the left of $\widehat{\psi}^\dagger(t')$ in the algebraic expression. The parts of the contour that follow the real axis are displaced slightly along the imaginary direction for clarity.

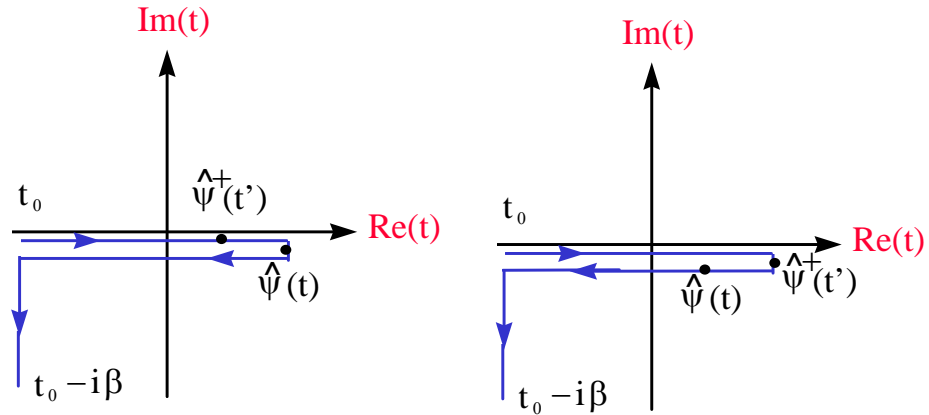


Figure 4-1 Kadanoff-Baym contour to compute $G^>(t-t')$.

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 $\widehat{U}(t', \infty) \widehat{U}(\infty, t') = 1$ to the left of $\widehat{\psi}^\dagger(t')$ in the algebraic expression Eq.(4.122).

In practice this greatly simplifies the calculations since the contour, illustrated in Fig.(4-2), 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..

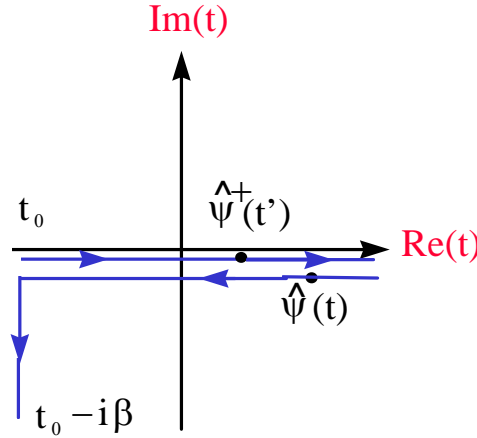


Figure 4-2 Keldysh-Schwinger contour.

In equilibrium, the analog of the fluctuation dissipation theorem in the form of Eq.(2.150) 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. 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.

4.5 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.(4-3) 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 functions as we wish, as long as we connect them to observable quantities in the corresponding manner at the end of the calculation. What makes this Green function extremely useful for calculations is the fact that in evaluating time-ordered products that occur in the perturbation series, a theorem (Wick's theorem) tells us that all correlations functions are related to products of time-ordered Green's functions. So we might as well focus on this quantity from the start. 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. 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. Also, the same tricks apply not only to Green's functions but also to general response functions such as the density-density 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 these functions are antiperiodic in imaginary time. This allows us to expand these functions in a Fourier series. The spectral representation and the so-called Lehman representation 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.

4.5.1 Definition

The Matsubara Green's function is defined by

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = - \left\langle T_\tau \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', \tau') \right\rangle \quad (4.126)$$

$$= - \left\langle \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', \tau') \right\rangle \theta(\tau - \tau') + \left\langle \psi^\dagger(\mathbf{r}', \tau') \psi(\mathbf{r}, \tau) \right\rangle \theta(\tau' - \tau) \quad (4.127)$$

The definition of Ref.([3]) has an overall minus sign difference with the definition given here.

Definition 12 *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. 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

$$\langle \mathcal{O} \rangle \equiv \frac{\text{Tr} [e^{-\beta(H-\mu N)} \mathcal{O}]}{\text{Tr} [e^{-\beta(H-\mu N)}]} \quad (4.128)$$

with μ the chemical potential and N is the total number of particle operator, while the time evolution of the operators is defined by

$$\psi(\mathbf{r}, \tau) \equiv e^{\tau(H-\mu N)} \psi_S(\mathbf{r}) e^{-\tau(H-\mu N)} \quad (4.129)$$

$$\psi^\dagger(\mathbf{r}, \tau) \equiv e^{\tau(H-\mu N)} \psi_S^\dagger(\mathbf{r}) e^{-\tau(H-\mu N)} \quad (4.130)$$

For convenience, it is useful to define

$$K \equiv H - \mu N \quad (4.131)$$

Several points should attract our attention:

- The correspondence with the real time evolution operators e^{-iHt} is done by noting that

$$\tau = -\text{Im}(t) \quad (4.132)$$

or, in general for complex time

$$\boxed{\tau = it}$$

- 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 $\widehat{\psi}(\mathbf{r}, \tau)$ 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 $\tau \rightarrow it$ 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 $\widehat{U}(-i\beta, 0) = T_c \left[\exp \left(- \int_C d\tau \widehat{V}(\tau) \right) \right]$ 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 ψ^\dagger : namely ψ^\dagger to the left of ψ and ψ^\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 $0 \leq \tau \leq \beta$.
- The last contour considered in the previous section for $\widehat{U}(-i\beta, 0) = T_c \left[\exp \left(- \int_C d\tau \widehat{V}(\tau) \right) \right]$ tells us that the time-ordering operator T_τ orders along the contour ($\text{Im}(t) = -\beta$) $>$ ($\text{Im}(t') = \beta$) which corresponds to $(\tau = \beta) > (\tau' = -\beta)$. The present contour is illustrated in Fig.(4-3).

Remark 72 *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. It corresponds to measuring energies with respect to the chemical potential as we will see with the Lehman representation below. 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 $(\psi^\dagger\psi)$ at equal time. Indeed in that case one has $\mathcal{O}^+(t) = e^{iHt}\mathcal{O}^+e^{-iHt} = e^{i(H-\mu N)t}\mathcal{O}^+e^{-i(H-\mu N)t}$. 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 single-particle energies with respect to the chemical potential.*

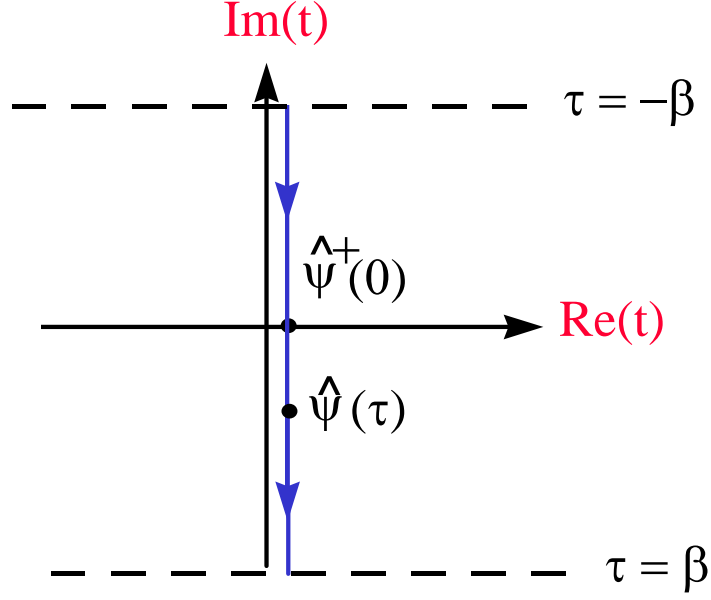


Figure 4-3 Contour for time ordering in imaginary time. Only the time difference is important. The contour is translated slightly along the real-time axis for clarity.

4.5.2 Antiperiodicity and Fourier expansion (Matsubara frequencies)

Suppose $\tau < 0$. Then

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = \langle \psi^+(\mathbf{r}', 0) \psi(\mathbf{r}, \tau) \rangle \quad (4.133)$$

Using the cyclic property of the trace twice, as in the demonstration of the fluctuation-dissipation theorem it is easy to show that

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = -\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau + \beta) \quad ; \quad \tau < 0} \quad (4.134)$$

This boundary condition is sometimes known as the Kubo-Martin-Schwinger (KMS) boundary condition.

Proof: Let

$$e^{-\beta\Omega} \equiv \text{Tr} [e^{-\beta K}] \quad (4.135)$$

then

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = e^{\beta\Omega} \text{Tr} [e^{-\beta K} \psi^+(\mathbf{r}') (e^{K\tau} \psi(\mathbf{r}) e^{-K\tau})] \quad (4.136)$$

The cyclic property of the trace then tells us that

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = e^{\beta\Omega} \text{Tr} [(e^{K\tau} \psi(\mathbf{r}) e^{-K\tau}) e^{-\beta K} \psi^+(\mathbf{r}')] \quad (4.137)$$

$$= e^{\beta\Omega} \text{Tr} [(e^{-\beta K} e^{\beta K}) (e^{K\tau} \psi(\mathbf{r}) e^{-K\tau}) e^{-\beta K} \psi^+(\mathbf{r}')] \quad (4.138)$$

$$= \langle \psi(\mathbf{r}, \tau + \beta) \psi^+(\mathbf{r}', 0) \rangle \quad (4.139)$$

$$= -\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau + \beta) \quad (4.140)$$

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 of the Matsubara Green's function.

If $\tau > 0$, the above arguments can be repeated to yield

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \beta) = -\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) \quad ; \quad \tau > 0} \quad (4.141)$$

However, for $\tau > 0$ note that

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) \neq -\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau + \beta) \quad ; \quad \tau > 0 \quad (4.142)$$

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

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n)} \quad (4.143)$$

where the so-called Matsubara frequencies for fermions are odd, namely

$$\boxed{k_n = (2n + 1) \pi T = \frac{(2n+1)\pi}{\beta}} \quad ; \quad n \text{ integer} \quad (4.144)$$

The antiperiodicity property will be automatically fulfilled because $e^{-ik_n \beta} = e^{-i(2n+1)\pi} = -1$.

The expansion coefficients are obtained as usual for Fourier series of antiperiodic functions from

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \int_0^\beta d\tau e^{ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau)} \quad (4.145)$$

Note that only the $\tau > 0$ region of the domain of definition is needed, as promised.

Remark 73 *Domain of definition of the Matsubara Green's function:* The value of $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau)$ given by the Fourier series (4.143) for τ outside the interval $-\beta < \tau < \beta$, is in general different from the actual value of Eq.(4.126) $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = -\langle T_\tau \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', \tau') \rangle$. 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 $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = -\langle T_\tau \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', \tau') \rangle$ 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 but we must beware.

4.5.3 Spectral representation, relation between G^R and \mathcal{G} and analytic continuation

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 is trivially related to $G^R(\mathbf{r}, \mathbf{r}'; \omega)$.

As before, we have

$$G^R(\mathbf{r}, \mathbf{r}'; t) = -i \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \right\} \right\rangle \theta(t) \quad (4.146)$$

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

$$K = H - \mu N$$

$$\psi(\mathbf{r}, t) \equiv e^{itK} \psi_S(\mathbf{r}) e^{-itK} \quad (4.147)$$

$$\psi^\dagger(\mathbf{r}, t) \equiv e^{itK} \psi_S^\dagger(\mathbf{r}) e^{-itK} \quad (4.148)$$

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

$$G^R(\mathbf{r}, \mathbf{r}'; t) = -iA(\mathbf{r}, \mathbf{r}'; t) \theta(t) \quad ; \quad \chi_{ij}^R(t) = 2i\chi_{ij}''(t) \theta(t) \quad (4.149)$$

where the *spectral weight* is defined by

$$A(\mathbf{r}, \mathbf{r}'; t) \equiv \langle \{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \} \rangle \quad ; \quad \chi_{ij}''(t) = \langle [A_i(\mathbf{r}, t), A_j(\mathbf{r}', 0)] \rangle \quad (4.150)$$

Then taking the Fourier transform, one obtains the spectral representation

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} \quad ; \quad \chi_{ij}^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi_{ij}''(\omega')}{\omega' - (\omega + i\eta)}. \quad (4.151)$$

The spectral weight will obey sum-rules, like χ'' did. For example

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{r}, \mathbf{r}'; \omega') = \langle \{ \psi(\mathbf{r}, 0), \psi^\dagger(\mathbf{r}', 0) \} \rangle = \delta(\mathbf{r} - \mathbf{r}') \quad (4.152)$$

From such sum rules, a high-frequency expansion can easily be found as usual. But that is not our subject for now.

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} , consider

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = -\langle \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', 0) \rangle \theta(\tau) + \langle \psi^\dagger(\mathbf{r}', 0) \psi(\mathbf{r}, \tau) \rangle \theta(-\tau) \quad (4.153)$$

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \int_0^\beta d\tau e^{ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) \quad (4.154)$$

$$= \int_0^\beta d\tau e^{ik_n \tau} [-\langle \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', 0) \rangle] \quad (4.155)$$

Assume that $k_n > 0$. Then, as illustrated in Fig.(4-4), we can deform the contour of integration within the domain of analyticity along $\text{Re}(t) = \text{Im}(\tau) > 0$. (The analyticity of $\langle \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', 0) \rangle$ 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.(4.162) and tricks for evaluating sums on Matsubara frequencies). For $\text{Im}(\tau) = \infty$ there will be no contribution from the small segment since $e^{ik_n \tau}$ becomes a decaying exponential. The integral becomes

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \quad (4.156)$$

$$\int_{t=0}^{t=\infty} d(it) [-\langle e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} \psi_S^\dagger(\mathbf{r}') \rangle] e^{ik_n(it)} \\ + \int_{t=-\infty}^{t=0} d(it) [-\langle e^{iK(t-i\beta)} \psi_S(\mathbf{r}) e^{-iK(t-i\beta)} \psi_S^\dagger(\mathbf{r}') \rangle] e^{(ik_n)i(t-i\beta)}$$

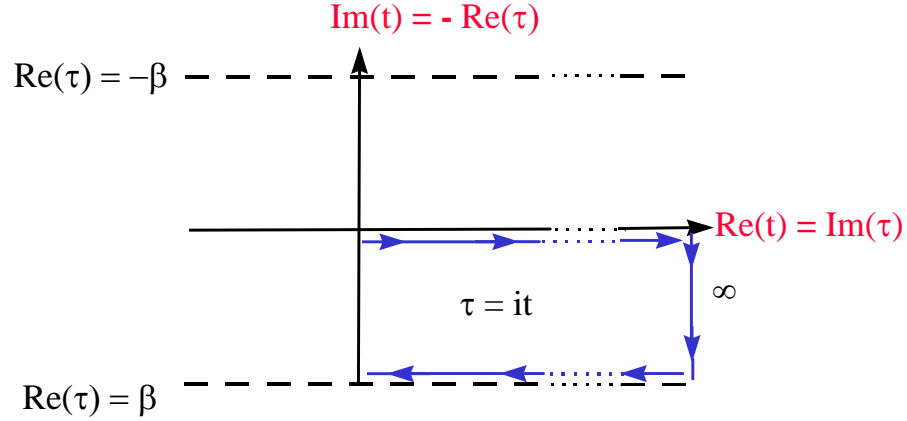


Figure 4-4 Deformed contour used to relate the Matsubara and the retarded Green's functions.

In the last integral, we then use the results

$$e^{(ik_n)i(-i\beta)} = e^{(ik_n)\beta} = -1 \quad (4.157)$$

$$\int_{-\infty}^0 = - \int_0^{\infty} \quad (4.158)$$

$$\left[- \left\langle e^{iK(t-i\beta)} \psi_S(\mathbf{r}) e^{-iK(t-i\beta)} \psi_S^\dagger(\mathbf{r}') \right\rangle \right] = \left[- \left\langle e^{\beta K} e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} e^{-\beta K} \psi_S^\dagger(\mathbf{r}') \right\rangle \right] \quad (4.159)$$

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,

$$= \left[- \left\langle \psi^\dagger(\mathbf{r}', 0) \psi(\mathbf{r}, t) \right\rangle \right]. \quad (4.160)$$

Overall then, the integral in Eq.(4.156) is equal to

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = -i \int_0^{\infty} dt \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \right\} \right\rangle e^{i(ik_n)t} \quad (4.161)$$

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{ik_n - \omega'}} \quad (4.162)$$

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 $\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n)$ for $k_n > 0$ with the expression for the retarded Green's function(4.151), we see that analytic continuation is possible.

$$\boxed{G^R(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{ik_n \rightarrow \omega + i\eta} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n)} \quad (4.163)$$

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 74 *Connectedness and periodicity:* For a general correlation function, similar spectral representations can also be defined for connected functions (see below) so that periodicity or anti-periodicity can be defined.

4.5.4 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.[4]

The key result for understanding the analytical properties of \mathcal{G} is the spectral representation Eq.(4.162)

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{ik_n - \omega'} \quad (4.164)$$

The spectral weight $A(\mathbf{r}, \mathbf{r}'; \omega')$ was discussed just in the previous subsection (See also Eq.(4.219)).

The Matsubara Green's function and the retarded functions are special case of a more general function defined in the complex frequency plane by

$$\boxed{G(\mathbf{r}, \mathbf{r}'; z) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{z - \omega'}} \quad (4.165)$$

This function is analytic everywhere except on the real axis. Physically interesting special cases are

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = G(\mathbf{r}, \mathbf{r}'; ik_n)$$

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\eta \rightarrow 0} G(\mathbf{r}, \mathbf{r}'; \omega + i\eta) \quad (4.166)$$

$$G^A(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\eta \rightarrow 0} G(\mathbf{r}, \mathbf{r}'; \omega - i\eta) \quad (4.167)$$

The function $G(\mathbf{r}, \mathbf{r}'; z)$ has a jump on the real axis given by

$$\boxed{A(\mathbf{r}, \mathbf{r}'; \omega') = i \lim_{\eta \rightarrow 0} [G(\mathbf{r}, \mathbf{r}'; \omega + i\eta) - G(\mathbf{r}, \mathbf{r}'; \omega - i\eta)]} \quad (4.168)$$

$$A(\mathbf{r}, \mathbf{r}'; \omega') = i [G^R(\mathbf{r}, \mathbf{r}'; \omega) - G^A(\mathbf{r}, \mathbf{r}'; \omega)]$$

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

$$A(\mathbf{r}, \mathbf{r}'; \omega') = -2 \text{Im} G^R(\mathbf{r}, \mathbf{r}'; \omega) \quad (4.169)$$

like we have often used in the one-body case.

The previous results are summarized in Fig.(4-5) 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.(4.168) 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 $G(z) (1 + (e^{\beta z} + 1))$ has the same value as $G(z)$ for all points $z = ik_n$ because $e^{ik_n \beta} + 1 = 0$. Baym and Mermin[5], using results from the theory of complex functions, have obtained the following result.

Theorem 13 *If*

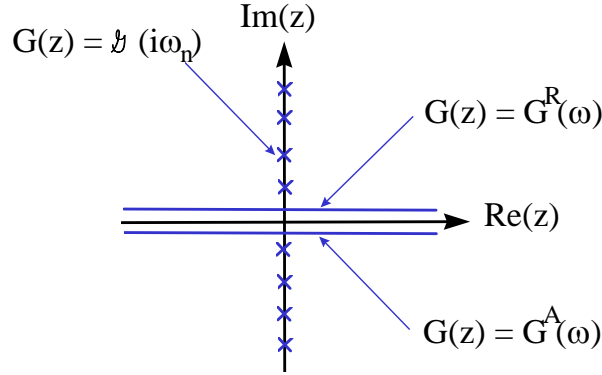


Figure 4-5 Analytical structure of $G(z)$ in the complex frequency plane. $G(z)$ reduces to either $G^R(\omega)$, $G^A(\omega)$ or $\mathcal{G}(i\omega_n)$ depending on the value of the complex frequency z . There is a branch cut along the real axis.

1. $G(z)$ is analytical in the upper half-plane
2. $G(z) = \mathcal{G}(ik_n)$ for all Matsubara frequencies
3. $\lim_{z \rightarrow \infty} zG(z) = cst$

then the analytical continuation is unique and

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{ik_n \rightarrow \omega + i\eta} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \quad (4.170)$$

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.(4.165) 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 $ik_n \rightarrow \omega + i\eta$ 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 (4.7.1).

4.5.5 Matsubara Green's function in momentum space and non-interacting case

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. With our definition of momentum and real space second quantized operators, and our normalization for momentum eigenstates Eq.(4.17) we have

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = - \left\langle T_\tau \psi(\mathbf{r}, \tau) \psi^\dagger(\mathbf{r}', \tau') \right\rangle = - \left\langle T_\tau \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle c_{\mathbf{k}}(\tau) \sum_{\mathbf{k}'} c_{\mathbf{k}'}^\dagger(\tau') \langle \mathbf{k}' | \mathbf{r}' \rangle \right\rangle \quad (4.171)$$

$$\langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k}' | \mathbf{r}' \rangle = \frac{1}{\mathcal{V}} e^{i\mathbf{k} \cdot \mathbf{r} - i\mathbf{k}' \cdot \mathbf{r}'} = \frac{1}{\mathcal{V}} e^{i(\mathbf{k} - \mathbf{k}') \cdot \left(\frac{\mathbf{r} + \mathbf{r}'}{2}\right) + i\left(\frac{\mathbf{k} + \mathbf{k}'}{2}\right) \cdot (\mathbf{r} - \mathbf{r}')}. \quad (4.172)$$

Assuming space translation invariance, we can integrate over the center of mass coordinate $\frac{1}{\mathcal{V}} \int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) = 1$. Since

$$\frac{1}{\mathcal{V}} \int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) e^{i(\mathbf{k}-\mathbf{k}')\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)} = \frac{1}{\mathcal{V}} (2\pi)^3 \delta(\mathbf{k}-\mathbf{k}') = \delta_{\mathbf{k},\mathbf{k}'} \quad (4.173)$$

we are left with

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = - \left\langle T_\tau \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} c_{\mathbf{k}'}(\tau) c_{\mathbf{k}'}^\dagger(\tau') e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')} \right\rangle \quad (4.174)$$

$$\mathcal{G}(\mathbf{k}; \tau - \tau') = \int d(\mathbf{r}-\mathbf{r}') e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \left[- \left\langle T_\tau \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} c_{\mathbf{k}'}(\tau) c_{\mathbf{k}'}^\dagger(\tau') e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')} \right\rangle \right] \quad (4.175)$$

$$\boxed{\mathcal{G}(\mathbf{k}; \tau - \tau') = - \left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(\tau') \right\rangle} \quad (4.176)$$

which could have been guessed from the start! Our definitions of Fourier transforms just make this work.

Remark 75 *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.

Example of non-interacting particles

For non-interacting particles let us consider a quadratic diagonal Hamiltonian

$$K_0 = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \quad (4.177)$$

The result for the Green's function may be obtained either directly from the definition or by integrating the equations of motion. Both ways of obtaining the simple result

$$\boxed{\mathcal{G}_0(\mathbf{k}; ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}}}} \quad (4.178)$$

are instructive, so let us do both. Assuming for one moment that the above result is correct, our rules for analytic continuation then immediately give us the retarded function

$$\boxed{G^R(\mathbf{k}; \omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}}} \quad (4.179)$$

that has precisely the form we expect from our experience with the one-body case. The only difference with the one-body case is in the presence of the chemical potential in $\zeta_{\mathbf{k}}$.

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,

$$\frac{\partial c_{\mathbf{k}}}{\partial \tau} = [K_0, c_{\mathbf{k}}] = -\zeta_{\mathbf{k}} c_{\mathbf{k}} \quad (4.180)$$

The anticommutator was easy to evaluate using our standard trick Eq.(4.49). The resulting differential equation is easy to integrate given the initial condition on Heisenberg operators. We obtain,

$$c_{\mathbf{k}}(\tau) = e^{-\zeta_{\mathbf{k}}\tau} c_{\mathbf{k}} \quad (4.181)$$

so that substituting in the definition,

$$\mathcal{G}_0(\mathbf{k}; \tau) = -\langle T_{\tau} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger} \rangle = -e^{-\zeta_{\mathbf{k}}\tau} [\langle c_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} \rangle \theta(\tau) - \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle \theta(-\tau)] \quad (4.182)$$

using the standard result from elementary statistical mechanics,

$$\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle = f(\zeta_{\mathbf{k}}) = \frac{1}{e^{\beta\zeta_{\mathbf{k}}} + 1} \quad (4.183)$$

and $\langle c_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} \rangle = 1 - \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle$ we obtain

$$\boxed{\mathcal{G}_0(\mathbf{k}; \tau) = -e^{-\zeta_{\mathbf{k}}\tau} [(1 - f(\zeta_{\mathbf{k}})) \theta(\tau) - f(\zeta_{\mathbf{k}}) \theta(-\tau)]}. \quad (4.184)$$

Remark 76 *Inadequacy of Matsubara representation outside the domain of definition: We see here clearly that if $\tau < 0$ the equality*

$$\mathcal{G}_0(\mathbf{k}; \tau + \beta) = -\mathcal{G}_0(\mathbf{k}; \tau) \quad (4.185)$$

is satisfied because $e^{-\zeta_{\mathbf{k}}\beta} (1 - f(\zeta_{\mathbf{k}})) = f(\zeta_{\mathbf{k}})$. On the other hand,

$$\mathcal{G}_0(\mathbf{k}; \tau + 3\beta) \neq \mathcal{G}_0(\mathbf{k}; \tau + \beta) \quad (4.186)$$

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 77 *Alternate evaluation of time evolution: We could have obtained the time evolution also by using the identity*

$$e^A C e^A = C + [A, C] + \frac{1}{2!} [A, [A, C]] + \frac{1}{3!} [A, [A, [A, C]]] + \dots \quad (4.187)$$

that follows from expanding the exponential operators. This is less direct.

Remark 78 *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.(4-6) to (4-8). 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.*

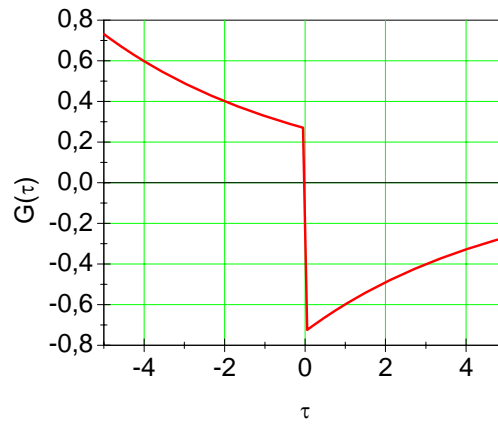


Figure 4-6 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum above the Fermi surface.

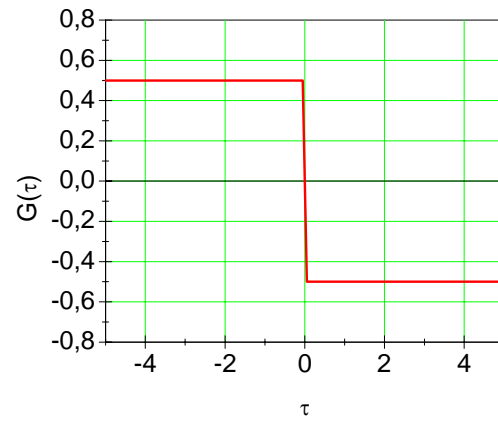


Figure 4-7 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum at the Fermi surface.

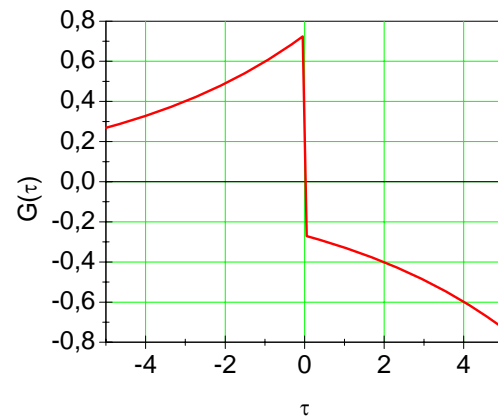


Figure 4-8 $\mathcal{G}_0(\mathbf{p}, \tau)$ for a value of momentum below the Fermi surface.

Let us continue with the derivation of the Matsubara frequency result $\mathcal{G}_0(\mathbf{k}; ik_n)$.

$$\mathcal{G}_0(\mathbf{k}; ik_n) = \int_0^\beta d\tau e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau) = -(1 - f(\zeta_{\mathbf{k}})) \int_0^\beta d\tau e^{ik_n\tau} e^{-\zeta_{\mathbf{k}}\tau} \quad (4.188)$$

$$= -(1 - f(\zeta_{\mathbf{k}})) \frac{e^{ik_n\beta} e^{-\zeta_{\mathbf{k}}\beta} - 1}{ik_n - \zeta_{\mathbf{k}}} \quad (4.189)$$

$$= -(1 - f(\zeta_{\mathbf{k}})) \frac{-e^{-\zeta_{\mathbf{k}}\beta} - 1}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{ik_n - \zeta_{\mathbf{k}}} \quad (4.190)$$

The last equality follows because

$$(1 - f(\zeta_{\mathbf{k}})) = \frac{e^{\zeta_{\mathbf{k}}\beta}}{e^{\zeta_{\mathbf{k}}\beta} + 1} = \frac{1}{e^{-\zeta_{\mathbf{k}}\beta} + 1} \quad (4.191)$$

We thus have our final result Eq.(4.178) for non-interacting particles.

From the equations of motion In complete analogy with the derivation in subsection (4.2.1) we can obtain the equations of motion in the quadratic case.

$$\frac{\partial}{\partial\tau} \mathcal{G}_0(\mathbf{k}; \tau) = -\frac{\partial}{\partial\tau} \left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \quad (4.192)$$

$$= -\delta(\tau) \left\langle \left\{ c_{\mathbf{k}}(\tau), c_{\mathbf{k}}^\dagger \right\} \right\rangle - \left\langle T_\tau \left(\frac{\partial}{\partial\tau} c_{\mathbf{k}}(\tau) \right) c_{\mathbf{k}}^\dagger \right\rangle \quad (4.193)$$

Using the equal-time anticommutation relations as well as the Heisenberg equations of motion for free particles Eq.(4.180) the above equation becomes,

$$\frac{\partial}{\partial\tau} \mathcal{G}_0(\mathbf{k}; \tau) = -\delta(\tau) + \zeta_{\mathbf{k}} \left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \quad (4.194)$$

so that the equation of motion for the Matsubara propagator is

$$\boxed{\left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}} \right) \mathcal{G}_0(\mathbf{k}; \tau) = -\delta(\tau)} \quad (4.195)$$

To obtain the Matsubara-frequency result, we only need to integrate on both sides using the general expression to obtain Fourier coefficients Eq.(4.145)

$$\int_{0^-}^{\beta^-} \left[\left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}} \right) \mathcal{G}_0(\mathbf{k}; \tau) \right] e^{ik_n\tau} d\tau = -1 \quad (4.196)$$

so that integrating by parts,

$$e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau) \Big|_{0^-}^{\beta^-} - ik_n \mathcal{G}_0(\mathbf{k}; ik_n) + \zeta_{\mathbf{k}} \mathcal{G}_0(\mathbf{k}; ik_n) = -1 \quad (4.197)$$

Note that we had to specify that the domain of integration includes 0. The integrated term disappears because of the KMS boundary conditions (antiperiodicity) Eq.(4.134). Indeed, antiperiodicity implies that

$$e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau) \Big|_{0^-}^{\beta^-} = -\mathcal{G}_0(\mathbf{k}; \beta^-) - \mathcal{G}_0(\mathbf{k}; 0^-) = 0 \quad (4.198)$$

Eq.(4.197) for the Matsubara Green's function then immediately gives us the desired result Eq.(4.178).

4.5.6 Sums over Matsubara frequencies

In doing practical calculations, we will have to become familiar with sums over Matsubara frequencies. When we have products of Green's functions, we will use partial fractions in such a way that we will basically always have to evaluate sums such as

$$T \sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \quad (4.199)$$

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

$$\mathcal{G}(\mathbf{k}; \tau) = T \sum_n \frac{e^{-ik_n \tau}}{ik_n - \zeta_{\mathbf{k}}} \quad (4.200)$$

We already know that the Green's function has a jump at $\tau = 0$. In other words,

$$\left[\lim_{\tau \rightarrow 0^+} \mathcal{G}(\mathbf{k}; \tau) = -\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \rangle \right] \neq \left[\lim_{\tau \rightarrow 0^-} \mathcal{G}(\mathbf{k}; \tau) = \langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \rangle \right] \quad (4.201)$$

This inequality in turn means that

$$T \sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} \neq T \sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} \neq T \sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \quad (4.202)$$

The sum does not converge uniformly in the interval including $\tau = 0$ because the $1/n$ decrease for $n \rightarrow \infty$ 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 $\tau \rightarrow 0^\pm$.

Remark 79 Remark 80 *The jump, $\lim_{\tau \rightarrow 0^-} \mathcal{G}(\mathbf{k}; \tau) - \lim_{\tau \rightarrow 0^+} \mathcal{G}(\mathbf{k}; \tau)$ 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 we will show as special cases that

$$\boxed{T \sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{e^{\beta \zeta_{\mathbf{k}} + 1}} = f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k}; 0^-)} \quad (4.203)$$

$$\boxed{T \sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} = \frac{-1}{e^{-\beta \zeta_{\mathbf{k}} + 1}} = -1 + f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k}; 0^+)} \quad (4.204)$$

Obviously, the non-interacting Green's function has the correct jump $\mathcal{G}_0(\mathbf{k}; 0^-) - \mathcal{G}_0(\mathbf{k}; 0^+) = 1$

Proof: [6] To perform the sum over Matsubara frequencies, the standard trick is to go to the complex plane. The following function

$$-\beta \frac{1}{e^{\beta z} + 1} \quad (4.205)$$

has poles for z equal to any fermionic Matsubara frequency: $z = ik_n$. Its residue at these poles is unity since for

$$z = ik_n + \delta z \quad (4.206)$$

we have

$$-\beta \frac{1}{e^{\beta z} + 1} = -\beta \frac{1}{e^{ik_n \beta + \beta \delta z} + 1} = -\beta \frac{1}{-1 e^{\beta \delta z} + 1} \quad (4.207)$$

$$\lim_{z - ik_n \rightarrow 0} \delta z \left[-\beta \frac{1}{e^{\beta z} + 1} \right] = 1 \quad (4.208)$$

Similarly the following function has the same poles and residues:

$$\lim_{z - ik_n \rightarrow 0} \delta z \left[\beta \frac{1}{e^{-\beta z} + 1} \right] = 1 \quad (4.209)$$

To evaluate the $\tau < 0$ case by contour integration, we use Cauchy's 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.(4.208) this allows us to establish the equality

$$\frac{1}{\beta} \sum_n \frac{e^{-ik_n \tau}}{ik_n - \zeta_{\mathbf{k}}} = -\frac{1}{2\pi i} \int_{C_1} \frac{dz}{e^{\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \quad (4.210)$$

This contour can be deformed, as illustrated in Fig.(4-9), into $C_2 + C_3$ (going through C'_1) with no contribution from the semi-circles at $\text{Re}(z) = \pm\infty$ because $\frac{1}{e^{\beta z} + 1}$ insures convergence when $\text{Re}(z) > 0$ despite $e^{-z\tau}$ in the numerator, and $e^{-z\tau}$ insures convergence when $\text{Re}(z) < 0$, $\tau < 0$. With the deformed contour $C_2 + C_3$, only the contribution from the pole in the clockwise direction is left so that we have

$$\boxed{\frac{1}{\beta} \sum_n \frac{e^{-ik_n \tau}}{ik_n - \zeta_{\mathbf{k}}} = \frac{e^{-\zeta_{\mathbf{k}} \tau}}{e^{\beta \zeta_{\mathbf{k}}} + 1} = e^{-\zeta_{\mathbf{k}} \tau} f(\zeta_{\mathbf{k}})} \quad (4.211)$$

which agrees with the value of $\mathcal{G}_0(\mathbf{k}; \tau)$ in Eq.(4.184) when $\tau < 0$. In particular, when $\tau = 0^-$ we have proven the identity (4.204). To evaluate the

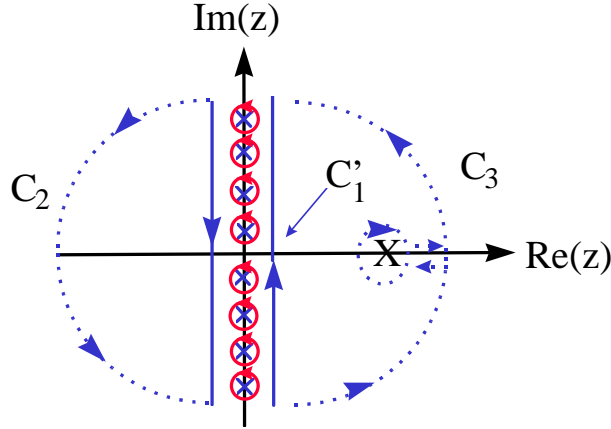


Figure 4-9 Evaluation of fermionic Matsubara frequency sums in the complex plane.

$\tau > 0$ case we use the same contour but with the other form of auxiliary function Eq.(4.209). We then obtain,

$$\frac{1}{\beta} \sum_n \frac{e^{-ik_n \tau}}{ik_n - \zeta_{\mathbf{k}}} = \lim_{\eta \rightarrow 0^+} \frac{1}{2\pi i} \int_{C_1} \frac{dz}{e^{-\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \quad (4.212)$$

This contour can be deformed into $C_2 + C_3$ with no contribution from the semi-circles at $\text{Re}(z) = \pm\infty$ because this time $e^{-z\tau}$ insures convergence when $\text{Re}(z) > 0$, $\tau > 0$ and $\frac{1}{e^{-\beta z} + 1}$ ensures convergence when $\text{Re}(z) < 0$ despite $e^{-z\tau}$ in the numerator. Again, from $C_2 + C_3$, only the contribution from the pole in the clockwise direction survives so that we have

$$\boxed{\frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{-\beta\zeta_{\mathbf{k}}} + 1} = -\frac{e^{-\zeta_{\mathbf{k}}\tau} e^{\beta\zeta_{\mathbf{k}}}}{e^{\beta\zeta_{\mathbf{k}}} + 1} = -e^{-\zeta_{\mathbf{k}}\tau} (1 - f(\zeta_{\mathbf{k}}))} \quad (4.213)$$

which agrees with the value of $\mathcal{G}_0(\mathbf{k}; \tau)$ in Eq.(4.184) when $\tau < 0$. In particular, when $\tau = 0^+$ we have proven the identity (4.203).

4.6 Physical meaning of the spectral weight: Quasiparticles, effective mass, wave function renormalization, momentum distribution.

To discuss the Physical meaning of the spectral weight, we first find it in the non-interacting case, then write a formal general expression, the Lehman 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.

4.6.1 Spectral weight for non-interacting particles

The general result for the spectral weight in terms of the Green's function Eq.(4.168) gives us for non-interacting particles

$$A_0(\mathbf{k}, \omega) = i \left[\frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}} - \frac{1}{\omega - i\eta - \zeta_{\mathbf{k}}} \right] \quad (4.214)$$

$$= 2\pi\delta(\omega - \zeta_{\mathbf{k}}) \quad (4.215)$$

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 an true excited eigenstate located an energy $\omega = \zeta_{\mathbf{k}}$ above or below the Fermi level. In the interacting case, the Lehman representation will show us clearly that what we just said is the correct interpretation

4.6.2 Lehman representation

For a general correlation function, not necessarily a Green's function, one establishes the connection between Matsubara functions and retarded functions by using the Lehman 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 Lehman representation in the one-body case when we wrote in Eq.(4.70),

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \sum_n \frac{\phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{\omega + i\eta - E_n}$$

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

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}'; t) &\equiv \langle \{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', 0) \} \rangle & (4.216) \\ &= e^{\beta\Omega} \sum_{m,n} \left[\langle n | e^{-\beta K} e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} | m \rangle \langle m | \psi_S^\dagger(\mathbf{r}') | n \rangle \right. \\ &\quad \left. + \langle n | e^{-\beta K} \psi_S^\dagger(\mathbf{r}') | m \rangle \langle m | e^{iKt} \psi_S(\mathbf{r}) e^{-iKt} | n \rangle \right] \end{aligned}$$

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

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}'; \omega') &= e^{\beta\Omega} \times & (4.217) \\ &\sum_{mn} \left[e^{-\beta K_n} \langle n | \psi_S(\mathbf{r}) | m \rangle \langle m | \psi_S^\dagger(\mathbf{r}') | n \rangle 2\pi\delta(\omega' - (E_m - \mu - E_n)) \right. \\ &\quad \left. + e^{-\beta K_n} \langle n | \psi_S^\dagger(\mathbf{r}') | m \rangle \langle m | \psi_S(\mathbf{r}) | n \rangle 2\pi\delta(\omega' - (E_n - \mu - E_m)) \right] \end{aligned}$$

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 81 *At zero temperature, we have*

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}'; \omega') &= Z^{-1} \sum_m \left[\langle 0 | \psi_S(\mathbf{r}) | m \rangle \langle m | \psi_S^\dagger(\mathbf{r}') | 0 \rangle 2\pi\delta(\omega' - (E_m - \mu - E_0)) \right. \\ &\quad \left. + \langle 0 | \psi_S^\dagger(\mathbf{r}') | m \rangle \langle m | \psi_S(\mathbf{r}) | 0 \rangle 2\pi\delta(\omega' - (E_0 - \mu - E_m)) \right] & (4.218) \end{aligned}$$

Since to add a particle we need at least an energy μ , then $E_m - \mu - E_0 > 0$ and the first term, that adds particles, contributes only to positive frequencies. On the other hand, if we remove a particle, $E_0 - \mu - E_m < 0$ since the thermodynamic result $\partial E / \partial N = \mu$ implies, with $dN = -1$, that $E_0 - E_m < \mu$ (the equality being satisfied only for the hole infinitesimally close to the Fermi surface) so that the second term, that adds holes, contributes only to the negative frequencies.

¹To 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.(4.162) 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,

$$A(\mathbf{r}, \mathbf{r}'; \omega') = e^{\beta\Omega} \sum_{mn} (e^{-\beta K_n} + e^{-\beta K_m}) \langle n| \psi_S(\mathbf{r}) |m\rangle \langle m| \psi_S^\dagger(\mathbf{r}') |n\rangle 2\pi\delta(\omega' - (K_m - K_n)) \quad (4.219)$$

Substituting in the spectral representation Eq.(4.162) we have,

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = e^{\beta\Omega} \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) \frac{\langle n| \psi_S(\mathbf{r}) |m\rangle \langle m| \psi_S^\dagger(\mathbf{r}') |n\rangle}{ik_n - (E_m - E_n - \mu)} \quad (4.220)$$

This is the Lehman representation. It tells us how to interpret the poles of the analytically continued $\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n)$.

Remark 82 *Standard way of proving analytical continuation formula: The standard way of proving that $G^R(\omega) = \lim_{ik_n \rightarrow \omega + i\eta} \mathcal{G}(ik_n)$ is to first find the Lehman representation for both quantities.*

4.6.3 Probabilistic interpretation of the spectral weight

For a different representation, for example for momentum, we have [7] in the translationally invariant case, by analogy with the above result for the spectral weight Eq.(4.219)

$$A(\mathbf{k}, \omega') = e^{\beta\Omega} \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) |\langle n| c_{\mathbf{k}} |m\rangle|^2 2\pi\delta(\omega' - (K_m - K_n)). \quad (4.221)$$

The overlap matrix element $|\langle n| c_{\mathbf{k}} |m\rangle|^2$ 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,

$$\int \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega') = \left\langle \left\{ c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger \right\} \right\rangle = 1. \quad (4.222)$$

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 83 *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 . 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 84 *Physical reason for high-frequency fall-off:* The explicit expression for the spectral weight Eq.(4.221) suggests why the spectral weight falls off fast at large frequencies for a given \mathbf{k} , as we have discussed in Subsection (4.7.1). 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.

4.6.4 Angle-resolved photoemission spectroscopy (ARPES) on a Fermi liquid compound.

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.(4-10). 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.

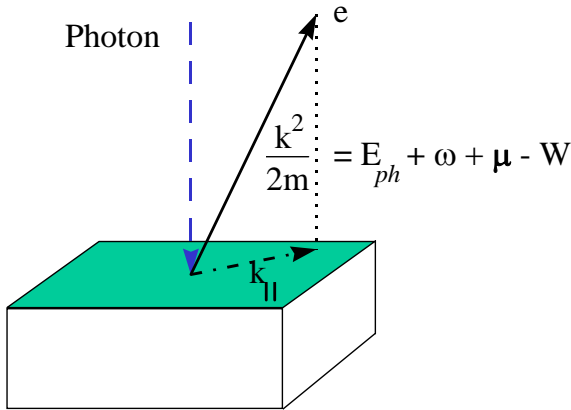


Figure 4-10 Schematic representation of an angle-resolved photoemission experiment.

The energy of the electron in the system ω will be mostly negative. The value of \mathbf{k}_{\parallel} 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}_{\parallel} that is conserved. Hence, it is only for layered systems that we really have access to both energy ω and total momentum \mathbf{k}_{\parallel} of the electron when it was in the system. Without going into details of the assumptions going into the derivation, Fermi's golden rule suggests, (see first section of Chapter 2) that the cross section for ejecting an electron of momentum \mathbf{k}_{\parallel} and energy ω (measured with respect to μ)

is proportional to

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} |\langle n | c_{\mathbf{k}_{||}} | m \rangle|^2 \delta(\omega + \mu - (E_m - E_n)) \quad (4.223)$$

$$\propto \sum_{mn} e^{-\beta K_m} |\langle n | c_{\mathbf{k}_{||}} | m \rangle|^2 \delta(\omega - (K_m - K_n)) \quad (4.224)$$

$$\propto \int dt e^{i\omega t} \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \rangle \quad (4.225)$$

which is “half” of the spectral weight (the mostly negative-energy part). More specifically, we can rewrite this result in terms of the spectral weight as follows,

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto f(\omega) A(\mathbf{k}_{||}, \omega). \quad (4.226)$$

Note the analogy with the cross section we found earlier for electron scattering. It was expressed in Eq.(2.1) in terms of a density-density correlation function. Through the fluctuation-dissipation theorem Eq.(2.146), it was related to a spectral weight χ'' (analogous to A) through the Bose function (analogous to the Fermi function).

Proof: The most direct and simple proof is from the Lehman representation Eq.(4.221). To get a few more general results about $G^<(\mathbf{k}_{||}, \omega)$ and $G^>(\mathbf{k}_{||}, \omega)$ we present the following alternate proof. The cross section is proportional to the Fourier transform of $G^<(\mathbf{k}_{||}, \omega)$ as defined in Eq.(4.124).

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto -iG^<(\mathbf{k}_{||}, \omega) \quad (4.227)$$

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

$$\begin{aligned} \langle c_{\mathbf{k}_{||}}(t) c_{\mathbf{k}_{||}}^\dagger \rangle &= Z^{-1} \text{Tr} \left[e^{-\beta K} (e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt}) c_{\mathbf{k}_{||}}^\dagger \right] \quad (4.228) \\ &= Z^{-1} \text{Tr} \left[(e^{\beta K} e^{-\beta K}) c_{\mathbf{k}_{||}}^\dagger e^{-\beta K} (e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt}) \right] \quad (4.229) \\ &= \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t + i\beta) \rangle \quad (4.230) \end{aligned}$$

one finds by simple use of definitions and change of integration variables,

$$A(\mathbf{k}_{||}, \omega) = \int dt e^{i\omega t} \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) + c_{\mathbf{k}_{||}}(t) c_{\mathbf{k}_{||}}^\dagger \rangle \quad (4.231)$$

$$= \int dt e^{i\omega t} \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \rangle + \int dt e^{i\omega(t+i\beta-i\beta)} \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t+i\beta) \rangle$$

$$= (1 + e^{\beta\omega}) \int dt e^{i\omega t} \langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \rangle \quad (4.232)$$

$$= f(\omega)^{-1} (-iG^<(\mathbf{k}_{||}, \omega)) \quad (4.233)$$

Substituting in Eq.(4.227) proves Eq.(4.226). Note that since

$$A(\mathbf{k}_{||}, \omega) = -i [G^<(\mathbf{k}_{||}, \omega) - G^>(\mathbf{k}_{||}, \omega)] \quad (4.234)$$

we also have the result

$$iG^>(\mathbf{k}_{||}, \omega) = (1 - f(\omega)) A(\mathbf{k}_{||}, \omega) \quad (4.235)$$

The theoretical formula for the photoemission cross-section Eq.(4.226) neglects 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”.

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-to-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[11] appear in Fig.(4-11).

Figure 4-11 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).

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.(4-10) is a fixed length vector. Hence, the angle with respect to the incident photon suffices to define the value of \mathbf{k}_{\parallel} . Each curve in Fig.(4-11) is for a given \mathbf{k}_{\parallel} , 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. 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 $A(\mathbf{k}_{\parallel}, \omega)$. From band structure calculations, one knows that the angle $\theta = 14.75^\circ$ 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.(4.6.6) below). The plots for angles $\theta < 14.75^\circ$ corresponds to wave vectors above the Fermi level. There, the intensity is *much* smaller than for the other peaks. For $\theta = 13^\circ$, the experimental results are scaled up by a factor 16. The intensity observed for wave-vectors above the Fermi wave vector comes from the overlap of particle-like excitations with eigenstates below the Fermi surface, a phenomenon we alluded to in the previous section.

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}_{\parallel} . 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.

4.6.5 Quasiparticles[9]

For a general interacting system, the one-particle Green’s function takes the form,

$$G^R(\mathbf{k}, \omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \Sigma^R(\mathbf{k}, \omega)} \quad (4.236)$$

The corresponding spectral weight is,

$$A(\mathbf{k}, \omega) = -2 \text{Im} G^R(\mathbf{k}, \omega) \quad (4.237)$$

$$= \frac{-2 \text{Im} \Sigma^R(\mathbf{k}, \omega)}{\left(\omega - \zeta_{\mathbf{k}} - \text{Re} \Sigma^R(\mathbf{k}, \omega)\right)^2 + \left(\text{Im} \Sigma^R(\mathbf{k}, \omega)\right)^2} \quad (4.238)$$

If the imaginary part of the self-energy, the scattering rate, is not too large and varies smoothly with frequency, the spectral weight will have a maximum whenever

$$\boxed{\omega - \zeta_{\mathbf{k}} - \text{Re} \Sigma^R(\mathbf{k}, \omega) = 0} \quad (4.239)$$

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*. 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 $\omega - \zeta_{\mathbf{k}} - \text{Re} \Sigma^R(\mathbf{k}, \omega)$ around $\omega - E_{\mathbf{k}} + \mu$ where $A(\mathbf{k}, \omega)$ is a maximum, we find

$$\omega - \zeta_{\mathbf{k}} - \text{Re} \Sigma^R(\mathbf{k}, \omega) \approx \left(1 - \left.\frac{\partial \text{Re} \Sigma^R(\mathbf{k}, \omega)}{\partial \omega}\right|_{E_{\mathbf{k}} - \mu}\right) (\omega - E_{\mathbf{k}} + \mu) + \dots \quad (4.240)$$

If we define the “quasiparticle weight” or square of the wave function renormalization by

$$\boxed{Z_{\mathbf{k}} = \frac{1}{1 - \left.\frac{\partial}{\partial \omega} \text{Re} \Sigma^R(\mathbf{k}, \omega)\right|_{\omega = E_{\mathbf{k}} - \mu}}} \quad (4.241)$$

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

$$A(\mathbf{k}, \omega) \approx 2\pi Z_{\mathbf{k}} \frac{1}{\pi} \frac{-Z_{\mathbf{k}} \text{Im} \Sigma^R(\mathbf{k}, \omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + \left(Z_{\mathbf{k}} \text{Im} \Sigma^R(\mathbf{k}, \omega)\right)^2} + inc \quad (4.242)$$

$$= 2\pi Z_{\mathbf{k}} \left[\frac{1}{\pi} \frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + (\Gamma_{\mathbf{k}}(\omega))^2} \right] + inc \quad (4.243)$$

The last equation needs some explanation. First, it is clear that we have defined the scattering rate

$$\boxed{\Gamma_{\mathbf{k}}(\omega) = -Z_{\mathbf{k}} \text{Im} \Sigma^R(\mathbf{k}, \omega)} \quad (4.244)$$

Second, the quantity in square brackets looks, as a function of frequency, like a Lorentzian. 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

$$Z_{\mathbf{k}} \leq 1 \quad (4.245)$$

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

$$v_{\mathbf{k}} = \nabla_{\mathbf{k}} \zeta_{\mathbf{k}} \quad (4.246)$$

and the renormalized velocity by

$$v_{\mathbf{k}}^* = \nabla_{\mathbf{k}} E_{\mathbf{k}} \quad (4.247)$$

Then the relation between both quantities is easily obtained by taking the gradient of the quasiparticle equation Eq.(4.239)

$$\nabla_{\mathbf{k}} [E_{\mathbf{k}} - \mu - \zeta_{\mathbf{k}} - \text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu) = 0] \quad (4.248)$$

$$v_{\mathbf{k}}^* - v_{\mathbf{k}} - \nabla_{\mathbf{k}} \text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu) - \left. \frac{\partial \text{Re} \Sigma^R(\mathbf{k}, \omega)}{\partial \omega} \right|_{E_{\mathbf{k}} - \mu} v_{\mathbf{k}}^* = 0 \quad (4.249)$$

where $\nabla_{\mathbf{k}}$ in the last equation acts only on the first argument of $\text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)$. 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, we have

$$\boxed{v_{\mathbf{k}}^* = v_{\mathbf{k}} \frac{1 + \frac{\partial}{\partial \zeta_{\mathbf{k}}} \text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma^R(\mathbf{k}, \omega) \Big|_{\omega = E_{\mathbf{k}} - \mu}}} \quad (4.250)$$

In cases where the 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

$$\boxed{\frac{m}{m^*} = \lim_{\mathbf{k} \rightarrow \mathbf{k}_F} \frac{1 + \frac{\partial}{\partial \zeta_{\mathbf{k}}} \text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma^R(\mathbf{k}, \omega) \Big|_{\omega = E_{\mathbf{k}} - \mu}}} \quad (4.251)$$

4.6.6 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.(4.243) is evaluated for $k = k_F$ so that only the frequency dependence of the remaining quantities is 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? 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. We cannot do it justice here. A simple way to make its main ingredients plausible, [10] is to assume that near the Fermi surface, at frequencies much less than 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 principle and available phase space that we do not discuss here.

Let us define real and imaginary parts of the retarded self-energy by

$$\Sigma^R = \Sigma' + i\Sigma'' \quad (4.252)$$

Our two hypothesis imply that Σ'' has the Taylor expansion

$$\Sigma''(\mathbf{k}_F; \omega) = \alpha\omega - \gamma\omega^2 + \dots \quad (4.253)$$

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.(4.236). 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 $d \geq 3$. The real part is then obtained from the Kramers-Kronig relation Eq.(3.86), (Sec.4.7.2) or from the spectral representation,

$$\lim_{\omega \rightarrow 0} [\Sigma'(\mathbf{k}_F; \omega) - \Sigma'(\mathbf{k}_F; \infty)] = \lim_{\omega \rightarrow 0} \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma''(\mathbf{k}_F; \omega')}{\omega' - \omega} \quad (4.254)$$

$$= \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma''(\mathbf{k}_F; \omega')}{\omega'} + \omega \left[\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma''(\mathbf{k}_F; \omega')}{(\omega')^2} \right] \quad (4.255)$$

The first term is the value of the real-part of the self-energy at zero-frequency. This constant contributes directly to the numerical value of the chemical potential (the Hartree-Fock shift $\Sigma'(\mathbf{k}_F; \infty)$ does not suffice to evaluate the chemical potential). The second term in the last equation tells us that

$$\left. \frac{\partial}{\partial \omega} \Sigma'(\mathbf{k}_F, \omega) \right|_{\omega=0} = \left[\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma''(\mathbf{k}_F; \omega')}{(\omega')^2} \right] \quad (4.256)$$

Since $\Sigma'' = -\gamma\omega^2$ the integral exists and is negative (if we assume a frequency cutoff as discussed below), hence

$$\left. \frac{\partial}{\partial \omega} \Sigma'(\mathbf{k}, \omega) \right|_{\omega=0} < 0 \quad (4.257)$$

This in turn means that the corresponding value of Z_{k_F} is less than unity, as we had concluded in Eqs.(4.241) and (4.245) above. In summary, the analyticity hypothesis along with the vanishing of $\Sigma''(0)$ implies the existence of quasiparticles.

Remark 85 *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.(4.256) fails when the integral diverges. Then, the low frequency expansion for the self-energy in Eq.(4.255) 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.(4.256). 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 [20]).*

The solid lines in Fig.(4-11) are two-parameter fits that also take into account the wave vector and energy resolution of the experiment [11]. 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.(4.244)

$$\Gamma_{k_F}(\omega) = Z_{k_F} \gamma \omega^2 = \gamma' \omega^2. \quad (4.258)$$

Contrary to E_k , the damping parameter γ' is the same for all curves. The solid-line fits are obtained with $\gamma' = 40 eV^{-1}$ (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 ($\theta < 14.75^0$) 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,[12] $\gamma = 0.067\omega_p/\varepsilon_F^2$. Using $\omega_p = 18.2 eV$, $\varepsilon_F = 0.3 eV$ and the extrapolated value of Z_{k_F} obtained by putting² $r_s = 10$ in electron gas results,[13] 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 [19]. Results are shown in Fig. (4-12). 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 $\hbar v_F = 0.73 \pm 0.1 eV \text{ \AA}$ close to band structure calculations, $\hbar v_F = 0.68 eV \text{ \AA}$ 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 there is much uncertainty still in the interpretation of ARPES data, even for Fermi liquids.

² r_s is the average electron spacing expressed in terms of the Bohr radius.

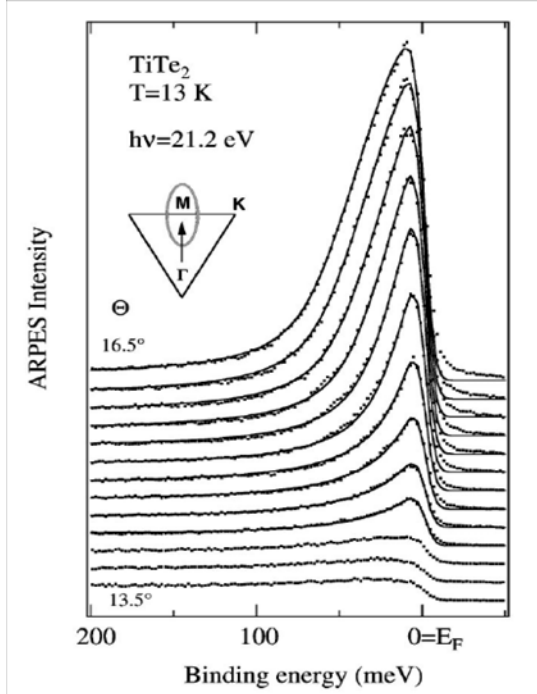


Figure 4-12 Figure 1 from Ref.[19] for the ARPES spectrum of 1T-TiTe₂ measured near the Fermi surface crossing along the high-symmetry ΓM direction ($\theta = 0$ is normal emission). The lines are results of Fermi liquid fits and the inset shows a portion of the Brillouin zone with the relevant ellipsoidal electron pocket.

Theoretical estimates for high-temperature superconductors are two orders of magnitude smaller than the observed result [11].

Remark 86 *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 87 *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 $1/ik_n$ as discussed below in subsection (4.7.1). Conversely, there is always a cutoff 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 88 *Destruction of quasiparticles by critical fluctuations in two dimensions: Note that it is only if Σ'' vanishes fast enough with frequency that it is correct to expand the Kramers-Kronig expression in powers of the frequency to obtain Eq.(4.256). When $\Sigma''(\omega)$ vanishes slower than ω^2 , then Eq.(4.256) 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 $\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k},\omega)|_{\omega=0} > 0$. 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 [14].

4.6.7 Momentum distribution in an interacting system

In an interacting system, momentum is not a good quantum number so $\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle$ is *not* equal to the Fermi distribution. On the other hand, $\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle$ can be computed from the spectral weight. Indeed,

$$\begin{aligned} \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle &= \lim_{\tau \rightarrow 0^-} \left[-\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \rangle \right] \\ &= \lim_{\tau \rightarrow 0^-} \mathcal{G}(\mathbf{k}, \tau) \end{aligned} \quad (4.259)$$

To compute the latter quantity from the spectral weight, it suffices to use the spectral representation Eq.(4.162)

$$\begin{aligned} \lim_{\tau \rightarrow 0^-} \mathcal{G}(\mathbf{k}, \tau) &= T \lim_{\tau \rightarrow 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \\ &= T \lim_{\tau \rightarrow 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}, \omega')}{ik_n - \omega'} \end{aligned} \quad (4.260)$$

Using the result Eq.(4.203) found above for the sum over Matsubara frequencies, we are left with

$$\boxed{\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = \lim_{\tau \rightarrow 0^-} \mathcal{G}(\mathbf{k}, \tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega') A(\mathbf{k}, \omega')} \quad (4.261)$$

with $f(\omega')$ the Fermi-Dirac distribution.

This 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.(4.238) for the spectral weight gives us a delta function.

Remark 89 *Jump of the momentum distribution at the Fermi level: Even if $\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle$ 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 $\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle$ at the Fermi level. The existence of this jump can be seen as follows. At zero temperature, our last result gives us*

$$\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = \int_{-\infty}^0 \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega') \quad (4.262)$$

Let us take the quasiparticle form Eq.(4.243) of the spectral weight with the Fermi liquid expression Eq.(4.258) 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 $k \rightarrow k_F$, or in other words when $E_{\mathbf{k}} - \mu \rightarrow 0$, as $Z_{k_F} \delta(\omega)$. At least crudely speaking. When $E_{\mathbf{k}} - \mu \rightarrow 0^-$, this

delta function is inside the integration domain hence it contributes to the integral, while when $E_{\mathbf{k}} - \mu \rightarrow 0^+$ 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

$$\lim_{\mathbf{k} \rightarrow \mathbf{k}_f^-} \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle - \lim_{\mathbf{k} \rightarrow \mathbf{k}_f^+} \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = Z_{k_F} \quad (4.263)$$

In the above argument, we have done as if $\Gamma_{\mathbf{k}}(\omega)$ was frequency independent and infinitesimally small in Eq.(4.243). 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 90 *Fermi surface and interactions:* The conclusion of the previous remark is that even in an interacting system, there is a sharp Fermi surface as in the free electron model. For simplicity we have discussed the spinless case. A qualitative sketch of the zero-temperature momentum distribution in an interacting system appears in Fig.(4-13). 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 Fermi surface is unaffected.

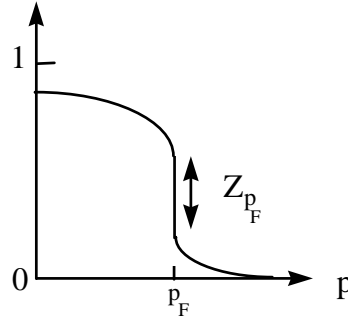


Figure 4-13 Qualitative sketch of the zero-temperature momentum distribution in an interacting system.

Remark 91 *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.

4.7 A few more formal matters : asymptotic behavior and causality

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.

4.7.1 Asymptotic behavior of $\mathcal{G}(\mathbf{k}; ik_n)$ and $\Sigma(\mathbf{k}; ik_n)$

As usual, the high-frequency asymptotic properties of the Green's function are determined by sum rules. From the spectral representation(4.162), we obtain, for the general interacting case

$$\lim_{ik_n \rightarrow \infty} \mathcal{G}(\mathbf{k}; ik_n) = \lim_{ik_n \rightarrow \infty} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}; \omega')}{ik_n - \omega'} \quad (4.264)$$

$$= \lim_{ik_n \rightarrow \infty} \frac{1}{ik_n} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') = \lim_{ik_n \rightarrow \infty} \frac{1}{ik_n} \langle \{c_{\mathbf{k}}, c_{\mathbf{k}}^+\} \rangle = \lim_{ik_n \rightarrow \infty} \frac{1}{ik_n} \quad (4.265)$$

Defining the self-energy as usual

$$\mathcal{G}(\mathbf{k}; ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k}, ik_n)} \quad (4.266)$$

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

$$\lim_{ik_n \rightarrow \infty} \Sigma(\mathbf{k}, ik_n) = cst. \quad (4.267)$$

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 [10] for the Green's function, is that if

$$\lim_{ik_n \rightarrow \infty} \mathcal{G}(\mathbf{k}; ik_n) = \lim_{ik_n \rightarrow \infty} \frac{1}{ik_n}$$

then that is all that is needed to obtain an approximation for the Green's function which obeys the anticommutation relation:

$$\mathcal{G}(\mathbf{k}; 0^-) - \mathcal{G}(\mathbf{k}; 0^+) = \langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \rangle + \langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \rangle = 1 \quad (4.268)$$

Proof :It suffices to notice that

$$\mathcal{G}(\mathbf{k}; 0^-) - \mathcal{G}(\mathbf{k}; 0^+) = \frac{1}{\beta} \sum_n \left[e^{-ik_n 0^-} - e^{-ik_n 0^+} \right] \mathcal{G}(\mathbf{k}; ik_n) \quad (4.269)$$

We can add and subtract the asymptotic behavior to obtain,

$$\frac{1}{\beta} \sum_n \left[\left(e^{-ik_n 0^-} - e^{-ik_n 0^+} \right) \left(\mathcal{G}(\mathbf{k}; ik_n) - \frac{1}{ik_n} \right) \right] + \frac{1}{\beta} \sum_n \left(e^{-ik_n 0^-} - e^{-ik_n 0^+} \right) \frac{1}{ik_n} \quad (4.270)$$

In the first sum, $\mathcal{G}(\mathbf{k}; ik_n) - \frac{1}{ik_n}$ 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 92 *High-frequency expansion for the Green's function and sum-rules: The coefficients of the high-frequency expansion of $\mathcal{G}(\mathbf{k}; ik_n)$ 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 $A(\mathbf{k}, \omega)$ falls fast enough to allow us to expand under the integral sign follows from the fact that all frequency moments of $A(\mathbf{k}, \omega)$, namely $\int d\omega \omega^n A(\mathbf{k}, \omega)$, exist and are given by equal-time commutators. Explicit expressions for $A(\mathbf{k}, \omega)$ in terms of matrix elements, as given in Subsection(4.6.3) above, show physically why $A(\mathbf{k}, \omega)$ 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 $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega')$ it is sufficient that $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} |\omega' A(\mathbf{k}; \omega')|$ exists.[8] This can be seen as follows,*

$$ik_n \mathcal{G}(\mathbf{k}; ik_n) - \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \left(\frac{ik_n}{ik_n - \omega'} - 1 \right) \quad (4.271)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \frac{\omega'}{ik_n - \omega'} \quad (4.272)$$

$$\leq \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left| A(\mathbf{k}; \omega') \frac{\omega'}{ik_n - \omega'} \right| \quad (4.273)$$

$$\leq \left| \frac{1}{ik_n} \right| \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} |A(\mathbf{k}; \omega') \omega'| \quad (4.274)$$

If the integral exists then, it is a rigorous result that

$$\lim_{ik_n \rightarrow \infty} ik_n \mathcal{G}(\mathbf{k}; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \quad (4.275)$$

This is an important result. It suggests that approximate theories that give 1 as the coefficient of $(ik_n)^{-1}$ in the high frequency expansion have a normalized spectral weight. However[8] the above proof assumes that there is indeed a spectral representation for $\mathcal{G}(\mathbf{k}; ik_n)$. 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 $G^R(\mathbf{k}, \omega)$ 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 $\mathcal{G}(\mathbf{k}; ik_n) = (ik_n - ia)^{-1}$. This has the correct high-frequency behavior but its analytical continuation does not satisfy causality. It has no spectral representation. On the other hand, $\mathcal{G}(\mathbf{k}; ik_n) = (ik_n + (k_n/|k_n|)ia)^{-1}$ has a Lorentzian as a spectral weight and is causal. It may also occur that the approximate theory may have $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') = 1$ but $A(\mathbf{k}; \omega') < 0$ 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.

4.7.2 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, $\text{Im} G^R$ and $\text{Im} \Sigma^R$ are both negative definite (except in the special case of non-interacting particles where $\text{Im} \Sigma^R = 0$).

In analogy with the Matsubara Green function Eq.(4.220) G^R has the Lehman representation

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = e^{\beta\Omega} \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) \frac{\langle n | \psi_S(\mathbf{r}) | m \rangle \langle m | \psi_S^\dagger(\mathbf{r}') | n \rangle}{\omega + i\eta - (E_m - E_n - \mu)}. \quad (4.276)$$

Taking the complex conjugate of the transpose, we obtain

$$\begin{aligned} \text{Re } G^R(\mathbf{r}', \mathbf{r}; \omega)^* &= e^{\beta\Omega} \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) \frac{\langle n | \psi_S(\mathbf{r}') | m \rangle^* \langle m | \psi_S(\mathbf{r}) | n \rangle^*}{\omega - (E_m - E_n - \mu)} \\ &= \text{Re } G^R(\mathbf{r}, \mathbf{r}'; \omega) \end{aligned} \quad (4.277)$$

$$\begin{aligned} \text{Im } G^R(\mathbf{r}', \mathbf{r}; \omega)^* &= -\pi \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) \langle n | \psi_S(\mathbf{r}') | m \rangle^* \langle m | \psi_S(\mathbf{r}) | n \rangle^* \\ &\quad \times \delta(\omega - (E_m - E_n - \mu)) \end{aligned} \quad (4.278)$$

$$= \text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega) \quad (4.279)$$

which means that the real and imaginary parts are both Hermitian matrices. In a basis where the matrix $\text{Im } G^R(\mathbf{r}, \mathbf{r}'; \omega)$ is diagonal, say for quantum number α , then

$$\begin{aligned} \text{Im } G^R(\alpha; \omega) &= -\pi \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) \langle n | c_\alpha | m \rangle \langle m | c_\alpha^\dagger | n \rangle \delta(\omega - (E_m - E_n - \mu)) \\ &= -\pi \sum_{mn} (e^{-\beta K_m} + e^{-\beta K_n}) |\langle n | c_\alpha | m \rangle|^2 \delta(\omega - (E_m - E_n - \mu)) \end{aligned} \quad (4.280)$$

which proves that the matrix for the imaginary part is negative definite in addition to being Hermitian. The negative sign comes from the $+i\eta$ in the original formula and is clearly a consequence of causality.

Following Potthoff [18] we show that the retarded self-energy as a matrix has the same properties as G^R . First, we need to prove that

$$\frac{1}{A \pm iB} = X \mp iY \quad (4.281)$$

with X and Y both Hermitian and Y positive definite if A and B are both Hermitian with B positive definite. This is true because

$$\frac{1}{A \pm iB} = B^{-1/2} \frac{1}{B^{-1/2} A B^{-1/2} \pm iI} B^{-1/2}. \quad (4.282)$$

Since $B^{-1/2} A B^{-1/2}$ is Hermitian as well, we can diagonalize it by a unitary transformation $B^{-1/2} A B^{-1/2} = U c U^\dagger$ where c is a diagonal matrix. Thus,

$$\frac{1}{A \pm iB} = B^{-1/2} U \frac{1}{c \pm iI} U^\dagger B^{-1/2} = B^{-1/2} U \frac{c \mp iI}{c^2 + 1} U^\dagger B^{-1/2} = X \mp iY \quad (4.283)$$

with X and Y Hermitians since $(U^\dagger B^{-1/2})^\dagger = B^{-1/2} U$. In addition, Y is positive definite since in the diagonal basis $Y \rightarrow (c^2 + 1)^{-1}$. Now, define $(G^R)^{-1} = (A - iB)^{-1} = X + iY$ and $(G_0^R)^{-1} = (A_0 - iB_0)^{-1} = X_0 + iY_0$ so that

$$(G^R)^{-1} = X + iY = (G_0^R)^{-1} - \Sigma^R = X_0 + iY_0 - \text{Re } \Sigma^R - i \text{Im } \Sigma^R. \quad (4.284)$$

Then, given that X, Y and X_0, Y_0 are Hermitians, we have that $\text{Re } \Sigma^R$ and $\text{Im } \Sigma^R$ are Hermitians. In addition, $\text{Im } \Sigma^R$ 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).

4.8 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 of

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.

4.8.1 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

$$\mathcal{G}(\tau) = -\frac{\text{Tr} \left[e^{-\beta H_0} T_\tau \left(\widehat{U}(\beta, \tau) \widehat{\psi}(\tau) \widehat{U}(\tau, 0) \widehat{\psi}^\dagger(0) \right) \right]}{\text{Tr} \left[e^{-\beta H_0} T_\tau \widehat{U}(\beta, 0) \right]} \quad (4.285)$$

Because $\widehat{U}(\tau, 0)$ always contains an even number of fermions, it can be commuted with creation-annihilation operators without paying the price of minus signs so that

$$\mathcal{G}(\tau) = -\frac{\text{Tr} \left[e^{-\beta H_0} T_\tau \left(\widehat{U}(\beta, 0) \widehat{\psi}(\tau) \widehat{\psi}^\dagger(0) \right) \right]}{\text{Tr} \left[e^{-\beta H_0} T_\tau \widehat{U}(\beta, 0) \right]} \quad (4.286)$$

More specifically the evolution operator is,

$$\widehat{U}(\beta, 0) = T_\tau \left[\exp \left(-\int_0^\beta d\tau_1 \widehat{V}(\tau_1) \right) \right] \quad (4.287)$$

Expanding this evolution operator to first order in the numerator of the Green's function one obtains

$$-\text{Tr} \left[e^{-\beta H_0} T_\tau \left(\widehat{\psi}(\tau) \widehat{\psi}^\dagger(0) \right) \right] + \int_0^\beta d\tau_1 \text{Tr} \left[e^{-\beta H_0} T_\tau \left(\widehat{V}(\tau_1) \widehat{\psi}(\tau) \widehat{\psi}^\dagger(0) \right) \right] \quad (4.288)$$

where in the case of a two-body interaction (Coulomb for example), $\widehat{V}(\tau_1)$ 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,

$$\left\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right\rangle_0 \quad (4.289)$$

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 14 *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

$$\langle a_1 a_1^\dagger \rangle = \frac{\text{Tr} \left[e^{-\beta H_0} a_1 a_1^\dagger \right]}{\text{Tr} \left[e^{-\beta H_0} \right]} \quad (4.290)$$

$$= \frac{\langle 0 | a_1 a_1^\dagger | 0 \rangle + e^{-\beta \epsilon_1} (\langle 0 | a_1) a_1 a_1^\dagger (a_1^\dagger | 0 \rangle)}{\langle 0 | 0 \rangle + e^{-\beta \epsilon_1} (\langle 0 | a_1) (a_1^\dagger | 0 \rangle)} = \frac{1}{1 + e^{-\beta \epsilon_1}} \quad (4.291)$$

For two fermion states 1, 2, then the complete set used to evaluate the trace is

$$|0\rangle |0\rangle, \quad a_1^\dagger |0\rangle |0\rangle, \quad |0\rangle a_2^\dagger |0\rangle, \quad a_1^\dagger |0\rangle a_2^\dagger |0\rangle \quad (4.292)$$

so that

$$\langle a_1 a_1^\dagger \rangle = \frac{1}{1 + e^{-\beta \epsilon_1}} \frac{1 + e^{-\beta \epsilon_2}}{1 + e^{-\beta \epsilon_2}} = \frac{1}{1 + e^{-\beta \epsilon_1}}. \quad (4.293)$$

The easiest way to understand the last result is to recall that $(1 + a_1^\dagger)(1 + a_2^\dagger)|0\rangle$ 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

$$\langle a_1 a_1^\dagger \rangle = \frac{1}{1 + e^{-\beta \epsilon_1}} \frac{\prod_{m \neq 1} (1 + e^{-\beta \epsilon_m})}{\prod_{m \neq 1} (1 + e^{-\beta \epsilon_m})} = \frac{1}{1 + e^{-\beta \epsilon_1}}. \quad (4.294)$$

Furthermore,

$$\langle a_1 a_1^\dagger a_2 a_2^\dagger \rangle = \frac{1}{1 + e^{-\beta \epsilon_1}} \frac{1}{1 + e^{-\beta \epsilon_2}} \frac{\prod_{m \neq 1,2} (1 + e^{-\beta \epsilon_m})}{\prod_{m \neq 1,2} (1 + e^{-\beta \epsilon_m})} \quad (4.295)$$

$$= \frac{1}{1 + e^{-\beta \epsilon_1}} \frac{1}{1 + e^{-\beta \epsilon_2}} \quad (4.296)$$

$$= \langle a_1 a_1^\dagger \rangle \langle a_2 a_2^\dagger \rangle \quad (4.297)$$

Theorem 15 Any expectation value such as $\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \rangle_0$ 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 $\langle a_j(\tau_j) a_k^\dagger(\tau_k) \rangle_0 \langle a_i(\tau_i) a_l^\dagger(\tau_l) \rangle_0$ 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.

Proof: It is somewhat pretentious to call a proof the plausibility argument that we give below, but let us go ahead anyway. The trick to prove the theorem ([15]) 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)

$$\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \rangle_0 = \quad (4.298)$$

$$\langle i | \alpha \rangle \langle j | \beta \rangle \langle a_\alpha(\tau_i) a_\beta(\tau_j) a_\gamma^\dagger(\tau_k) a_\delta^\dagger(\tau_l) \rangle_0 \langle \gamma | k \rangle \langle \delta | l \rangle \quad (4.299)$$

We already know from Eq.(4.181) that

$$a_\alpha(\tau_i) = e^{-\zeta_\alpha \tau_i} a_\alpha \quad ; \quad a_\alpha^\dagger(\tau_i) = a_\alpha^\dagger e^{\zeta_\alpha \tau_i} \quad (4.300)$$

so that

$$\left\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right\rangle_0 \quad (4.301)$$

$$= \langle i | \alpha \rangle e^{-\zeta_\alpha \tau_i} \langle j | \beta \rangle e^{-\zeta_\beta \tau_j} \left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 e^{\zeta_\gamma \tau_k} \langle \gamma | k \rangle e^{\zeta_\delta \tau_l} \langle \delta | l \rangle \quad (4.302)$$

What we need to evaluate then are expectation values of the type

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0. \quad (4.303)$$

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

$$\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger \right\rangle_0 = \langle a_\alpha a_\alpha^\dagger \rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0 \quad (4.304)$$

If instead, $\beta = \delta$, $\alpha = \gamma$ and $\alpha \neq \beta$, then

$$\left\langle a_\alpha a_\beta a_\alpha^\dagger a_\beta^\dagger \right\rangle_0 = - \left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger \right\rangle_0 = - \langle a_\alpha a_\alpha^\dagger \rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0. \quad (4.305)$$

The last case to consider is $\alpha = \beta$, $\beta = \delta$, $\alpha = \gamma$

$$\left\langle a_\alpha a_\alpha a_\alpha^\dagger a_\alpha^\dagger \right\rangle_0 = 0. \quad (4.306)$$

All these results, Eqs.(4.304)(4.305) and the last equation can be combined into one formula

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 = \langle a_\alpha a_\alpha^\dagger \rangle_0 \left\langle a_\beta a_\beta^\dagger \right\rangle_0 (\delta_{\alpha,\delta} \delta_{\beta,\gamma} - \delta_{\alpha,\gamma} \delta_{\beta,\delta}) \quad (4.307)$$

$$= \left\langle a_\alpha a_\delta^\dagger \right\rangle_0 \left\langle a_\beta a_\gamma^\dagger \right\rangle_0 - \langle a_\alpha a_\gamma^\dagger \rangle_0 \left\langle a_\beta a_\delta^\dagger \right\rangle_0 \quad (4.308)$$

which is easiest to remember as follows,

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger \right\rangle_0 = \left\langle a_{\alpha \uparrow}^\downarrow a_{\beta \uparrow}^\downarrow a_{\gamma \uparrow}^\uparrow a_{\delta \uparrow}^\uparrow \right\rangle_0 + \left\langle a_{\alpha \uparrow}^\downarrow a_{\beta \uparrow}^\downarrow a_{\gamma \uparrow}^\uparrow a_{\delta \uparrow}^\uparrow \right\rangle_0 \quad (4.309)$$

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.(4.308) back into the expression for the original average expressed in the diagonal basis Eq.(4.302) we have

$$\begin{aligned} & \left\langle a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right\rangle_0 \quad (4.310) \\ &= \left\langle a_i(\tau_i) a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_j(\tau_j) a_k^\dagger(\tau_k) \right\rangle_0 - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0 \end{aligned}$$

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 16 *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

$$\boxed{\left\langle T_\tau \left[a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right] \right\rangle_0 =} \quad (4.311)$$

$$\boxed{\left\langle T_\tau \left[a_i(\tau_i) a_l^\dagger(\tau_l) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j) a_k^\dagger(\tau_k) \right] \right\rangle_0 - \left\langle T_\tau \left[a_i(\tau_i) a_k^\dagger(\tau_k) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j) a_l^\dagger(\tau_l) \right] \right\rangle_0.} \quad (4.312)$$

The only simplification that occurs with time-ordered products is the following. Note that, given the definition of time-ordered product, we have

$$\left\langle T_\tau \left[a_i(\tau_i) a_k^\dagger(\tau_k) \right] \right\rangle_0 = - \left\langle T_\tau \left[a_k^\dagger(\tau_k) a_i(\tau_i) \right] \right\rangle_0 \quad (4.313)$$

Indeed, the left-hand side and right-hand side of the above equation are, respectively

$$\left\langle T_\tau \left[a_i(\tau_i) a_k^\dagger(\tau_k) \right] \right\rangle_0 = \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \theta(\tau_i - \tau_k) \quad (4.314)$$

$$- \left\langle a_k^\dagger(\tau_k) a_i(\tau_i) \right\rangle_0 \theta(\tau_k - \tau_i) \quad (4.315)$$

$$- \left\langle T_\tau \left[a_k^\dagger(\tau_k) a_i(\tau_i) \right] \right\rangle_0 = - \left\langle a_k^\dagger(\tau_k) a_i(\tau_i) \right\rangle_0 \theta(\tau_k - \tau_i) \quad (4.316)$$

$$+ \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \theta(\tau_i - \tau_k) \quad (4.317)$$

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.

On the other hand, if we apply Wick's theorem to a product that is not time ordered, then we have to remember that

$$\left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \neq - \left\langle a_k^\dagger(\tau_k) a_i(\tau_i) \right\rangle_0 \quad (4.318)$$

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 17 *To make the example of Wick's theorem Eq.(4.312) more plausible, we give a few examples, Suppose first that the time order to the left of Eq.(4.312) is such that the destruction operators are inverted. Then,*

$$\left\langle T_\tau \left[a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right] \right\rangle_0 = - \left\langle a_j(\tau_j) a_i(\tau_i) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right\rangle_0 \quad (4.319)$$

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.(4.312). 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.(4.310). Doing this and substituting above, we obtain

$$\left\langle a_j(\tau_j) a_i(\tau_i) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right\rangle_0 = \left\langle a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 - \left\langle a_j(\tau_j) a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_i(\tau_i) a_l^\dagger(\tau_l) \right\rangle_0 \quad (4.320)$$

which we substitute in the previous equation to obtain exactly what the right-hand side of Eq.(4.312) would have predicted. To take another example, suppose that the time orders are such that

$$\left\langle T_\tau \left[a_i(\tau_i) a_j(\tau_j) a_k^\dagger(\tau_k) a_l^\dagger(\tau_l) \right] \right\rangle_0 = - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0. \quad (4.321)$$

Then, to do the contractions we proceed as above, being careful not to permute creation and annihilation operators within an expectation value

$$\begin{aligned} & - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0 \\ = & - \left\langle a_i(\tau_i) a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_k^\dagger(\tau_k) a_j(\tau_j) \right\rangle_0 - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0 \end{aligned}$$

The right-hand side of Eq.(4.312) gives us

$$\begin{aligned} & \left\langle T_\tau \left[a_i(\tau_i) a_l^\dagger(\tau_l) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j) a_k^\dagger(\tau_k) \right] \right\rangle_0 - \left\langle T_\tau \left[a_i(\tau_i) a_k^\dagger(\tau_k) \right] \right\rangle_0 \left\langle T_\tau \left[a_j(\tau_j) a_l^\dagger(\tau_l) \right] \right\rangle_0 \\ = & - \left\langle a_i(\tau_i) a_l^\dagger(\tau_l) \right\rangle_0 \left\langle a_k^\dagger(\tau_k) a_j(\tau_j) \right\rangle_0 - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_j(\tau_j) a_l^\dagger(\tau_l) \right\rangle_0 \end{aligned} \quad (4.324)$$

with the minus sign in the first term because we had to exchange the order in one of the time-ordered products.

4.8.2 Linked cluster theorems

Suppose we want to evaluate the Green's function by expanding the time-ordered product in the evolution operator Eq.(4.287). The expansion has to be done both in the numerator and in the denominator of the general expression for the average Eq.(4.285). 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

$$\ln Z = \ln \left(T_\tau \left[e^{-\beta H_0} \widehat{U}(\beta, 0) \right] \right) = \ln \left(Z_0 \left\langle \widehat{U}(\beta, 0) \right\rangle_0 \right) \quad (4.325)$$

$$= \ln \left(\left\langle T_\tau \left[\exp \left(- \int_0^\beta d\tau_1 \widehat{V}(\tau_1) \right) \right] \right\rangle_0 \right) + \ln Z_0 \quad (4.326)$$

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 theorem for normalized averages

Consider the calculation of

$$\frac{\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \rangle}{\langle e^{-f(\mathbf{x})} \rangle} \quad (4.327)$$

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

$$\frac{\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \rangle}{\langle e^{-f(\mathbf{x})} \rangle} = \frac{\sum_{n=0}^{\infty} \frac{1}{n!} \langle (-f(\mathbf{x}))^n A(\mathbf{x}) \rangle}{\sum_{n=0}^{\infty} \frac{1}{n!} \langle (-f(\mathbf{x}))^n \rangle} \quad (4.328)$$

When computing a term of a given order n , such as $\frac{1}{n!} \langle (-f(\mathbf{x}))^n A(\mathbf{x}) \rangle$, we may always write

$$\frac{1}{n!} \langle (-f(\mathbf{x}))^n A(\mathbf{x}) \rangle = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} \delta_{n,m+\ell} \frac{1}{n!} \frac{n!}{\ell! m!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c \langle (-f(\mathbf{x}))^m \rangle \quad (4.329)$$

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

$$\frac{\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \rangle}{\langle e^{-f(\mathbf{x})} \rangle} = \frac{\sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{m! \ell!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c \langle (-f(\mathbf{x}))^m \rangle}{\sum_{n=0}^{\infty} \frac{1}{n!} \langle (-f(\mathbf{x}))^n \rangle} \quad (4.330)$$

The numerator can now be factored so as to cancel the denominator which proves the theorem

Theorem 18 *Linked cluster theorem for normalized averages:*

$$\boxed{\frac{\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \rangle}{\langle e^{-f(\mathbf{x})} \rangle} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c = \langle e^{-f(\mathbf{x})} A(\mathbf{x}) \rangle_c} \quad (4.331)$$

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 $\left(-\int_0^\beta d\tau \widehat{V}(\tau)\right)$ can be moved within the T_τ product without costing any additional minus sign.

Linked cluster theorem for characteristic functions or free energy

We now wish to show the following general theorem for a multivariate probability distribution.

Theorem 19 *Linked cluster theorem (cumulant expansion).*

$$\boxed{\ln \langle e^{-f(\mathbf{x})} \rangle = \sum_{n=1}^{\infty} \frac{1}{n!} \langle (-f(\mathbf{x}))^n \rangle_c = \langle e^{-f(\mathbf{x})} \rangle_c - 1} \quad (4.332)$$

The proof is inspired by Enz[16]. When $f(\mathbf{x}) = i\mathbf{k} \cdot \mathbf{x}$, the quantity $\langle e^{-i\mathbf{k} \cdot \mathbf{x}} \rangle$ 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 $\ln \langle e^{-i\mathbf{k} \cdot \mathbf{x}} \rangle$ is the generating function for the cumulant averages.

Proof: To prove the theorem, we introduce first an auxiliary variable λ

$$\frac{\partial}{\partial \lambda} \langle e^{-\lambda f(\mathbf{x})} \rangle = \langle e^{-\lambda f(\mathbf{x})} [-f(\mathbf{x})] \rangle \quad (4.333)$$

We can apply to the right-hand side the theorem we just proved

$$\langle e^{-\lambda f(\mathbf{x})} [-f(\mathbf{x})] \rangle = \langle e^{-\lambda f(\mathbf{x})} [-f(\mathbf{x})] \rangle_c \langle e^{-\lambda f(\mathbf{x})} \rangle \quad (4.334)$$

so that

$$\frac{1}{\langle e^{-\lambda f(\mathbf{x})} \rangle} \frac{\partial}{\partial \lambda} \langle e^{-\lambda f(\mathbf{x})} \rangle = \left\langle \frac{\partial}{\partial \lambda} e^{-\lambda f(\mathbf{x})} \right\rangle_c. \quad (4.335)$$

Integrating both sides from 0 to 1, we obtain

$$\ln \langle e^{-\lambda f(\mathbf{x})} \rangle \Big|_0^1 = \langle e^{-f(\mathbf{x})} \rangle_c - 1 \quad (4.336)$$

QED

Example 20 *It is instructive to check the meaning of the above result explicitly to second order*

$$\ln \langle e^{-\lambda f(x)} \rangle \approx \ln \left\langle 1 - \lambda f(x) + \frac{1}{2} (\lambda f(x))^2 \right\rangle \approx \left(-\langle \lambda f(x) \rangle + \frac{1}{2} \langle (\lambda f(x))^2 \rangle \right) - \frac{1}{2} \langle \lambda f(x) \rangle^2 \quad (4.337)$$

$$\langle e^{-\lambda f(x)} \rangle_c - 1 \approx -\langle \lambda f(x) \rangle_c + \frac{1}{2} \langle (\lambda f(x))^2 \rangle_c \quad (4.338)$$

so that equating powers of λ , we find as expected,

$$\langle (f(\mathbf{x}))^2 \rangle_c = \langle (f(\mathbf{x}))^2 \rangle - \langle f(\mathbf{x}) \rangle^2. \quad (4.339)$$

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,

$$F = -T \ln \left[Z_0 \left\langle T_\tau \left[e^{-\int_0^\beta d\tau \hat{V}(\tau)} \right] \right\rangle_0 \right] = -T \sum_{n=1}^{\infty} \frac{1}{n!} \left\langle T_\tau \left[-\int_0^\beta d\tau \hat{V}(\tau) \right]^n \right\rangle_{0c} - T \ln Z_0 \quad (4.340)$$

$$\boxed{F = -T \ln Z = -T \left[\left\langle T_\tau \left[e^{-\int_0^\beta d\tau \hat{V}(\tau)} \right] \right\rangle_{0c} - 1 \right] - T \ln Z_0.} \quad (4.341)$$

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.

4.8.3 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.

Thermodynamic variational principle for classical systems

One can base the thermodynamic variational principle for classical systems on the inequality

$$\boxed{e^x \geq 1 + x} \quad (4.342)$$

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.* $d^2 e^x / dx^2 \geq 0$ 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 equality occurs when $x = 0$. For $x \leq -1$, $e^x \geq 0$ while $1 + x < 0$, hence the inequality is satisfied. For the remaining two intervals, notice that $e^x \geq 1 + x$ is equivalent to

$$\sum_{n=2}^{\infty} \frac{1}{n!} x^n \geq 0. \quad (4.343)$$

For $x \geq 0$, all terms in the sum are positive so the inequality is trivially satisfied. In the only remaining interval, $-1 < x < 0$, the odd powers of x in the infinite-sum version of the inequality are less than zero but the magnitude of each odd power of x is less than the magnitude of the preceding positive power of x , so the inequality (4.343) survives. *QED*

Moving back to our initial purpose, let \tilde{H}_0 be a trial Hamiltonian. Then take $e^{-\beta(\tilde{H}_0 - \mu N)} / Z_0$ as the trial density matrix corresponding to averages $\langle \cdot \rangle_{\tilde{0}}$. We will use the above inequality Eq.(4.342) to prove that

$$\boxed{-T \ln Z \leq -T \ln Z_{\tilde{0}} + \langle H - \tilde{H}_0 \rangle_{\tilde{0}}} \quad (4.344)$$

This inequality is a variational principle because \tilde{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.(4.341), 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

$$\tilde{V} = H - \tilde{H}_0 \quad (4.345)$$

we have

$$F = -T \ln Z = -T \left[\langle e^{-\beta \tilde{V}} \rangle_{\tilde{0},c} - 1 \right] - T \ln Z_{\tilde{0}}. \quad (4.346)$$

Using our basic inequality Eq.(4.342) for $e^{-\beta \tilde{V}}$ we immediately obtain the desired result

$$F \leq -T \langle -\beta \tilde{V} \rangle_{\tilde{0},c} + F_{\tilde{0}} \quad (4.347)$$

which is just another way of rewriting Eq.(4.344).

It is useful to note that in the language of density matrices, $\rho_0 = e^{-\beta(\tilde{H}_0 - \mu N)} / Z_0$ the variational principle Eq.(4.344) reads,

$$\boxed{-T \ln Z \leq Tr [\rho_0 (H - \mu N)] + TTr [\rho_0 \ln \rho_0]} \quad (4.348)$$

which looks as if we had the function $(E - \mu N) - TS$ to minimize, quite a satisfactory state of affairs.

Thermodynamic variational principle for quantum systems

For quantum systems, the general result Eq.(4.344) 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 $T_\tau \exp \left[- \int_0^\beta d\tau \tilde{V}(\tau) \right]$. If \tilde{V} was not time dependent, as in the classical case, then matters would be different since \tilde{V}^n would be diagonal in the same basis as \tilde{V} and one could apply our inequality Eq.(4.342) 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. As far as I know, the proof is due to Feynman [17].

Proof: First, let

$$H(\alpha) = \tilde{H}_0 + \alpha (H - \tilde{H}_0) \quad (4.349)$$

$$= \tilde{H}_0 + \alpha \tilde{V} \quad (4.350)$$

then

$$H(0) = \tilde{H}_0 \quad (4.351)$$

and

$$H(1) = H \quad (4.352)$$

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

$$F(1) \leq F(0) + \left. \frac{\partial F(\alpha)}{\partial \alpha} \right|_{\alpha=0} \quad (4.353)$$

as illustrated in Fig.(4-14). Eq.(4.353) is the variational principle that we want Eq.(4.344). Indeed, let us compute the first derivative of $F(\alpha)$ by going to the interaction representation where \tilde{H}_0 plays the role of the unperturbed Hamiltonian and use the result for F in terms of connected graphs Eq.(4.341) to obtain

$$\left. \frac{\partial F(\alpha)}{\partial \alpha} \right|_{\alpha=0} = \frac{\partial}{\partial \alpha} \left\{ -T \left[\left\langle T_\tau \left[e^{-\alpha \int_0^\beta d\tau (\hat{H}(\tau) - \tilde{H}_0)} \right] \right\rangle_{\tilde{0}_c} - 1 \right] \right\}_{\alpha=0} \quad (4.354)$$

$$= T \left\langle \int_0^\beta d\tau (\hat{H}(\tau) - \tilde{H}_0) \right\rangle_{\tilde{0}} \quad (4.355)$$

$$= \left\langle H - \tilde{H}_0 \right\rangle_{\tilde{0}} \quad (4.356)$$

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 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

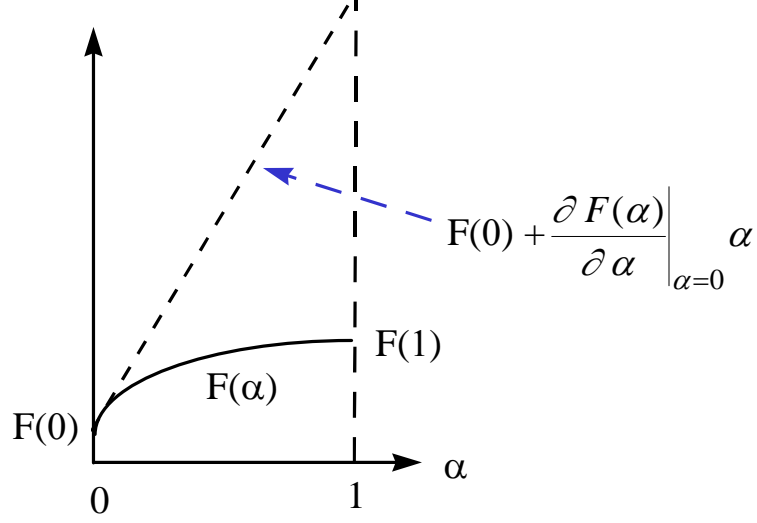


Figure 4-14 Geometrical significance of the inequalities leading to the quantum thermodynamic variational principle.

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 $\gamma(H - \tilde{H}_0)$ is the perturbation. Then,

$$F(\alpha + \gamma) = -T \left[\left\langle T_\tau \left[e^{-\gamma \int_0^\beta d\tau (\hat{H}(\tau) - \tilde{H}_0)} \right] \right\rangle_{\alpha, c} - 1 \right] - T \ln Z(\alpha) \quad (4.357)$$

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 \tilde{V} Eq.(4.350) we find

$$\begin{aligned} F(\alpha + \gamma) &= F(\alpha) + \gamma \langle \tilde{V} \rangle_\alpha - \frac{1}{2} \gamma^2 \left(\frac{1}{\beta} \left\langle T_\tau \left[-\gamma \int_0^\beta d\tau \tilde{V}(\tau) \right]^2 \right\rangle_{\alpha, c} \right) + \dots \\ F(\alpha + \gamma) &= F(\alpha) + \frac{\partial F(\alpha)}{\partial \alpha} \gamma + \frac{1}{2} \gamma^2 \frac{\partial^2 F(\alpha)}{\partial \alpha^2} + \dots \end{aligned} \quad (4.358)$$

so that the second derivative, using the expression we found above for the second cumulant Eq.(4.339) is,

$$\begin{aligned} \frac{\partial^2 F(\alpha)}{\partial \alpha^2} &= -\frac{1}{\beta} \left\langle T_\tau \left[\left(-\int_0^\beta d\tau \tilde{V}(\tau) \right)^2 \right] \right\rangle_{\alpha, c} \\ &= -\frac{1}{\beta} \left\langle T_\tau \left[\left(-\int_0^\beta d\tau \tilde{V}(\tau) \right)^2 \right] \right\rangle_\alpha + \frac{1}{\beta} \left\langle \int_0^\beta d\tau \tilde{V}(\tau) \right\rangle_\alpha^2 \end{aligned} \quad (4.359)$$

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,

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} = -2 \frac{1}{\beta} \left\langle \int_0^\beta d\tau \tilde{V}(\tau) \int_0^\tau d\tau' \tilde{V}(\tau') \right\rangle_\alpha + \beta \langle \tilde{V} \rangle_\alpha^2 \quad (4.360)$$

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,

$$\left\langle \int_0^\beta d\tau \tilde{V}(\tau) \int_0^\tau d\tau' \tilde{V}(\tau') \right\rangle_\alpha \quad (4.361)$$

$$\begin{aligned} &= \frac{1}{Z(\alpha)} \sum_{m,n} e^{-K_n \beta} \int_0^\beta d\tau \int_0^\tau d\tau' e^{K_n(\tau-\tau')} e^{-K_m(\tau-\tau')} |\langle n | \tilde{V} | m \rangle|^2 \\ &= \frac{1}{Z(\alpha)} \sum_{m \neq n} e^{-K_n \beta} \int_0^\beta d\tau e^{(K_n - K_m)\tau} \frac{e^{(K_m - K_n)\tau'}}{K_m - K_n} \Big|_0^\tau |\langle n | \tilde{V} | m \rangle|^2 \\ &\quad + \frac{1}{Z(\alpha)} \sum_n e^{-K_n \beta} \int_0^\beta d\tau \tau |\langle n | \tilde{V} | n \rangle|^2 \end{aligned} \quad (4.362)$$

$$= \frac{1}{Z(\alpha)} \sum_{m \neq n} e^{-K_n \beta} \int_0^\beta d\tau \frac{1 - e^{(K_n - K_m)\tau}}{K_m - K_n} |\langle n | \tilde{V} | m \rangle|^2 \quad (4.363)$$

$$+ \frac{\beta^2}{2Z(\alpha)} \sum_n e^{-K_n \beta} |\langle n | \tilde{V} | n \rangle|^2 \quad (4.364)$$

The first term on the right-hand side is easily evaluated as follows

$$\begin{aligned} &\frac{1}{Z(\alpha)} \sum_{m \neq n} e^{-K_n \beta} \left[\frac{\beta}{K_m - K_n} + \frac{e^{(K_n - K_m)\beta} - 1}{(K_m - K_n)^2} \right] |\langle n | \tilde{V} | m \rangle|^2 \\ &= \frac{\beta}{Z(\alpha)} \sum_{m \neq n} e^{-K_n \beta} \frac{|\langle n | \tilde{V} | m \rangle|^2}{K_m - K_n} \end{aligned} \quad (4.365)$$

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.(4.360) we finally obtain

$$\begin{aligned} \frac{\partial^2 F(\alpha)}{\partial \alpha^2} &= -\frac{2}{Z(\alpha)} \sum_{m \neq n} e^{-K_n \beta} \frac{|\langle n | \tilde{V} | m \rangle|^2}{K_m - K_n} \\ &\quad - \beta \left(\frac{\sum_n e^{-K_n \beta} |\langle n | \tilde{V} | n \rangle|^2}{Z(\alpha)} - \left(\frac{\sum_n e^{-K_n \beta} \langle n | \tilde{V} | n \rangle}{Z(\alpha)} \right)^2 \right) \end{aligned} \quad (4.366)$$

The terms on the last line gives a negative contribution, as can be seen from the Cauchy-Schwarz inequality

$$\left[\sum_n |a_n|^2 \right] \left[\sum_n |b_n|^2 \right] \geq \left| \sum_n a_n b_n \right|^2 \quad (4.367)$$

when we substitute

$$a_n = \sqrt{\frac{e^{-K_n \beta}}{Z(\alpha)}} \quad (4.368)$$

$$b_n = \sqrt{\frac{e^{-K_n\beta}}{Z(\alpha)}} \langle n | \tilde{V} | n \rangle \quad (4.369)$$

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.(4.366) in the form

$$-\frac{2}{Z(\alpha)} \sum_{m \neq n} e^{-K_n\beta} \frac{|\langle n | \tilde{V} | m \rangle|^2}{K_m - K_n} = -\frac{1}{Z(\alpha)} \sum_{m \neq n} \frac{e^{-K_n\beta} - e^{-K_m\beta}}{K_m - K_n} |\langle n | \tilde{V} | m \rangle|^2 \quad (4.370)$$

and to use the Cauchy-Schwartz inequality to obtain

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} \leq -\frac{1}{Z(\alpha)} \sum_{m \neq n} \frac{e^{-K_n\beta} - e^{-K_m\beta}}{K_m - K_n} |\langle n | \tilde{V} | m \rangle|^2 \leq 0 \quad (4.371)$$

QED

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

$$\tilde{H}_0 = \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}^*(\mathbf{x}) \left(-\frac{\nabla^2}{2m} \right) \phi_{\alpha}(\mathbf{x}) c_{\alpha}^{\dagger} c_{\alpha} \quad (4.372)$$

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!

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5. 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 many-body theory in the context of Solid State physics. In this chapter, we assume that the uniform neutralizing background has infinite inertia. In a subsequent chapter we will allow it to move, in other words to support sound waves, or phonons. In subsequent chapters 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 establishing the rules for Feynman diagrams in an interacting electron gas, and then start to do calculations. 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.

5.1 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 [3],[2].

5.1.1 Hamiltonian and notation

The Hamiltonian we consider is the following. Note that we now introduce spin indices denoted by Greek indices:

$$K = H - \mu N = H_0 + V + V_n - \mu N \quad (5.1)$$

$$H_0 = \frac{1}{2m} \sum_{\sigma_1} \int d\mathbf{x}_1 \nabla \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \cdot \nabla \psi_{\sigma_1}(\mathbf{x}_1) \quad (5.2)$$

$$V = \frac{1}{2} \sum_{\sigma_1, \sigma_2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 v(\mathbf{x}_1 - \mathbf{x}_2) \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \psi_{\sigma_2}^\dagger(\mathbf{x}_2) \psi_{\sigma_2}(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_1)$$

$$V_n = - \sum_{\sigma_1} \int d\mathbf{x}_1 \int d\mathbf{x}_2 v(\mathbf{x}_1 - \mathbf{x}_2) \psi_{\sigma_1}^\dagger(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_2) n_0 \quad (5.3)$$

The last piece, V_n represents the interaction between a “neutralizing background” of the same uniform density n_0 as the electrons. The potential is the Coulomb potential

$$v(\mathbf{x}_1 - \mathbf{x}_2) = \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|} \quad (5.4)$$

Let us say we want to compute the one-body Green’s function in the interaction representation

$$\begin{aligned} \mathcal{G}_{\sigma_1 \sigma_2}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) &= - \frac{\text{Tr} \left[e^{-\beta K_0} T_\tau \left(\widehat{U}(\beta, \tau_1) \widehat{\psi}_{\sigma_1}(\mathbf{x}_1, \tau_1) \widehat{U}(\tau_1, \tau_2) \widehat{\psi}_{\sigma_2}^\dagger(\mathbf{x}_2, \tau_2) \widehat{U}(\tau_2, 0) \right) \right]}{\text{Tr} \left[e^{-\beta K_0} \widehat{U}(\beta, 0) \right]} \\ &= - \frac{\text{Tr} \left[e^{-\beta K_0} T_\tau \left(\widehat{U}(\beta, 0) \widehat{\psi}_{\sigma_1}(\mathbf{x}_1, \tau_1) \widehat{\psi}_{\sigma_2}^\dagger(\mathbf{x}_2, \tau_2) \right) \right]}{\text{Tr} \left[e^{-\beta K_0} \widehat{U}(\beta, 0) \right]} \end{aligned} \quad (5.5)$$

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

$$\widehat{U}(\beta, 0) = T_\tau \left[\exp \left(- \int_0^\beta d\tau_1 \widehat{V}(\tau_1) \right) \right]$$

Note that by definition of the interaction representation,

$$\widehat{V}(\tau_1) = e^{K_0 \tau_1} \left[\frac{1}{2} \sum_{\sigma_1, \sigma_2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 v(\mathbf{x}_1 - \mathbf{x}_2) \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \psi_{\sigma_2}^\dagger(\mathbf{x}_2) \psi_{\sigma_2}(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_1) \right] e^{-K_0 \tau_1} \quad (5.6)$$

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

$$\begin{aligned} \widehat{U}(\beta, 0) &= T_\tau \left[\exp \left(- \frac{1}{2} \sum_{\sigma_1, \sigma_2} \int_0^\beta d\tau_1 \int d\mathbf{x}_1 \int d\mathbf{x}_2 \right. \right. \\ &\quad \left. \left. v(\mathbf{x}_1 - \mathbf{x}_2) \widehat{\psi}_{\sigma_1}^\dagger(\mathbf{x}_1, \tau_1) \widehat{\psi}_{\sigma_2}^\dagger(\mathbf{x}_2, \tau_1) \widehat{\psi}_{\sigma_2}(\mathbf{x}_2, \tau_1) \widehat{\psi}_{\sigma_1}(\mathbf{x}_1, \tau_1) \right) \right] \end{aligned} \quad (5.7)$$

This can be made even more symmetrical by defining the potential,

$$\boxed{V_{\sigma_1, \sigma_2}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) = \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|} \delta(\tau_1 - \tau_2)} \quad (5.8)$$

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

$$V(1, 2) \quad (5.9)$$

where

$$(1) = (\mathbf{x}_1, \tau_1; \sigma_1) \quad (5.10)$$

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

$$\int_1 = \int_0^\beta d\tau_1 \int d\mathbf{x}_1 \sum_{\sigma_1=\pm 1} \quad (5.11)$$

and

$$\psi(1) = \widehat{\psi}_{\sigma_1}(\mathbf{x}_1, \tau_1) \quad (5.12)$$

Note that we have taken this opportunity to remove hats 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.(5.5) and the time evolution operator Eq.(5.7) take the simpler looking form

$$\mathcal{G}(1, 2) = - \frac{\text{Tr}[e^{-\beta K_0} T_\tau(U(\beta, 0)\psi(1)\psi^\dagger(2))]}{\text{Tr}[e^{-\beta K_0} U(\beta, 0)]} \quad (5.13)$$

$$U(\beta, 0) = T_\tau \left[\exp \left(-\frac{1}{2} \int_1 \int_2 V(1, 2) \psi^\dagger(1) \psi^\dagger(2) \psi(2) \psi(1) \right) \right] \quad (5.14)$$

5.1.2 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 $1/\text{Tr}[e^{-\beta K_0}]$ we can use the linked cluster theorem in Subsection (4.8.2) 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.(5.13) only connected terms are kept. The perturbation expansion for the Green's function thus takes the form

$$\mathcal{G}(1, 2) = - \left\langle T_\tau \left(U(\beta, 0) \psi(1) \psi^\dagger(2) \right) \right\rangle_{0,c} \quad (5.15)$$

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

$$-\frac{1}{n!} \left\langle T_\tau \left[\left(-\frac{1}{2} \int_{1'} \int_{2'} V(1', 2') \psi^\dagger(1') \psi^\dagger(2') \psi(2') \psi(1') \right)^n \psi(1) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (5.16)$$

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.(5.16) 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.(5-1). Following the convention of Ref. [4] 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. [5]. 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 an 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 ψ^\dagger attached to any given end of a dotted line. The arrow heads in Fig.(5-1) just remind 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 5-1 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

$$-\left\langle T_\tau \left[-\frac{1}{2} \int_{1'} \int_{2'} V(1', 2') \psi_1^\dagger(1') \psi_2^\dagger(2') \psi_3(2') \psi_2(1') \psi_1(1) \psi_3^\dagger(2) \right] \right\rangle_{0,c} \quad (5.17)$$

We have marked by a the same number every operator that belongs to the same contraction. The corresponding algebraic expression is

$$-\frac{1}{2} \int_{1'} \int_{2'} V(1', 2') \mathcal{G}(1, 1') \mathcal{G}(1', 2') \mathcal{G}(2', 2) \quad (5.18)$$

and we can represent it by a diagram, as in Fig.(5-2) Clearly, exactly the same

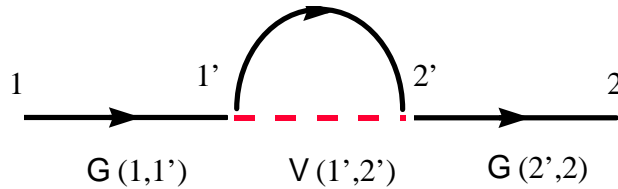


Figure 5-2 A typical contraction for the first-order expansion of the Green's function. The Fock term.

contribution is obtained if the roles of the fields at the points $1'$ and $2'$ above are interchanged. More specifically, the set of contractions

$$-\left\langle T_\tau \left[-\frac{1}{2} \int_{1'} \int_{2'} V(1', 2') \psi_2^\dagger(1') \psi_1^\dagger(2') \psi_2(2') \psi_3(1') \psi_1(1) \psi_3^\dagger(2) \right] \right\rangle_{0,c} \quad (5.19)$$

gives the algebraic expression

$$-\frac{1}{2} \int_{1'} \int_{2'} V(1', 2') \mathcal{G}(2', 1') \mathcal{G}(1, 2') \mathcal{G}(1', 2) \quad (5.20)$$

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.(5-3). 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.(5.18)(5.20). 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.

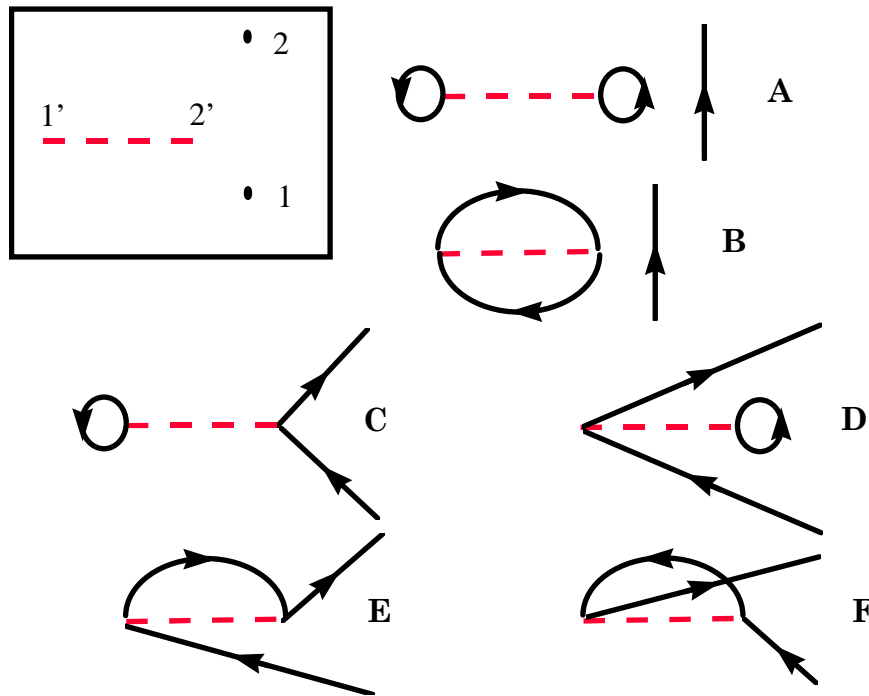


Figure 5-3 All possible contractions for the first-order contribution to the Green's function. A line must start at point 1 illustrated in the box on the left, and one line must end at 2. Lines must also come in and go out on either side of the dotted line.

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.(5-4). 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 $1/(2^n n!)$ coming from the expansion of the exponential and the $1/2$ in front of each interaction $V(1', 2')$.

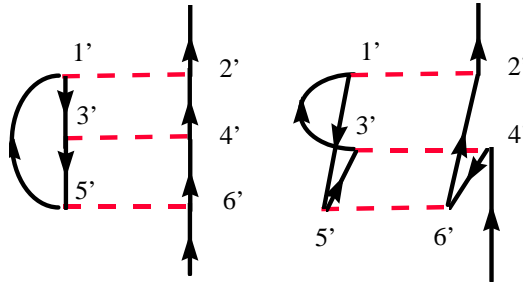


Figure 5-4 Two topologically equivalent diagrams of order 3.

From what precedes then, it is clear that we can find all contributions for $\mathcal{G}(1, 2)$ 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 $\mathcal{G}(1, 2)$ to every line going from a vertex or external point labeled 1 to a vertex or external point labeled 2.
4. Associate a factor $V(1', 2')$ 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.(5.7). (And now the last two rules that we have not proven yet)
6. Associate a factor $(-1)^n (-1)^F$ 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.(5-5)) the factor

$$\mathcal{G}(1, 2^+) \equiv \lim_{\eta \rightarrow 0} \mathcal{G}_{\sigma_1, \sigma_2}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_1 + \eta) \quad (5.21)$$

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 5-5 Pieces of diagrams for which lead to equal-time Green's functions and for which it is necessary to specify how the $\tau \rightarrow 0$ limit is taken.

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.

$$- (-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \dots \int_{2n-1} \int_{2n} \psi^\dagger(1') \psi^\dagger(2') \psi(2') \psi(1') \dots \right. \right. \quad (5.22)$$

$$\left. \dots \psi^\dagger(2n-1) \psi^\dagger(2n) \psi(2n) \psi(2n-1) \psi(1) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (5.23)$$

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

$$- (-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \dots \int_{2n-1} \int_{2n} \left(\psi^\dagger(1'^+) \psi(1') \right) \left(\psi^\dagger(2'^+) \psi(2') \right) \dots \right. \right. \quad (5.24)$$

$$\left. \dots \left(\psi^\dagger((2n-1)^+) \psi(2n-1) \right) \left(\psi^\dagger((2n)^+) \psi(2n) \right) \psi(1) \psi^\dagger(2) \right] \right\rangle_{0,c}$$

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.(5.21) 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

$$- (-1)^n \left\langle T_\tau \left[\int_{1'} \int_{2'} \dots \int_{2n-1} \int_{2n} \psi^\dagger(1'^+) \psi(1') \psi^\dagger(2'^+) \psi(2') \dots \right. \right. \quad (5.25)$$

$$\left. \dots \psi^\dagger_{2n-2} \psi^\dagger_{2n-2} \left((2n-1)^+ \right) \psi_{2n-1} \psi_{2n-1} \psi^\dagger_{2n-1} \left((2n)^+ \right) \psi_{2n+1} \psi_{2n} \psi_{2n} \psi(1) \psi^\dagger_{2n+1}(2) \right] \right\rangle_{0,c}$$

Not taking into account the $- (-1)^n$ already in front of the average, the contractions labeled 1 to $2n-1$ give a contribution

$$(-1)^{2n-1} \mathcal{G}(1', 2') \mathcal{G}(2'3') \dots \mathcal{G}(2n-1, 2n) \quad (5.26)$$

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

$$-(-1)^n(-1)^{2n-1}(-1)^2 = (-1)^n \quad (5.27)$$

In the contractions we have just done there is no closed fermion loop, as illustrated in Fig.(5-6) for the special case where $2n = 4$.

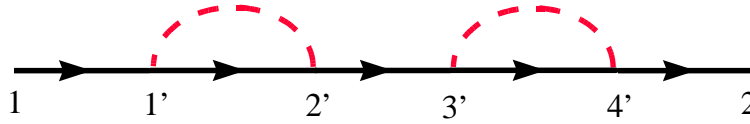


Figure 5-6 Example of a contraction without closed fermion loop.

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,

$$\left\langle T_\tau \left[\psi^\dagger(1') \left(\psi^\dagger \psi \psi \dots \psi \right) \psi^\dagger(2) \right] \right\rangle_{0,c} \quad (5.28)$$

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 $\psi^\dagger(2)$ 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 permutation 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.(5-6) and interchange the role of two creation operators, as in Fig.(5-7), then we go from a situation with no fermion loops to one with one fermion loop. Fig.(5-8) 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.

Spin sums

A remark is in order concerning spin. In a diagram without loops, as in Fig.(5-6), 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

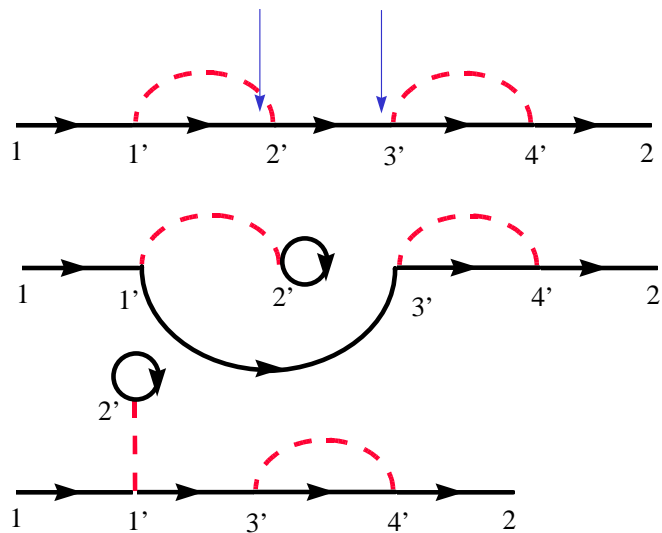


Figure 5-7 Creation of loops in diagrams by interchange of operators: The role of the two creation operators indicated by light arrows is interchanged, leading from a diagram with no loop, as on top, to a diagram with one loop. The diagram on the bottom is the same as the one in the middle. It is simply redrawn for clarity.

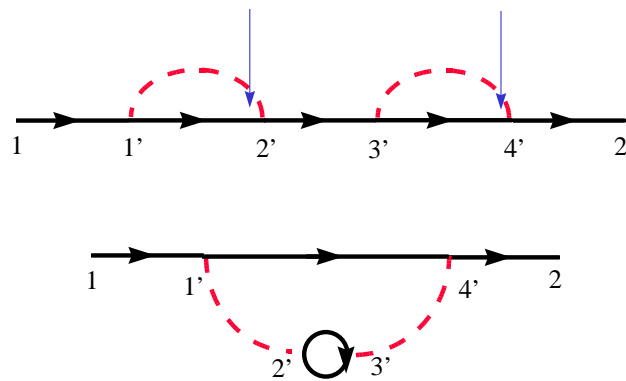


Figure 5-8 Interchange of two fermion operators creating a fermion loop.

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.

5.1.3 In momentum space

Starting from our results for Feynman's rule in position space, we can derive the rules in momentum space.[8] First introduce, for a translationally and spin rotationally invariant system, the definition

$$\mathcal{G}_\sigma(k) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2) e^{-i\mathbf{k}\cdot(\mathbf{x}_1 - \mathbf{x}_2)} e^{ik_n(\tau_1 - \tau_2)} \mathcal{G}_\sigma(1 - 2) \quad (5.29)$$

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

$$V_{\sigma, \sigma'}(q) = \int d(\mathbf{x}_1 - \mathbf{x}_2) \int_0^\beta d(\tau_1 - \tau_2) e^{-i\mathbf{q}\cdot(\mathbf{x}_1 - \mathbf{x}_2)} e^{iq_n(\tau_1 - \tau_2)} V_{\sigma, \sigma'}(1 - 2) \quad (5.30)$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_n = 2n\pi T \quad (5.31)$$

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 93 *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

$$\mathcal{G}_\sigma(1 - 2) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1 - \mathbf{x}_2)} e^{-ik_n(\tau_1 - \tau_2)} \mathcal{G}_\sigma(k) \quad (5.32)$$

$$V_{\sigma, \sigma'}(1 - 2) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1 - \mathbf{x}_2)} e^{-iq_n(\tau_1 - \tau_2)} V_{\sigma, \sigma'}(q) \quad (5.33)$$

Then we consider an internal vertex, as illustrated in Fig.(5-9), where one has to 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

$$\int d\mathbf{x}'_1 \int_0^\beta d\tau'_1 e^{-i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{q})\cdot\mathbf{x}'_1} e^{i(k_{1,n} - k_{2,n} + q_n)\tau'_1} \quad (5.34)$$

$$= (2\pi)^3 \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{q}) \beta \delta_{(k_{1,n} - k_{2,n}), q_n} \quad (5.35)$$

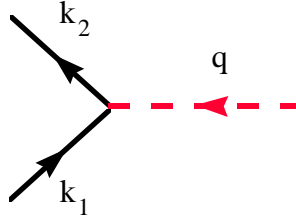


Figure 5-9 A typical interaction vertex and momentum conservation at the vertex.

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.(5.32) and (5.33) 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

$$\boxed{\mathcal{G}_\sigma^0(k) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)}} \quad (5.36)$$

(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.(5-5), 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.

5.1.4 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 Lehman representation tells us that the interacting Green's function has simple poles.
- High order poles can lead to negative spectral weight.[7] For example, the first order contribution to the spectral weight $A(k) = -2\text{Im}G^R$ would be given by a term proportional to

$$\begin{aligned} -2\text{Im}\left(\frac{1}{(\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu))^2}\right) &= 2\text{Im}\frac{\partial}{\partial\omega}\left(\frac{1}{\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu)}\right) \\ &= -2\pi\frac{\partial}{\partial\omega}\delta(\omega - (\varepsilon_{\mathbf{k}} - \mu)) \end{aligned} \quad (5.37)$$

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

$$\boxed{\mathcal{G}_\sigma(k) = \mathcal{G}_\sigma^0(k) + \mathcal{G}_\sigma^0(k) \Sigma_\sigma(k) \mathcal{G}_\sigma(k)} \quad (5.38)$$

or

$$\mathcal{G}_\sigma(k) = \frac{1}{(\mathcal{G}_\sigma^0(k))^{-1} - \Sigma_\sigma(k)} \quad (5.39)$$

This is the so-called Dyson equation. The iterative solution of this equation

$$\mathcal{G}_\sigma(k) = \mathcal{G}_\sigma^0(k) + \mathcal{G}_\sigma^0(k) \Sigma_\sigma(k) \mathcal{G}_\sigma^0(k) + \mathcal{G}_\sigma^0(k) \Sigma_\sigma(k) \mathcal{G}_\sigma^0(k) \Sigma_\sigma(k) \mathcal{G}_\sigma^0(k) + \dots$$

clearly shows that all diagrams that can be cut in two pieces by cutting one fermion line $\mathcal{G}_\sigma^0(k)$ 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 $\mathcal{G}_\sigma^0(k)$ line. As an example, the diagram on the left of Fig.(5-10) 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.

Remark 94 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.*

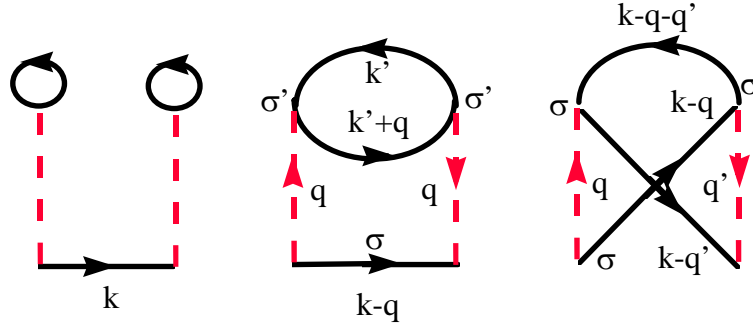


Figure 5-10 Diagram on the left is one-particle reducible, and hence is not an acceptable contribution to the self-energy. The two diagrams on the right however are acceptable contributions to the one-particle irreducible self-energy. In these diagrams, k is the external momentum and Matsubara frequency label while σ is the external spin label. There is a sum over the variables k' , q and q' and over the spin σ' .

5.1.5 Feynman diagrams and the Pauli principle

Since operators can be anticommutated 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 principle. On the other hand, if we look at a self-energy diagram like the middle one in Fig.(5-10) there are contributions that violate the Pauli 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 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.(5-10). 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 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 principle.

5.2 Collective modes and dielectric 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.(2.276) measures

$$S_{nn}(\mathbf{q}, \omega) = \frac{2}{1 - e^{-\beta\omega}} \text{Im} [\chi_{nn}^R(\mathbf{q}, \omega)] = -\frac{2}{1 - e^{-\beta\omega}} \frac{q^2}{4\pi} \text{Im} \left[\frac{1}{\epsilon^L(\mathbf{q}, \omega)} \right]. \quad (5.40)$$

The longitudinal dielectric constant itself is given by Eq.(2.275)

$$\boxed{\frac{1}{\epsilon^L(\mathbf{q}, \omega)} = 1 - \frac{4\pi}{q^2} \chi_{nn}^R(\mathbf{q}, \omega)}. \quad (5.41)$$

The physical phenomenon of screening will manifest itself in the zero-frequency limit of the longitudinal dielectric constant, $\epsilon^L(\mathbf{q}, 0)$. Plasma oscillations on the other hand should come out from the finite frequency zeros of this same function $\epsilon^L(\mathbf{q}, \omega) = 0$, as we expect from our general discussion of collective modes.

We will start this section by a discussion of the Lindhard function, namely $\chi_{nn}^R(\mathbf{q}, \omega)$ 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.

5.2.1 Definitions and analytic continuation

We want the Fourier transform of the density-density response function. First note that

$$n_{\mathbf{q}} \equiv \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} n(\mathbf{r}) = \sum_{\sigma=\pm 1} \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \quad (5.42)$$

$$= \frac{1}{(\sqrt{\mathcal{V}})^2} \sum_{\sigma} \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k}',\sigma} \quad (5.43)$$

$$= \sum_{\sigma} \sum_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q},\sigma} \quad (5.44)$$

As before, \mathcal{V} is the quantization volume of the system. We can obtain the retarded density-density response function from

$$\boxed{\chi_{nn}^R(\mathbf{q}, \omega) = \lim_{iq_n \rightarrow \omega + i\eta} \chi_{nn}(\mathbf{q}, iq_n)} \quad (5.45)$$

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

$$\chi_{nn}(\mathbf{q}, iq_n) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_0^\beta d\tau e^{iq_n\tau} \langle T_\tau [\delta n(\mathbf{r}, \tau) \delta n(\mathbf{r}', 0)] \rangle \quad (5.46)$$

$$= \frac{1}{\mathcal{V}} \int_0^\beta e^{iq_n\tau} \langle T_\tau [\delta n_{\mathbf{q}}(\tau) \delta n_{-\mathbf{q}}(0)] \rangle d\tau \quad (5.47)$$

$$\chi_{nn}^R(\mathbf{q}, \omega) = \frac{1}{\mathcal{V}} \int_{-\infty}^{\infty} e^{i\omega t} i \langle [\delta n_{\mathbf{q}}(t), \delta n_{-\mathbf{q}}(0)] \rangle \theta(t) dt \quad (5.48)$$

Analytic continuation for density response To prove the analytic continuation formula for the density response Eq.(5.45), one can simply use the Lehman representation or deform the integration contour in the Matsubara representation, as we did for propagators in Sec.(4.5.3). (See Eqs.(4.161) and (4.157) in particular). The fact that we have bosonic Matsubara frequencies means that we will have a commutator in real frequency instead of an anti-commutator 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

$$\delta n(\mathbf{q}, t) = n(\mathbf{q}, t) - \langle n(\mathbf{q}, t) \rangle = n(\mathbf{q}, t) - n_0 (2\pi)^3 \delta(\mathbf{q})$$

is irrelevant since a constant commutes with any operator.

Remark 95 *The density response function is also called charge susceptibility.*

5.2.2 Density response in the non-interacting limit: Lindhard function

To do the calculation in the non-interacting case, it suffices to use Wick's theorem.

$$\chi_{nn}^0(\mathbf{q}, iq_n) = \frac{1}{\mathcal{V}} \int_0^\beta d\tau e^{iq_n\tau} \sum_{\sigma} \sum_{\mathbf{k}} \sum_{\sigma'} \sum_{\mathbf{k}'} \left[\left\langle T_\tau \left[c_{\mathbf{k},\sigma}^\dagger(\tau) c_{\mathbf{k}+\mathbf{q},\sigma}(\tau) c_{\mathbf{k}',\sigma'}^\dagger c_{\mathbf{k}'-\mathbf{q},\sigma'} \right] \right\rangle_0 - \left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle_0 \left\langle c_{\mathbf{k}',\sigma'}^\dagger c_{\mathbf{k}',\sigma'} \right\rangle_0 \delta_{\mathbf{q},0} \right] \quad (5.49)$$

Only the contractions indicated survive. The other possible set of contractions is canceled by the disconnected piece $\left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle_0 \left\langle c_{\mathbf{k}',\sigma'}^\dagger c_{\mathbf{k}',\sigma'} \right\rangle_0$. Using momentum conservation, all that is left is

$$\chi_{nn}^0(\mathbf{q}, iq_n) = -\frac{1}{\mathcal{V}} \int_0^\beta d\tau e^{iq_n\tau} \sum_{\sigma} \sum_{\mathbf{k}} \mathcal{G}_{\sigma}^0(\mathbf{k} + \mathbf{q}, \tau) \mathcal{G}_{\sigma}^0(\mathbf{k}, -\tau) \quad (5.50)$$

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

$$\chi_{nn}^0(\mathbf{q}, iq_n) = -\frac{1}{\mathcal{V}} \sum_{\sigma} \sum_{\mathbf{k}} T \sum_{ik_n} \mathcal{G}_{\sigma}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \mathcal{G}_{\sigma}^0(\mathbf{k}, ik_n) \quad (5.51)$$

where as usual we will do the replacement in the infinite volume limit

$$\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \rightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3} \quad (5.52)$$

Remark 96 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.(5-11) 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.

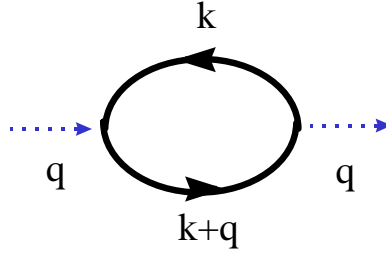


Figure 5-11 Diagram for non-interacting charge susceptibility. Note that the dotted lines just indicate the flow of momentum. No algebraic expression is associated with them.

The sums over Matsubara frequency should be performed first and they are easy to do. The technique is standard. First introduce the notation

$$\boxed{\zeta_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu} \quad (5.53)$$

then use partial fractions

$$T \sum_{ik_n} \mathcal{G}_{\sigma}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \mathcal{G}_{\sigma}^0(\mathbf{k}, ik_n) = T \sum_{ik_n} \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \frac{1}{ik_n - \zeta_{\mathbf{k}}} \quad (5.54)$$

$$\chi_{nn}^0(\mathbf{q}, iq_n) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \left[\frac{1}{ik_n - \zeta_{\mathbf{k}}} - \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \right] \frac{1}{iq_n - \zeta_{\mathbf{k}+\mathbf{q}} + \zeta_{\mathbf{k}}}. \quad (5.55)$$

The factor of two comes from the sum over spins. Before the partial fractions, the terms in the ik_n series decreased like $(ik_n)^{-2}$ so no convergence factor is needed. 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.(4.203) and (4.204), it is clear that as long as we take the same convergence factor for both terms, the result is

$$\chi_{nn}^0(\mathbf{q}, iq_n) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{iq_n + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.56)$$

independently of the choice of convergence factor.

The retarded function is easy to obtain by analytic continuation. It is the so-called Lindhard function

$$\boxed{\chi_{nn}^{0R}(\mathbf{q}, \omega) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}}} \quad (5.57)$$

This form is very close to the Lehman 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 97 *Diagrammatic form of particle-hole excitations:* If we return to the diagram in Fig.(5-11), 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 98 *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 $f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}}) = (1 - f(\zeta_{\mathbf{k}+\mathbf{q}}))f(\zeta_{\mathbf{k}}) - (1 - f(\zeta_{\mathbf{k}}))f(\zeta_{\mathbf{k}+\mathbf{q}})$. 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.

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

$$\begin{aligned} \text{Im } \chi_{nn}^{0R}(\mathbf{q}, \omega) &= 2\pi \int \frac{d^3\mathbf{k}}{(2\pi)^3} [f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})] \delta(\omega + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}) \quad (5.58) \\ &= 2\pi \int \frac{d^3\mathbf{k}}{(2\pi)^3} f(\zeta_{\mathbf{k}}) [\delta(\omega + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}) - \delta(\omega + \zeta_{\mathbf{k}-\mathbf{q}} - \zeta_{\mathbf{k}})]. \end{aligned}$$

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

$$\text{Im } \chi_{nn}^{0R}(\mathbf{q}, \omega) = \frac{1}{2\pi} \int_0^{k_F} k^2 dk \int_{-1}^1 d(\cos\theta) \frac{m}{kq} \left[\delta\left(\frac{\omega - \varepsilon_{\mathbf{q}}}{kq/m} - \cos\theta\right) - \delta\left(\frac{\omega + \varepsilon_{\mathbf{q}}}{kq/m} - \cos\theta\right) \right] \quad (5.59)$$

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 [10]

$$\varepsilon_{\mathbf{k}} = \sum_{i=1}^d \frac{k_i^2}{2m_i} \quad (5.60)$$

$$\begin{aligned} \text{Im } \chi_{nn}^{0R}(\mathbf{q}, \omega) &= \frac{\prod_{i=1}^d (\sqrt{2m_i})}{2^d \pi^{(d-1)/2} \Gamma\left(\frac{d+1}{2}\right) \sqrt{\varepsilon_{\mathbf{q}}}} \times \\ &\left\{ \theta\left(\mu - \frac{(\omega - \varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right) \left[\mu - \frac{(\omega - \varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}} - \theta\left(\mu - \frac{(\omega + \varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right) \left[\mu - \frac{(\omega + \varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}} \right\} \end{aligned}$$

The real part is also calculable [10] but we do not quote it here.

The appearance of this function in low dimension is quite interesting. Figures (5-12)(5-13) and (5-14) 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 $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ on the vertical axis, frequency going from left to right and wave vector 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 will lead to the famous spin-charge separation as we will see in later chapters. 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.[10] By contrast, the three-dimensional function is much smoother, despite a discontinuity in slope at $q = 2k_F$. The region in \mathbf{q} and ω space where there is absorption is referred to as the particle-hole continuum.

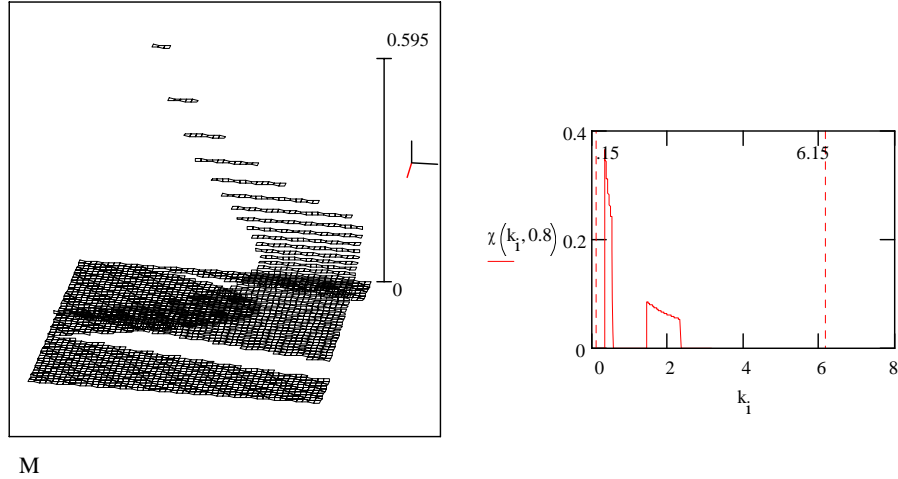
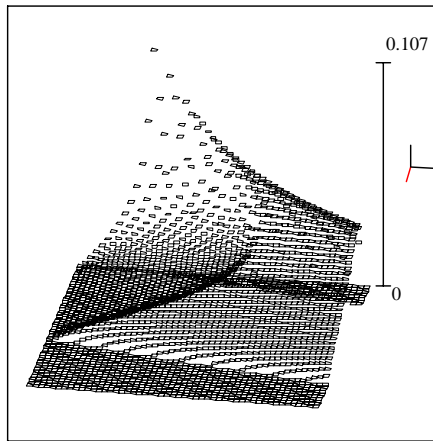


Figure 5-12 Imaginary part of the Lindhard function in $d = 1$ on the vertical axis. Frequency increases from left to right and wave vector from back to front.

To understand the existence of the particle-hole continuum and its shape, it is preferable to return to the original expression Eq.(5.58). In Fig.(5-15) we draw the geometry for the *three-dimensional case*. [11] 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 all wave vectors \mathbf{k} located in the plane

$$\omega - \frac{q^2}{2m} = \frac{kq}{m} \cos \theta \quad (5.61)$$

are allowed. This plane must be inside the left most sphere and outside the right most one or vice versa (not shown). It cannot however be inside both or outside both. That is why when the plane 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 $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$. This occurs when the vectors $\mathbf{k} + \mathbf{q}$ and \mathbf{k} are antiparallel to each other and when \mathbf{k} is on the Fermi



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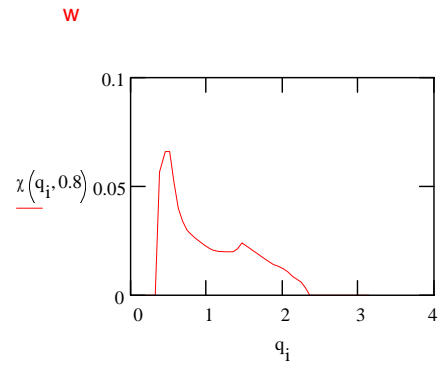
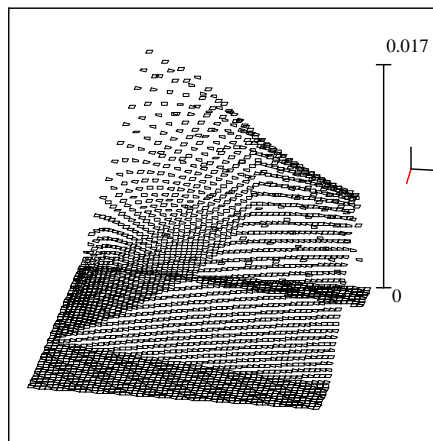


Figure 5-13 Imaginary part of the Lindhard function in $d = 2$. Axes like in the $d = 1$ case.



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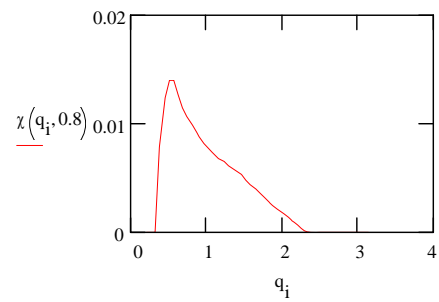


Figure 5-14 Imaginary part of the Lindhard function in $d = 3$. Axes like in the $d = 1$ case.

surface. The corresponding energy is

$$\omega_{change} = \frac{k_F^2}{2m} - \frac{(k_F - q)^2}{2m} = v_F q - \varepsilon_{\mathbf{q}} \quad (5.62)$$

This line, $\omega_{change}(q)$, is shown in Fig.(5-16). Clearly the cases $q < 2k_F$ and $q > 2k_F$ are also different. The figure (5-15) illustrates the case $q < 2k_F$. In the latter case, the maximum value of ω is found by letting $\mathbf{k} + \mathbf{q}$ and \mathbf{k} be parallel to each other while \mathbf{k} sits right on the Fermi surface. This gives

$$\omega_{\max} = \frac{(k_F + q)^2}{2m} - \frac{k_F^2}{2m} \quad (5.63)$$

$$= \varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q < 2k_F \quad (5.64)$$

The minimum allowed value of ω vanishes since both arrows can be right at the Fermi surface in the annulus region.

$$\omega_{\min} = 0 \quad ; \quad q < 2k_F \quad (5.65)$$

For the other case, namely $q > 2k_F$ the maximum allowed value of ω is exactly the same as above, but there is now a minimum value, given by the case where $\mathbf{k} + \mathbf{q}$ and \mathbf{k} are antiparallel and \mathbf{k} is on the Fermi surface

$$\omega_{\min} = \frac{(k_F - q)^2}{2m} - \frac{k_F^2}{2m} = \varepsilon_{\mathbf{q}} - v_F q; \quad q > 2k_F \quad (5.66)$$

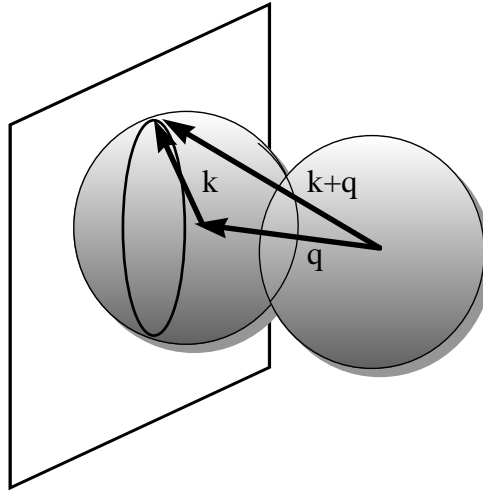


Figure 5-15 Geometry for the integral giving the imaginary part of the $d = 3$ Lindhard function. The wave vectors in the plane satisfy energy conservation as well as the restrictions imposed by the Pauli principle. The plane located symmetrically with respect to the mirror plane of the spheres corresponds to energies of opposite sign.

The region in ω and q space where $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ is non-vanishing, the particle-hole continuum, is illustrated schematically in Fig.(5-16) for positive frequency. Since $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ is odd in frequency, there is a symmetrical region at $\omega < 0$.

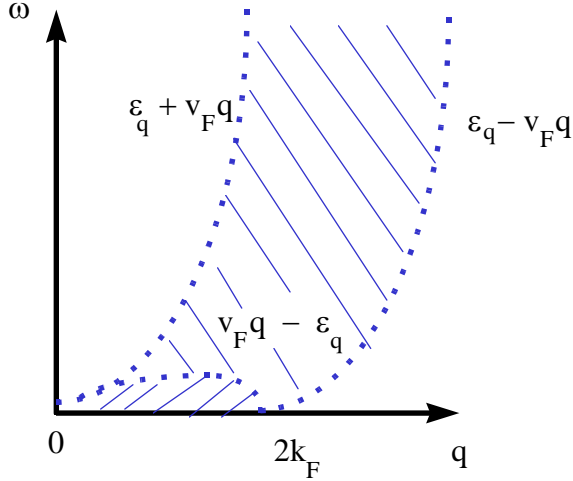


Figure 5-16 Schematic representation of the domain of frequency and wave vector where there is a particle-hole continuum.

5.2.3 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 $1/(ma_0^2)$ and the value of a_0 itself is obtained by equating this to the potential energy

$$\frac{1}{ma_0^2} = \frac{e^2}{a_0} \quad (5.67)$$

giving us for the Bohr radius, in standard units,

$$a_0 = \frac{\hbar^2}{me^2} = 0.529 \times 10^{-10} m \sim 0.5 \text{ \AA} \quad (5.68)$$

It is standard practice to define the dimensionless parameter r_s by setting the density of electrons n_0 equal to $1/(\text{volume of the sphere of radius } r_s a_0 \text{ occupied by a single electron})$. In other words, we have

$$n_0 \equiv \frac{1}{\frac{4\pi}{3} r_s^3 a_0^3} \quad (5.69)$$

where

$$n_0 = \frac{k_F^3}{3\pi^2} \quad (5.70)$$

is the density of electrons. Another way to write r_s is then

$$r_s \equiv \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{k_F a_0} \quad (5.71)$$

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

$$\frac{\text{Potential}}{\text{Kinetic}} \sim \frac{e^2 k_F}{k_F^2/2m} \sim \frac{me^2}{k_F} \sim \frac{1}{k_F a_0} \sim \left(\frac{1}{n_0 a_0^3} \right)^{1/3} \sim r_s \quad (5.72)$$

These estimates are obtained as follows. The average momentum exchanged in interactions is of order k_F so that $e^2/r \sim e^2 k_F$ 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.

5.2.4 Elementary approaches to screening and plasma oscillations

Thomas-Fermi screening

The elementary theory of screening is the Thomas-Fermi theory.[9] 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 impurity charge ρ_i

$$-\nabla^2 \phi(\mathbf{r}) = 4\pi [\rho_i(\mathbf{r}) + \delta\rho(\mathbf{r})] \quad (5.73)$$

The quantity $\delta\rho(\mathbf{r})$ is the change in charge density of the background produced by the charged impurity

$$\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0 = -e [n(\mathbf{r}) - n_0] \quad (5.74)$$

We need to find $n(\mathbf{r})$. 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

$$\frac{n(\mathbf{r})}{n_0} = \frac{k_F^3(\mathbf{r})}{k_F^3} \quad (5.75)$$

and electrochemical equilibrium

$$\frac{k_F^2(\mathbf{r})}{2m} + (-e\phi(\mathbf{r})) = E_F = \frac{k_F^2}{2m} \quad (5.76)$$

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

$$\frac{n(\mathbf{r})}{n_0} = \frac{k_F^3(\mathbf{r})}{k_F^3} = \left[\frac{k_F^2(\mathbf{r})/2m}{k_F^2/2m} \right]^{3/2} = \left[1 - \frac{(-e\phi(\mathbf{r}))}{E_F} \right]^{3/2} \quad (5.77)$$

Substituting this back into Poisson's equation, we have a closed equation for potential

$$\boxed{-\nabla^2 \phi(\mathbf{r}) = 4\pi \rho_i(\mathbf{r}) - 4\pi n_0 e \left[\left(1 - \frac{(-e\phi(\mathbf{r}))}{E_F} \right)^{3/2} - 1 \right]} \quad (5.78)$$

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,

$$\frac{n(\mathbf{r})}{n_0} \approx \left[1 - \frac{3(-e\phi(\mathbf{r}))}{2E_F} \right] \quad (5.79)$$

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.(5.78) becomes

$$-\nabla^2\phi(\mathbf{r}) = 4\pi\rho_i(\mathbf{r}) + \frac{6\pi n_0 e}{E_F}(-e\phi(\mathbf{r})) \quad (5.80)$$

We could have arrived directly at this equation by posing

$$-\nabla^2\phi(\mathbf{r}) = 4\pi \left[\rho_i(\mathbf{r}) - e \frac{\partial n}{\partial \mu} (+e\phi(\mathbf{r})) \right] \quad (5.81)$$

We now proceed to solve this equation, but first let us define

$$\boxed{q_{TF}^2 = \frac{6\pi n_0 e^2}{E_F} = 4\pi e^2 \frac{\partial n}{\partial \mu}} \quad (5.82)$$

Then we can write

$$(-\nabla^2 + q_{TF}^2)\phi(\mathbf{r}) = 4\pi\rho_i(\mathbf{r}) \quad (5.83)$$

whose solution, by Fourier transforms, is

$$\boxed{\phi(\mathbf{q}) = \frac{4\pi\rho_i(\mathbf{q})}{q^2 + q_{TF}^2}} \quad (5.84)$$

The Thomas-Fermi dielectric constant follows immediately since the definition,

$$\phi(\mathbf{q}) = \frac{1}{\varepsilon^L(\mathbf{q},0)} \frac{4\pi\rho_i(\mathbf{q})}{q^2} \quad (5.85)$$

immediately yields, the value of the zero-frequency dielectric constant

$$\boxed{\varepsilon^L(\mathbf{q},0) = \frac{q^2 + q_{TF}^2}{q^2} = 1 + \frac{q_{TF}^2}{q^2}} \quad (5.86)$$

Let us pause to give a physical interpretation of this result. At small distances (large q) the charge is unscreened since $\varepsilon_L \rightarrow 1$. On the contrary, at large distance (small q) the screening 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.(5.69) or (5.71)

$$\lambda^2 \equiv q_{TF}^{-2} = \frac{E_F}{6\pi n_0 e^2} = \frac{k_F^2/2m}{6\pi n_0 e^2} = \frac{k_F^2 a_0}{12\pi n_0} \quad (5.87)$$

$$= \frac{k_F^2 a_0^4}{12\pi} \left(\frac{4\pi}{3} r_s^3 \right) = a_0^2 \left(\frac{1}{9} \left(\frac{9\pi}{4} \right)^{2/3} \right) r_s \quad (5.88)$$

Roughly speaking then, for $r_s \ll 1$ we have that the screening length

$$\boxed{\lambda \sim \left(a_0 \sqrt{r_s} = \frac{a_0 r_s}{\sqrt{r_s}} \right)} \quad (5.89)$$

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. It makes less sense to think that the free electron Hamiltonian is a good perturbative starting point. Electrons start to localize. For sodium, $r_s \sim 4$ while for aluminum, $r_s \sim 2$ but still, these should be considered good metals.

Remark 99 *Two dimensional case: As an exercise, note that if the material is two dimensional, then the density is confined to a surface so that $n_0 \rightarrow n_s \delta(z)$ and $\rho \rightarrow \rho_s \delta(z)$ where n_s and ρ_s are surface density and charge surface density. Then, Eq.(5.81) in Fourier space becomes*

$$(q_z^2 + q_{||}^2) \phi(\mathbf{q}) = 4\pi \left[\rho_s(\mathbf{q}_{||}) - e \frac{\partial n_s}{\partial \mu} (e\phi(\mathbf{q}_{||}, z=0)) \right] \quad (5.90)$$

Dividing by $q_z^2 + q_{||}^2$ we obtain

$$\begin{aligned} \int \phi(\mathbf{q}) \frac{dq_z}{2\pi} &= \phi(\mathbf{q}_{||}, z=0) \\ &= 4\pi \left[\rho_s(\mathbf{q}_{||}) - e \frac{\partial n_s}{\partial \mu} (e\phi(\mathbf{q}_{||}, z=0)) \right] \int \frac{1}{q_z^2 + q_{||}^2} \frac{dq_z}{2\pi}. \end{aligned} \quad (5.91)$$

The last integral is equal to $(2q_{||})^{-1}$ so that

$$\left[1 + \frac{2\pi e^2}{q_{||}} \frac{\partial n_s}{\partial \mu} \right] \phi(\mathbf{q}_{||}, z=0) = \frac{2\pi \rho_s(\mathbf{q}_{||})}{q_{||}} \quad (5.92)$$

and

$$\phi(\mathbf{q}_{||}, z=0) = \frac{2\pi \rho_s(\mathbf{q}_{||})}{\varepsilon_L(\mathbf{q}_{||}) q_{||}} = \frac{2\pi \rho_s(\mathbf{q}_{||})}{q_{||} + 2\pi e^2 \frac{\partial n_s}{\partial \mu}} \quad (5.93)$$

$$\varepsilon_L(\mathbf{q}_{||}) = 1 + \frac{2\pi e^2}{q_{||}} \frac{\partial n_s}{\partial \mu}. \quad (5.94)$$

This result was obtained by Stern in *Phys. Rev. Lett.* 1967.

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

$$\mathbf{j} = -en_0 \mathbf{v} \quad (5.95)$$

Taking the time derivative and using Newton's equations,

$$\frac{\partial \mathbf{j}}{\partial t} = -en_0 \frac{\partial \mathbf{v}}{\partial t} = -\frac{en_0}{m} (-e\mathbf{E}) \quad (5.96)$$

we are in a position where one more time derivative

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = \frac{n_0 e^2}{m} \frac{\partial \mathbf{E}}{\partial t} \quad (5.97)$$

and an appeal to the *longitudinal* part of Maxwell's fourth equation

$$0 = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \quad (5.98)$$

should give us the desired result, namely

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = -\frac{4\pi n_0 e^2}{m} \mathbf{j} \quad (5.99)$$

This equation has an oscillatory solution at a frequency ω_p

$$\boxed{\omega_p^2 \equiv \frac{4\pi n_0 e^2}{m}} \quad (5.100)$$

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

$$\boxed{\lim_{\omega \rightarrow \omega_p} \epsilon^L(\mathbf{q} = \mathbf{0}, \omega) = a(\omega - \omega_p)} \quad (5.101)$$

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.

An alternate derivation that is more easily extended to films or wires takes the divergence of Eq.(5.96) and then uses current conservation with Maxwell's first equation to obtain

$$\frac{\partial \nabla \cdot \mathbf{j}}{\partial t} = -\frac{en_0}{m} (-e \nabla \cdot \mathbf{E}) \quad (5.102)$$

$$-\frac{\partial^2 \rho}{\partial t^2} = \frac{e^2 n_0}{m} 4\pi \rho \quad (5.103)$$

which immediately leads to the desired expression for the plasma frequency. Note that writing $\nabla \cdot \mathbf{E} = -\nabla^2 \phi = 4\pi \rho$ 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 100 *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,*

$$\frac{\partial \rho_s}{\partial t} + \nabla_s \cdot \mathbf{j}_s = 0. \quad (5.104)$$

Taking the two-dimensional divergence of Newton's equation Eq.(5.96) on both sides, we obtain

$$\frac{\partial \nabla_s \cdot \mathbf{j}_s}{\partial t} \delta(z) = \frac{e^2 n_s}{m} \delta(z) \nabla_s \cdot \mathbf{E} \quad (5.105)$$

so that Fourier transforming and using charge conservation, we obtain

$$-\frac{\partial^2 \rho_s(q_{||})}{\partial t^2} = \frac{e^2 n_s}{m} i\mathbf{q}_{||} \cdot \mathbf{E}(\mathbf{q}_{||}, z=0). \quad (5.106)$$

We can express the electric field in terms of the surface density to close the system of equations,

$$\mathbf{E}(\mathbf{q}_{||}, z=0) = -i\mathbf{q}_{||} \phi(\mathbf{q}_{||}, z=0) = -i\mathbf{q}_{||} \frac{2\pi \rho_s}{q_{||}} \quad (5.107)$$

where we used the unscreened Poisson equation for a film (two-dimensional material). This leads to

$$\frac{\partial^2 \rho_s(q_{||})}{\partial t^2} = -\frac{e^2 n_s}{m} q_{||} 2\pi \rho_s \quad (5.108)$$

which means that the plasma frequency is

$$\omega_p^2 = \frac{2\pi e^2 n_s}{m} q_{||} \quad (5.109)$$

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.

5.2.5 Density response in the presence of interactions

We are now ready to start our diagrammatic analysis. Fig.(5-17) 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 $4\pi/q^2$ that diverges at small wave vectors. On the other hand, the contribution from the other diagram is proportional to

$$\begin{aligned} & -2 \int \frac{d^3 k}{(2\pi)^3} T \sum_{ik_n} \int \frac{d^3 k'}{(2\pi)^3} T \sum_{ik'_n} \mathcal{G}_\sigma^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \mathcal{G}_\sigma^0(\mathbf{k}, ik_n) \times \\ & \frac{4\pi}{|\mathbf{k} - \mathbf{k}'|^2} \mathcal{G}_\sigma^0(\mathbf{k}' + \mathbf{q}, ik'_n + iq_n) \mathcal{G}_\sigma^0(\mathbf{k}', ik'_n) \end{aligned} \quad (5.110)$$

which is a convergent integral with no singularity at $q = 0$.

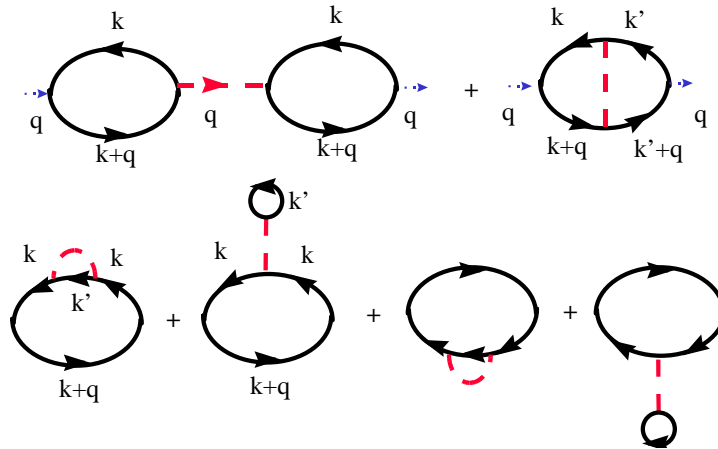


Figure 5-17 Charge susceptibility diagrams to first order in the interaction

Remark 101 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 $q \rightarrow 0$, it has additional pathologies. Indeed, it has double poles at the particle-hole excitations of the non-interacting problem while the Lehman 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 illustrated in Fig.(5-18). 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.

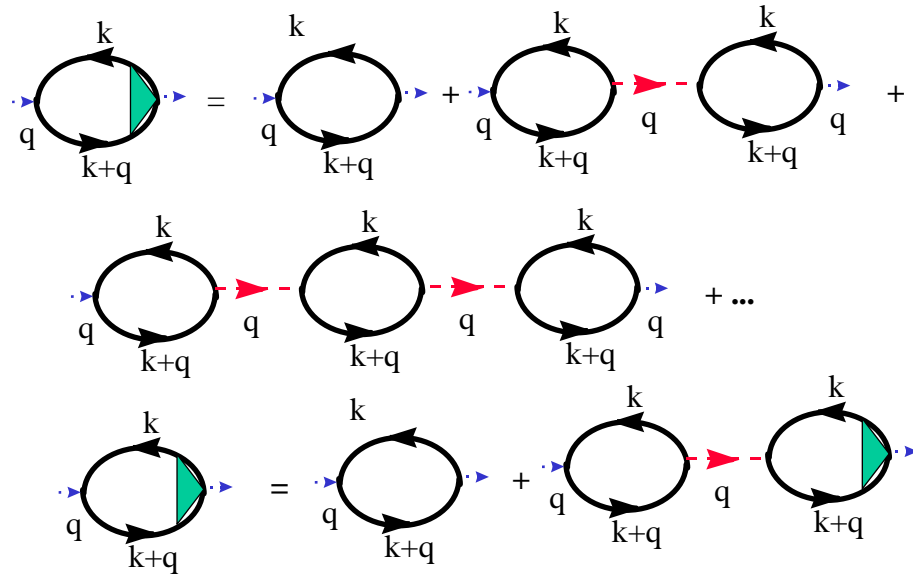


Figure 5-18 Bubble diagrams. Random phase approximation.

From our calculation of the susceptibility for non-interacting electrons we know that Feynman's rules apply for the diagrams on Fig.(5-18). Each bubble is associated with a factor $\chi_{nm}^0(\mathbf{q}, iq_n)$, 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 $-V_{\mathbf{q}} = -4\pi e^2/q^2$, 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.(5-18) is

easy to do since it is just a geometric series. The result is.

$$\boxed{\chi_{nn}(\mathbf{q}, iq_n) = \frac{\chi_{nn}^0(\mathbf{q}, iq_n)}{1 + V_{\mathbf{q}} \chi_{nn}^0(\mathbf{q}, iq_n)}} \quad ; \quad V_{\mathbf{q}} = \frac{4\pi e^2}{q^2} \quad (5.111)$$

The corresponding result for the dielectric constant Eq.(5.41) is

$$\boxed{\frac{1}{\epsilon^L(\mathbf{q}, \omega)} = 1 - \frac{4\pi e^2}{q^2} \chi_{nn}^R(\mathbf{q}, \omega) = \frac{1}{1 + V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q}, \omega)}} \quad (5.112)$$

Remark 102 *Irreducible polarization: It is customary to call $-\chi_{nn}^{0R}(\mathbf{q}, \omega)$ the first order irreducible polarization $\prod^{(1)R}(\mathbf{q}, \omega)$ (Irreducible here means that the diagrams can be connected at each end to an interaction but cannot be cut in two by cutting an interaction line).*

Using our previous results for the susceptibility of non-interacting particles, the explicit expression for the real and imaginary parts of the dielectric function in three dimensions at zero temperature is, for positive frequencies

$$\text{Re} [\epsilon^L(\mathbf{q}, \omega)] \equiv \epsilon_1^L(\mathbf{q}, \omega) \quad (5.113)$$

$$= 1 + \frac{q_{TF}^2}{q^2} \left\{ \frac{1}{2} + \frac{k_F}{4q} \left[\left(1 - \frac{(\omega - \varepsilon_q)^2}{q^2 v_F^2} \right) \ln \left| \frac{\omega - v_F q - \varepsilon_q}{\omega + v_F q - \varepsilon_q} \right| \right. \right. \\ \left. \left. + \left(1 - \frac{(\omega + \varepsilon_q)^2}{q^2 v_F^2} \right) \ln \left| \frac{\omega + v_F q + \varepsilon_q}{\omega - v_F q + \varepsilon_q} \right| \right] \right\} \quad (5.114)$$

$$\text{Im} [\epsilon^L(\mathbf{q}, \omega)] \equiv \epsilon_2^L(\mathbf{q}, \omega) \quad (5.115)$$

$$= \left\{ \begin{array}{ll} \frac{\pi}{2} \frac{\omega}{v_F q} \frac{q_{TF}^2}{q^2} \quad ; & \omega \leq v_F q - \varepsilon_q \\ \frac{\pi k_F}{4q} \frac{q_{TF}^2}{q^2} \left(1 - \frac{(\omega - \varepsilon_q)^2}{q^2 v_F^2} \right) ; & v_F q - \varepsilon_q \leq \omega \leq \varepsilon_q + v_F q \\ 0 \quad ; & \omega \geq \varepsilon_q + v_F q \end{array} \right\} \quad q < 2k_F$$

$$\left\{ \begin{array}{ll} \frac{\pi k_F}{4q} \frac{q_{TF}^2}{q^2} \left(1 - \frac{(\omega - \varepsilon_q)^2}{q^2 v_F^2} \right) ; & \varepsilon_q - v_F q \leq \omega \leq \varepsilon_q + v_F q \end{array} \right\} \quad q > 2k_F$$

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.

Particle-hole continuum

Let us first think of a finite system with M discrete poles to see that these have been shifted. The spectral representation tells us, using the fact that, $\chi_{nn}''(\mathbf{q}, \omega')$ is odd

$$\begin{aligned} \chi_{nn}^{0R}(\mathbf{q}, \omega) &= \int \frac{d\omega'}{\pi} \frac{\chi_{nn}^{0''}(\mathbf{q}, \omega')}{\omega' - \omega - i\eta} = \int \frac{d\omega'}{\pi} \frac{\omega' \chi_{nn}^{0''}(\mathbf{q}, \omega')}{(\omega')^2 - (\omega + i\eta)^2} \\ &= \sum_{i=1}^{M/2} \frac{A_i}{u_i^2 - (\omega + i\eta)^2} = \frac{B \prod_{i=1}^{(M/2)-1} ((\omega + i\eta)^2 - v_i^2)}{\prod_{i=1}^{M/2} (u_i^2 - (\omega + i\eta)^2)} \end{aligned} \quad (5.116)$$

where $A_i > 0$ and u_i are respectively the residue and the location of each pole. 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.(5.111) for the RPA susceptibility we find,

$$\chi_{nn}^R(\mathbf{q}, \omega) = \frac{B \prod_{i=1}^{(M/2)-1} \left((\omega + i\eta)^2 - v_i^2 \right)}{\prod_{i=1}^{M/2} \left(u_i^2 - (\omega + i\eta)^2 \right) + V_{\mathbf{q}} B \prod_{i=1}^{(M/2)-1} \left((\omega + i\eta)^2 - v_i^2 \right)} \quad (5.117)$$

The denominator can be rewritten as a polynomial of the same order as the non-interacting susceptibility, namely of order $M/2$ 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.(5.111) and simple algebra

$$\text{Im} \left(\frac{x + iy}{1 + x + iy} \right) = \frac{y}{(1 + x)^2 + y^2} \quad (5.118)$$

we find the following result for the imaginary part

$$\text{Im} \chi_{nn}^R(\mathbf{q}, \omega) = \frac{\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)}{(1 + V_{\mathbf{q}} \text{Re} \chi_{nn}^{0R}(\mathbf{q}, \omega))^2 + (V_{\mathbf{q}} \text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega))^2} \quad (5.119)$$

In a discrete system $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ 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

$$\frac{1}{V_{\mathbf{q}}} + \text{Re} \chi_{nn}^{0R}(\mathbf{q}, \omega) = \frac{1}{V_{\mathbf{q}}} + \sum_{i=1}^{M/2} \frac{A_i}{u_i^2 - \omega^2} = 0 \quad (5.120)$$

The solution of this equation may in principle be found graphically as illustrated in Fig.(5-19). We have taken the simple case $M = 6$ for clarity. In reality, $M \rightarrow \infty$ and the separation between each discrete pole is inversely proportional to a power of the size of the system $1/\mathcal{V}$. The poles of the non-interacting susceptibility are right on the vertical asymptotes while those of the interacting system are at 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. In other words, 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 103 *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(5-19), there are six non-interacting poles and six interacting ones.*

Since $\text{Im} (\epsilon^L(\mathbf{q}, \omega))^{-1} = 1 + V_{\mathbf{q}} \text{Im} \chi_{nn}^R(\mathbf{q}, \omega)$ the zeros of the dielectric constant are at the same location as the poles of $\chi_{nn}^R(\mathbf{q}, \omega)$ and, from what we just said, these poles are located basically in the same (ω, \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.(5-20), that generalizes Fig.(5-16)

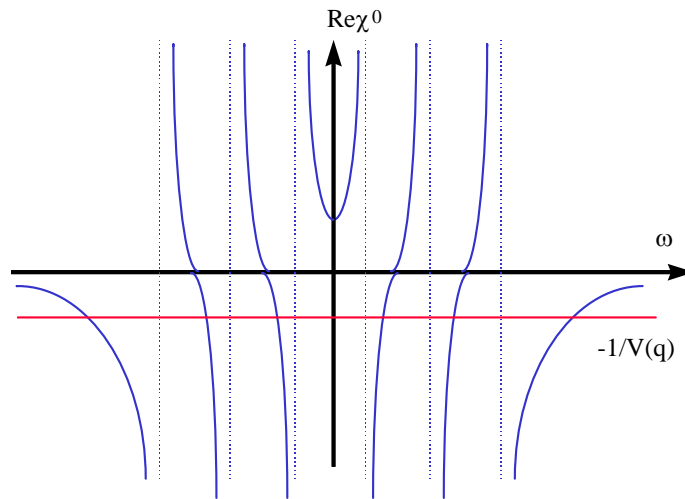


Figure 5-19 Graphical solution for the poles of the charge susceptibility in the interacting system.

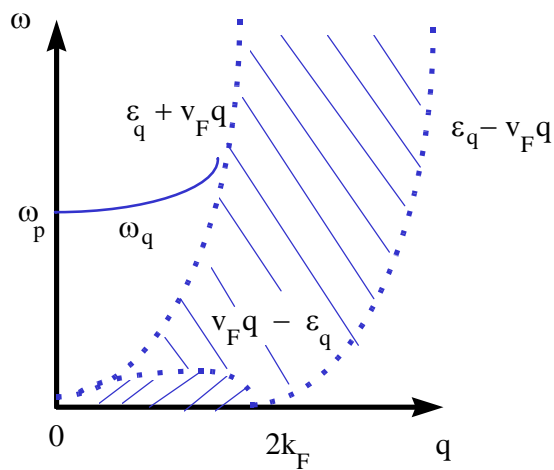


Figure 5-20 Schematic representation of the domain of frequency and wave vector where there are poles in the charge susceptibility, or zeros in the longitudinal dielectric function. In addition to the particle-hole continuum, there is a plasma pole.

Screening

At zero frequency, namely for a static charge perturbation, the imaginary part of the dielectric constant vanishes, as shown by Eq.(5.115), while the real part Eq.(5.113) becomes

$$\varepsilon_1^L(\mathbf{q}, 0) = 1 + \frac{q_{TF}^2}{q^2} \left[\frac{1}{2} + \frac{k_F}{2q} \left(1 - \frac{q^2}{(2k_F)^2} \right) \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right] \quad (5.121)$$

In the long wave length limit, we recover our Thomas Fermi result Eq.(5.86). This limit can also be obtained directly by approximating the integral defining Lindhard function Eq.(5.57) that enters the RPA dielectric function Eqs.(5.112)

$$\lim_{\mathbf{q} \rightarrow 0} \varepsilon_1^L(\mathbf{q}, 0) = \lim_{\mathbf{q} \rightarrow 0} \left[1 - 2V_{\mathbf{q}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \right] \quad (5.122)$$

$$= \left[1 - 2V_{\mathbf{q}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\partial f(\zeta_{\mathbf{k}})}{\partial \zeta_{\mathbf{k}}} \right] \quad (5.123)$$

$$= 1 + V_{\mathbf{q}} \frac{\partial}{\partial \mu} \left[2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} f(\zeta_{\mathbf{k}}) \right] \quad (5.124)$$

$$= 1 + \frac{4\pi e^2}{q^2} \frac{\partial n}{\partial \mu} \quad (5.125)$$

$$= 1 + \frac{q_{TF}^2}{q^2} \quad (5.126)$$

The definition of q_{TF} is in Eq.(5.82). The corresponding potential

$$V_{eff}(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{q^2 + q_{TF}^2} e^{i\mathbf{q}\cdot\mathbf{r}} \propto \frac{4\pi e^2}{r} e^{-r q_{TF}} \quad (5.127)$$

is the screened Coulomb interaction.

Remark 104 The expression $\varepsilon_1^L(\mathbf{q}, 0) = (1 + V_{\mathbf{q}}\chi_{nn}^0(\mathbf{q}, 0))$ would be replaced by $\varepsilon_1^L(\mathbf{q}, 0) = (1 - V_{\mathbf{q}}\Pi_{nn}^{R(1)}(\mathbf{q}, 0))$ in the general case, with $-\Pi_{nn}^{R(1)}(\mathbf{q}, 0)$ the irreducible polarization. That quantity 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.(5.125) would be different from the non-interacting result. This is relevant in effective models such as the Hubbard model.

Friedel oscillations

If instead of using the limiting Thomas-Fermi form for small wave vectors one does a more careful evaluation[12] of the Fourier transform of $\varepsilon_1(\mathbf{q}, 0)$ Eq.(5.121), one finds

$$\lim_{r \rightarrow \infty} V_{eff}(r) \propto \frac{\cos(2k_F r)}{r^3} \quad (5.128)$$

These oscillations are the real-space manifestation of the discontinuity in slope of the dielectric function that appears in the logarithm at $q = 2k_F$. These are so-called Friedel oscillations. They manifest themselves 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 $k_B T$ equal to $v_F \hbar \Delta k$ and identifying the spread in wave vector around k_F as $\Delta k \sim \xi_{th}^{-1}$.

Plasmons

We have already suggested in Fig.(5-19) that at small wave numbers, a large frequency pole far from the particle-hole continuum appears. Let us look at this parameter range. Taking $v_F q/\omega$ as a small parameter, the imaginary part of the dielectric constant Eq.(5.115) 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.(5.112) and (5.57). Indeed, when the frequency is large and outside the particle-hole continuum, we can write

$$\lim_{\mathbf{q} \rightarrow 0} \lim_{\omega \rightarrow v_F q - \varepsilon_q} \varepsilon_1^L(\mathbf{q}, \omega) = \lim_{\omega \gg v_F q - \varepsilon_q} \left[1 - 2V_{\mathbf{q}} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \right] \quad (5.129)$$

$$= \lim_{\mathbf{q} \rightarrow 0} \left[1 + 2V_{\mathbf{q}} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2} (\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}) \right] \quad (5.130)$$

$$= 1 + 2V_{\mathbf{q}} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2} (\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}) \quad (5.131)$$

$$= 1 + \frac{4V_{\mathbf{q}}}{\omega^2} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} f(\zeta_{\mathbf{k}}) (\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}) \quad (5.132)$$

To obtain the last expression we did the change of variables $\mathbf{k} \rightarrow -\mathbf{k} - \mathbf{q}$ 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

$$\lim_{\mathbf{q} \rightarrow 0} \lim_{\omega \gg v_F q - \varepsilon_q} \varepsilon_1^L(\mathbf{q}, \omega) = 1 - \frac{2V_{\mathbf{q}} n}{\omega^2} \frac{q^2}{2m} = 1 - \frac{\omega_p^2}{\omega^2} \quad (5.133)$$

with the value of ω_p^2 defined in Eq.(5.100). One can continue the above approach to higher order or proceed directly with a tedious Taylor series expansion of the real part Eq.(5.113) in powers of $v_F q/\omega$ to obtain

$$\varepsilon_1^L(\mathbf{q} \rightarrow 0, \omega) = 1 - \frac{\omega_p^2}{\omega^2} - \frac{3}{5} \frac{\omega_p^2}{\omega^2} \frac{(v_F q)^2}{\omega^2} + \dots \quad (5.134)$$

Several physical remarks follow directly from this result

- Even at long wave lengths ($q \rightarrow 0$), the interaction becomes unscreened at sufficiently high frequency. More specifically,

$$\varepsilon_1^L(\mathbf{q} \rightarrow 0, \omega \gg \omega_p) \rightarrow 1 \quad (5.135)$$

- The collective plasma oscillation that we expected does show up. Indeed, $\varepsilon_1(\mathbf{q} \rightarrow 0, \omega) = 0$ when

$$0 = \omega^2 - \omega_p^2 - \frac{3}{5} \frac{\omega_p^2}{\omega^2} (v_F q)^2 + \dots \quad (5.136)$$

$$\omega^2 \approx \omega_p^2 + \frac{3}{5} (v_F q)^2 + \dots \quad (5.137)$$

Letting this solution be called ω_q we have in the vicinity of this solution $\omega \approx \omega_q$

$$\varepsilon_1^L(\mathbf{q} \rightarrow 0, \omega) \approx 1 - \frac{\omega_q^2}{\omega^2} \approx \frac{2}{\omega_q} (\omega - \omega_q) \quad (5.138)$$

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.(5.101) has the value $a = 2/\omega_q$.

Fig.(5-21) 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 $\varepsilon_1(\mathbf{q}, \infty) \rightarrow 1$ but the zero crossing is illustrated by the maximum in $\text{Im}(1/\varepsilon)$. There is another zero crossing of ε_1 but it occurs in the region where ε_2 is large. Hence this is an overdamped mode.

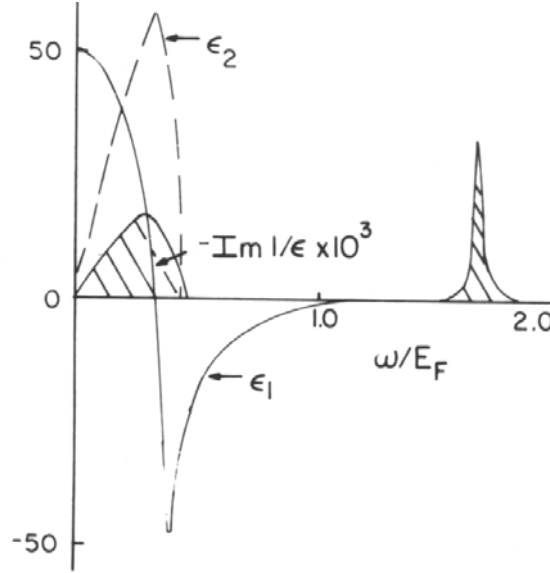


Figure 5-21 Real and imaginary parts of the dielectric constant and $\text{Im}(1/\varepsilon)$ as a function of frequency, calculated for $r_s = 3$ and $q = 0.2k_F$. Shaded plots correspond to $\text{Im}(1/\varepsilon)$. Taken from Mahan *op. cit.* p.430

f -sum rule

We have not checked yet whether the f -sum rule is satisfied. Let us first recall that it takes the form,

$$2 \int_0^\infty \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q}, \omega) = \frac{nq^2}{m}. \quad (5.139)$$

Using our relation between dielectric constant and density fluctuations Eq.(5.41) we obtain the corresponding sum rule for the longitudinal dielectric constant

$$\int_0^\infty \frac{d\omega}{2\pi} \omega \text{Im} \left[\frac{1}{\varepsilon^L(\mathbf{q} \rightarrow 0, \omega)} \right] = -\frac{4\pi ne^2}{4m} = -\frac{\omega_p^2}{4} \quad (5.140)$$

Let us obtain the plasmon contribution to this sum rule by using the approximate form Eq.(5.138)

$$\int_0^\infty \frac{d\omega}{2\pi} \omega \operatorname{Im} \left[\frac{1}{\frac{2}{\omega_q} (\omega - \omega_q) + i\eta} \right] = -\pi \int_0^\infty \frac{d\omega}{2\pi} \omega \left| \frac{\omega_q}{2} \right| \delta(\omega - \omega_q) \quad (5.141)$$

$$= -\frac{\omega_q^2}{4} \quad (5.142)$$

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

$$-\frac{\omega_p^2}{4} + \frac{\omega_q^2}{4} = \frac{3}{20} (v_F q)^2 \quad (5.143)$$

as necessary to satisfy the f -sum rule.

Remark 105 *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. We will discuss this problem in more details later.*

5.3 More formal matters: Consistency relations between single-particle self-energy, collective modes, potential energy and free energy

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.

5.3.1 Consistency between self-energy and density fluctuations

We start from the equations of motion for the Green's function. We need first those for the field operators.

$$\frac{\partial \psi(1)}{\partial \tau_1} = -[\psi(1), K] \quad (5.144)$$

Using $[A, BC] = \{A, B\}C - B\{A, C\}$ and Eq.(5.1) for K we have

$$\begin{aligned} \frac{\partial \psi_{\sigma_1}(\mathbf{x}_1, \tau_1)}{\partial \tau_1} &= \frac{\nabla_1^2}{2m} \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) + \mu \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \\ &\quad - \sum_{\sigma_{1'}} \int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \psi_{\sigma_{1'}}^\dagger(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \end{aligned} \quad (5.145)$$

Remark 106 *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*

$$+n_0 \left[\int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \right] \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \quad (5.146)$$

The $\mathbf{q} = \mathbf{0}$ contribution of the potential in the above equation of motion gives on the other hand a contribution

$$- \left[\int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \right] \left[\frac{1}{\mathcal{V}} \int d\mathbf{x}_{1'} \sum_{\sigma_{1'}} \psi_{\sigma_{1'}}^\dagger(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \right] \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \quad (5.147)$$

While the quantity in bracket is an operator and not a number, its deviations from n_0 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.(5.8) the above result can be written in the shorthand notation

$$\frac{\partial \psi(1)}{\partial \tau_1} = \frac{\nabla_1^2}{2m} \psi(1) + \mu \psi(1) - \int_{1'} \psi^\dagger(1') V(1-1') \psi(1') \psi(1) \quad (5.148)$$

From this, we can easily find the equation of motion for the Green's function

$$\mathcal{G}(1, 2) = - \langle T_\tau [\psi(1) \psi^\dagger(2)] \rangle \quad (5.149)$$

namely,

$$\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu \right) \mathcal{G}(1, 2) = -\delta(1-2) + \left\langle T_\tau \left[\int_{1'} \psi^\dagger(1') V(1-1') \psi(1') \psi(1) \psi^\dagger(2) \right] \right\rangle \quad (5.150)$$

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

$$\mathcal{G}_0^{-1} \mathcal{G} = 1 + \Sigma \mathcal{G} \quad (5.151)$$

we have that

$$\boxed{\int_{1''} \Sigma(1, 1'') \mathcal{G}(1'', 2) = - \left\langle T_\tau \left[\int_{1'} \psi^\dagger(1') V(1'-1) \psi(1') \psi(1) \psi^\dagger(2) \right] \right\rangle} \quad (5.152)$$

which, in all generality, can be taken as a *definition* of the self-energy.

In the limit $2 \rightarrow 1^+$ where

$$1^+ \equiv (\mathbf{x}_1, \tau_1 + 0^+; \sigma_1) \quad (5.153)$$

the term on the right-hand side is

$$\left\langle T_\tau \left[\int_{1'} \psi^\dagger(1^+) \psi^\dagger(1') V(1' - 1) \psi(1') \psi(1) \right] \right\rangle$$

Note that we have placed $\psi^\dagger(2) \rightarrow \psi^\dagger(1^+)$ to the far left of the three fermion operators $\psi^\dagger(1') \psi(1') \psi(1)$ 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

$$2 \langle V \rangle = \sum_{\sigma_1} \int d^3 \mathbf{x}_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger(1^+) \psi^\dagger(1') V(1' - 1) \psi(1') \psi(1) \right] \right\rangle \quad (5.154)$$

we directly get from Eq.(5.152) above a relation between self-energy and potential energy

$$\sum_{\sigma_1} \int d^3 \mathbf{x}_1 \int_{1'} \Sigma(1, 1') \mathcal{G}(1', 1^+) = 2 \langle V \rangle \quad (5.155)$$

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

$$\boxed{\int_1 \int_{1'} \Sigma(1, 1') \mathcal{G}(1', 1^+) = 2 \langle V \rangle \beta = \int_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger(1^+) \psi^\dagger(1') V(1' - 1) \psi(1') \psi(1) \right] \right\rangle} \quad (5.156)$$

Remark 107 *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

$$\begin{aligned} 2 \langle V \rangle \beta &= \int_{1'} \int_1 \left\langle \psi^\dagger(1^+) \psi^\dagger(1') V(1' - 1) \psi(1') \psi(1) \right\rangle \quad (5.157) \\ &= -\beta \sum_{\sigma_1, \sigma_{1'}} \int d^3 \mathbf{x}_{1'} \int d^3 \mathbf{x}_1 \left\langle \psi_{\sigma_{1'}}^\dagger(\mathbf{x}_{1'}) v(\mathbf{x}_{1'} - \mathbf{x}_1) \psi_{\sigma_1}(\mathbf{x}_1) \right\rangle \delta_{\sigma_1, \sigma_{1'}} \delta(\mathbf{x}_{1'} - \mathbf{x}_1) \\ &\quad + \beta \sum_{\sigma_1, \sigma_{1'}} \int d^3 \mathbf{x}_{1'} \int d^3 \mathbf{x}_1 \left\langle \psi_{\sigma_{1'}}^\dagger(\mathbf{x}_{1'}) \psi_{\sigma_{1'}}(\mathbf{x}_{1'}) v(\mathbf{x}_{1'} - \mathbf{x}_1) \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \psi_{\sigma_1}(\mathbf{x}_1) \right\rangle \\ &= -n_0 \mathcal{V} \beta v(0) + \beta \int d^3 \mathbf{x}_{1'} \int d^3 \mathbf{x}_1 \langle n(\mathbf{x}_{1'}) v(\mathbf{x}_{1'} - \mathbf{x}_1) n(\mathbf{x}_1) \rangle \quad (5.158) \end{aligned}$$

where in the last equation we have used

$$\int d^3 \mathbf{x}_1 \sum_{\sigma_1} \left\langle \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \psi_{\sigma_1}(\mathbf{x}_1) \right\rangle = N = n_0 \mathcal{V} \quad (5.159)$$

Going to Fourier space, we have

$$\int d^3 \mathbf{x}_{1'} \int d^3 \mathbf{x}_1 \langle n(\mathbf{x}_{1'}) v(\mathbf{x}_{1'} - \mathbf{x}_1) n(\mathbf{x}_1) \rangle \quad (5.160)$$

$$= \int d^3 \mathbf{x}_{1'} \int d^3 \mathbf{x}_1 v(\mathbf{x}_{1'} - \mathbf{x}_1) \chi_{nn}(\mathbf{x}_{1'}, 0; \mathbf{x}_1 0) \quad (5.161)$$

$$= \int \frac{d^3 q}{(2\pi)^3} V_{\mathbf{q}} \left[\lim_{\tau \rightarrow 0} \mathcal{V} \chi_{nn}(\mathbf{q}, \tau) \right] \quad (5.162)$$

We did not have to take into account the disconnected piece that appears in Eq.(5.160) 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.(5.158) we have

$$\begin{aligned} 2 \langle V \rangle \beta &= \int_{1'} \int_1 \langle \psi^\dagger(1^+) \psi^\dagger(1') V(1' - 1) \psi(1') \psi(1) \rangle = \quad (5.163) \\ &= \beta \mathcal{V} \left[-n_0 v(0) + \int \frac{d^3 q}{(2\pi)^3} V_{\mathbf{q}} T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) \right] \\ &= \beta \mathcal{V} \left[\int \frac{d^3 q}{(2\pi)^3} V_{\mathbf{q}} \left[T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) - n_0 \right] \right] \end{aligned}$$

Substituting the above Eq.(5.163) into the consistency relation between self-energy and potential energy Eq.(5.156) 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

$$\int_{1'} \Sigma(1, 1') \mathcal{G}(1', 1^+) = \quad (5.164)$$

$$T \sum_{ik_n} \int \frac{d^3 k}{(2\pi)^3} \Sigma(\mathbf{k}, ik_n) G(\mathbf{k}, ik_n) e^{ik_n \eta} \quad (5.165)$$

$$= \frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} V_{\mathbf{q}} \left[T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) - n_0 \right]. \quad (5.166)$$

Remark 108 *In short range models, we need to restore the $v_{\mathbf{q}=0}$ 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.*

5.3.2 General theorem on free-energy calculations

The diagram rules for the free energy are more complicated than for the Green's function. 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. This trick is apparently due to Pauli [13]. The proof is simple. First, notice that

$$-\frac{1}{\beta} \frac{\partial \ln Z}{\partial \lambda} = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial \text{Tr} [e^{-\beta(H_0 + \lambda V - \mu N)}]}{\partial \lambda} = \frac{1}{Z} \text{Tr} [e^{-\beta(H_0 + \lambda V - \mu N)} V] = \frac{1}{\lambda} \langle \lambda V \rangle_\lambda. \quad (5.167)$$

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 $\langle \lambda V \rangle_\lambda$ 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

$$\boxed{\Omega = -T \ln Z = -T \ln Z_0 + \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda V \rangle_\lambda.} \quad (5.168)$$

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 109 Recall that the free energy in this grand-canonical ensemble is related to the pressure.

$$\Omega = -P\mathcal{V}. \quad (5.169)$$

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 the previous section, Eq.(5.163), how the potential energy may be obtained from density correlations,

$$\begin{aligned} \Omega &= -T \ln Z = -T \ln Z_0 \\ &+ \frac{\mathcal{V}}{2} \int_0^1 \frac{d\lambda}{\lambda} \left\langle \lambda \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) - n_0 \right] \right\rangle_\lambda. \end{aligned} \quad (5.170)$$

Using our previous relation between self-energy and potential energy, Eq.(5.156) the coupling-constant integration in Eq.(5.168) may also be done with

$$\Omega = -T \ln Z_0 + \frac{T}{2} \int_0^1 \frac{d\lambda}{\lambda} \int d1 \int d1'' \Sigma_\lambda(1, 1'') \mathcal{G}_\lambda(1'', 1^+). \quad (5.171)$$

where the subscript λ reminds oneself that the interaction Hamiltonian must be multiplied by a coupling constant λ .

5.4 Single-particle properties

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 the consistency relations we just derived. 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 chapter in the context of photoemission experiments.

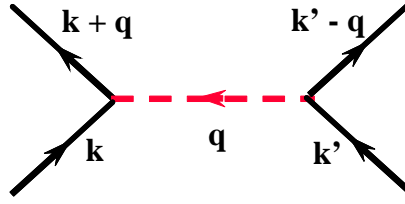


Figure 5-22 Momentum conservation for the Coulomb interaction.

5.4.1 Hartree-Fock theory

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.

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

$$H_0 = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}, \sigma} = \sum_{\mathbf{k}, \sigma} \frac{k^2}{2m} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}, \sigma} \quad (5.172)$$

where the spin-sum is represented by a sum over σ . The interacting part, written in Fourier space, takes the form

$$H - H_0 = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}, \sigma} \sum_{\mathbf{k}', \sigma'} \sum_{\mathbf{q}} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}', \sigma'}^+ V_{\mathbf{q}} c_{\mathbf{k}' - \mathbf{q}, \sigma'} c_{\mathbf{k} + \mathbf{q}, \sigma} \quad (5.173)$$

with $V_{\mathbf{q}}$ the Fourier transform of the Coulomb potential

$$V_{\mathbf{q}} = \frac{4\pi e^2}{q^2}. \quad (5.174)$$

Electroneutrality leads to $V_{\mathbf{q}=0} = 0$ 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.(5-22). 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, $(\mathcal{V}^{-1/2})^4$, 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

$$\boxed{\tilde{H}_0 = \sum_{\mathbf{k}, \sigma} \tilde{\epsilon}_{\mathbf{k}} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}, \sigma}} \quad (5.175)$$

with the variational parameter $\tilde{\epsilon}_{\mathbf{k}}$. We then minimize

$$-T \ln Z_0 + \langle H - \tilde{H}_0 \rangle_0 \quad (5.176)$$

The partition function for $\tilde{H}_0 - \mu N$ is computed as usual for non-interacting electrons

$$-T \ln Z_0 = -T \ln \prod_{\mathbf{k}, \sigma} \left(1 + e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} \right) = -T \sum_{\mathbf{k}, \sigma} \ln \left(1 + e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} \right). \quad (5.177)$$

Then the quantity $\langle H - \tilde{H}_0 \rangle_0$ is easily evaluated using Wick's theorem since \tilde{H}_0 is quadratic in creation-annihilation operators

$$\langle H - \tilde{H}_0 \rangle_0 = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) \langle c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} \rangle_0 \quad (5.178)$$

$$+ \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}, \sigma} \sum_{\mathbf{k}', \sigma'} \sum_{\mathbf{q}} V_{\mathbf{q}} \left[\langle c_{\mathbf{k}', \sigma'}^{\dagger} c_{\mathbf{k}' - \mathbf{q}, \sigma'} \rangle_0 \langle c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k} + \mathbf{q}, \sigma} \rangle_0 - \langle c_{\mathbf{k}', \sigma'}^{\dagger} c_{\mathbf{k} + \mathbf{q}, \sigma} \rangle_0 \langle c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}' - \mathbf{q}, \sigma'} \rangle_0 \right]. \quad (5.179)$$

which may be simplified by using

$$\langle c_{\mathbf{k}', \sigma'}^{\dagger} c_{\mathbf{k}, \sigma} \rangle_0 = \delta_{\sigma, \sigma'} \delta_{\mathbf{k}, \mathbf{k}'} \langle c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} \rangle_0 \equiv \delta_{\sigma, \sigma'} \delta_{\mathbf{k}, \mathbf{k}'} f(\tilde{\zeta}_{\mathbf{k}}) = \frac{1}{e^{\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} + 1} \quad (5.180)$$

to obtain

$$\langle H - \tilde{H}_0 \rangle_0 = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) f(\tilde{\zeta}_{\mathbf{k}}) - 2 \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}} \sum_{\mathbf{q}} V_{\mathbf{q}} f(\tilde{\zeta}_{\mathbf{k} + \mathbf{q}}) f(\tilde{\zeta}_{\mathbf{k}}) \quad (5.181)$$

where the overall factor of 2 comes from what is left of the spin sums. We have dropped the term that leads to $V_{\mathbf{q}=0}$ as usual because of the neutralizing background.

We can now determine our variational parameter $\tilde{\epsilon}_{\mathbf{k}}$ by minimizing with respect to it:

$$\frac{\partial}{\partial \tilde{\epsilon}_{\mathbf{k}}} \left[-T \sum_{\mathbf{k}, \sigma} \ln \left(1 + e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} \right) \right] = \frac{2e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)}}{(1 + e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)})} = 2f(\tilde{\zeta}_{\mathbf{k}}) \quad (5.182)$$

$$\frac{\partial}{\partial \tilde{\epsilon}_{\mathbf{k}}} \langle H - \tilde{H}_0 \rangle_0 = -2f(\tilde{\zeta}_{\mathbf{k}}) + \frac{\partial f(\tilde{\zeta}_{\mathbf{k}})}{\partial \tilde{\epsilon}_{\mathbf{k}}} \left[2(\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) - \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} V_{\mathbf{q}} \left(f(\tilde{\zeta}_{\mathbf{k} + \mathbf{q}}) + f(\tilde{\zeta}_{\mathbf{k} - \mathbf{q}}) \right) \right]. \quad (5.183)$$

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

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} V_{\mathbf{q}} f(\tilde{\zeta}_{\mathbf{k} + \mathbf{q}}) = \epsilon_{\mathbf{k}} - \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} V_{\mathbf{k} - \mathbf{k}'} f(\tilde{\zeta}_{\mathbf{k}'}) \quad (5.184)$$

$$\boxed{\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} \frac{1}{e^{\beta(\tilde{\epsilon}_{\mathbf{k}'} - \mu)} + 1}} \quad (5.185)$$

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.

Hartree-Fock from the point of view of Green's functions, renormalized perturbation theory and effective medium theories

We want to do perturbation theory but using this time for the Hamiltonian

$$H = \tilde{H}_0 + (H_0 - \tilde{H}_0 + V) \quad (5.186)$$

The unperturbed Hamiltonian is now \tilde{H}_0 and we assume that it takes the same form as Eq.(5.175) above. In addition to the usual perturbation V , there is now a translationally invariant one-body potential $H_0 - \tilde{H}_0$. One determines the self-energy in such a way that \tilde{H}_0 becomes the best “effective medium” in the sense that to first order in $(H_0 - \tilde{H}_0 + V)$ the self-energy calculated in this effective medium vanishes completely. This is illustrated in Fig.(5-23). This kind of approach is also known as renormalized perturbation theory [22].

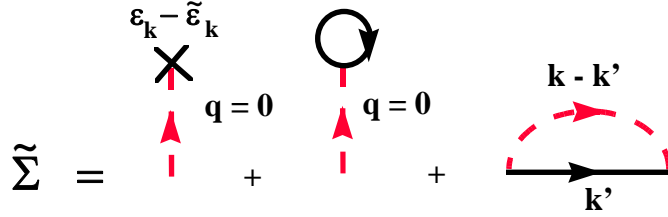


Figure 5-23 Effective medium point of view for the Hartree-Fock approximation. In this figure, the propagators are evaluated with the effective medium \tilde{H}_0 .

The 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 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.(5-23) gives

$$\tilde{\Sigma} = \epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) = 0 \quad (5.187)$$

Using the diagram rules to evaluate the exchange, or Fock, diagram $\Sigma^{(1)}(\mathbf{k})$ we get a minus sign because we compute to first order and there is no fermion loop. Furthermore, we have the $e^{ik'_n\eta}$ convergence factor. Hence, we obtain for $\Sigma^{(1)}(\mathbf{k})$

$$\Sigma^{(1)}(\mathbf{k}) = - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} \tilde{\mathcal{G}}^0(\mathbf{k}', ik'_n) e^{ik'_n\eta} \quad (5.188)$$

that we can evaluate using our formula for Matsubara sums. Substituting back into Eq.(5.187) we get precisely our Hartree-Fock result Eq.(5.185) obtained from the variational principle.

To close this section, we note that there is another instructive way of rewriting the last equation for $\Sigma^{(1)}(\mathbf{k})$. Using Eq.(5.187) for $\tilde{\epsilon}_{\mathbf{k}}$ we can remove all reference to $\tilde{\epsilon}_{\mathbf{k}}$ and write

$$\Sigma^{(1)}(\mathbf{k}) = - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} \frac{1}{ik'_n - (\epsilon_{\mathbf{k}} - \mu) - \Sigma^{(1)}(\mathbf{k})} e^{ik'_n\eta} \quad (5.189)$$

Performing the summation over Matsubara frequencies and using Eq.(5.187) to relate $\tilde{\epsilon}_{\mathbf{k}}$ to $\Sigma^{(1)}(\mathbf{k})$, this expression is found identical to our earlier variational result Eq.(5.185). The above equation Eq.(5.189) looks as if the perturbation expansion for the full Green’s function, illustrated by a thick arrow in Fig.(5-24), 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. One commonly says that all the “rainbow” diagrams have been summed. In principle this Hartree-Fock Green’s function may be used in further perturbative calculations. We just have to be careful not to double-count the diagrams we have already included.

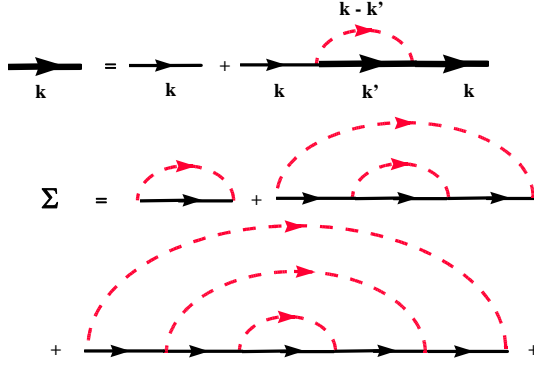


Figure 5-24 Hartree-Fock as a self-consistent approximation for the Green's function. This self-consistent approximation is equivalent to a self-energy that sums all the rainbow diagrams illustrated on the bottom part of the figure. The thick line is the full Green's function.

The pathologies of the Hartree-Fock approximation for the electron gas.

To evaluate our expression for the Hartree-Fock self-energy $\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k})$ Eq.(5.185) 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

$$n = 2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \tilde{\mathcal{G}}^0(\mathbf{k}, ik_n) e^{ik_n \eta} \quad (5.190)$$

$$= 2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) - \mu)} + 1} \quad (5.191)$$

Let us focus on the zero temperature case. Then the Fermi function is a step function and the last integral reduces to

$$n = 2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \theta(k_F - |\mathbf{k}|) \quad (5.192)$$

where the chemical potential is given by

$$\epsilon_{\mathbf{k}_F} + \Sigma^{(1)}(\mathbf{k}_F) - \mu = 0 \quad (5.193)$$

The equation Eq.(5.192) 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

$$\Sigma^{(1)}(\mathbf{k}) = - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} \theta(k_F - |\mathbf{k}'|) \quad (5.194)$$

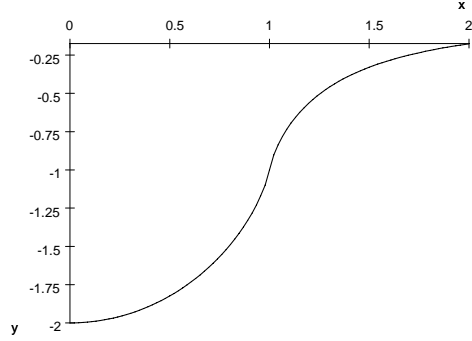
$$= - \frac{4\pi e^2}{8\pi^3} \int_0^{k_F} (k')^2 dk' \int_{-1}^1 \frac{2\pi d(\cos \theta)}{k^2 + (k')^2 - 2kk' \cos \theta} \quad (5.195)$$

$$= - \frac{e^2}{\pi} \int_0^{k_F} k' \frac{1}{-2k} \ln \left(\left| \frac{(k' - k)^2}{(k + k')^2} \right| \right) dk' \quad (5.196)$$

We evaluated the integral as a principal part integral because we have argued that the potential should have no $q = 0$ component which means $|\mathbf{k} - \mathbf{k}'|^2 \neq 0$. Pursuing the calculation, we have

$$\Sigma^{(1)}(\mathbf{k}) = -\frac{e^2}{\pi} k_F \left[1 + \frac{1-y^2}{2y} \ln \left(\left| \frac{1+y}{1-y} \right| \right) \right] ; \quad y \equiv \frac{k}{k_F} \quad (5.197)$$

The function $\Sigma^{(1)}(\mathbf{k}) / \left(\frac{e^2}{\pi} k_F \right)$ is plotted in Fig.(??).



$\Sigma^{(1)}(k/k_F) / \left(\frac{e^2}{\pi} k_F \right)$ Plot of the Hartree-Fock self-energy at zero temperature.

Since $\lim_{x \rightarrow 0} x \ln x = 0$, we have that

$$\Sigma^{(1)}(\mathbf{k}_F) = -\frac{e^2}{\pi} k_F \quad (5.198)$$

The ratio of this term to the zeroth order term, namely the kinetic energy $k_F^2/2m$ is of order r_s

$$\propto \frac{m e^2 k_F}{k_F^2} \propto \frac{1}{k_F a_0} \propto r_s \quad (5.199)$$

as can be seen using the definitions Eqs.(5.68)(5.71).

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.(4.251)

$$\frac{m}{m^*} = \lim_{\mathbf{k} \rightarrow \mathbf{k}_F} \frac{1 + \frac{\partial}{\partial \zeta_{\mathbf{k}}} \text{Re} \Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma^R(\mathbf{k}, \omega) \Big|_{\omega = E_{\mathbf{k}} - \mu}} = 1 + \frac{dk}{d\zeta_{\mathbf{k}}} \frac{\partial \Sigma^{(1)}(\mathbf{k})}{\partial k} \Big|_{k=k_F} \quad (5.200)$$

we have

$$\frac{\partial \Sigma^{(1)}(\mathbf{k})}{\partial k} \Big|_{k=k_F} \propto k_F \left(\frac{dy}{dk} \right)_{y=1} \frac{d \left[1 + \frac{1-y^2}{2y} \ln \left(\left| \frac{1+y}{1-y} \right| \right) \right]}{dy} \Big|_{y=1} \quad (5.201)$$

The problem comes from $\ln(1-y)$. Let us concentrate on the contributions proportional to this term

$$\begin{aligned} \frac{d}{dy} \left[\left(\frac{1}{2y} - \frac{y}{2} \right) \ln(1-y) \right] &= \left(-\frac{1}{2y^2} - \frac{1}{2} \right) \ln(1-y) \\ &\quad - \left(\frac{1}{2y} - \frac{y}{2} \right) \frac{1}{1-y} \end{aligned} \quad (5.202)$$

As $y \rightarrow 1$ we obtain a singularity from $\ln(0) = \infty$. This corresponds to the unphysical result $m^* = 0$. Already an effective mass smaller than the bare mass would require explanation since we expect that in general interactions will make quasiparticles look heavier. But the result obtained here, $m^* = 0$, 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.

5.4.2 Curing Hartree-Fock theory: screened interaction in the self-energy

In this subsection we present the solution to the failure of Hartree-Fock that was found by Gell-Man and Brueckner[14], interpret the results, and compare with experiments. In particular, we will recover theoretically the Fermi liquid regime, compute the free energy and compare with experiment.

An approximation for Σ that is consistent with the Physics of screening

We have seen in the previous section Eq.(5.164) 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.(5-25). The diagram on the left is built from the rainbow self-energy of Fig.(5-24) 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.(5.164) 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.

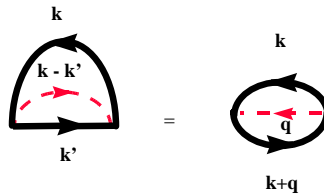


Figure 5-25 Approximation for the density fluctuations that corresponds to the Hartree-Fock self-energy.

Remark 110 *Equality (5.164) for the Hartree-Fock approximation. Let us check just the sums over Matsubara frequencies on both sides of Eq.(5.164) to see that they are identical. First, the sum on the left hand-side.*

$$T \sum_{ik_n} T \sum_{ik'_n} \frac{e^{ik_n \eta}}{ik_n - \zeta_{\mathbf{k}}} \frac{e^{ik'_n \eta}}{ik'_n - \zeta_{\mathbf{k}'}} = f(\zeta_{\mathbf{k}}) f(\zeta_{\mathbf{k}'}) \quad (5.203)$$

While the sum on the right-hand side is

$$T \sum_{ik_n} T \sum_{iq_n} \frac{1}{ik_n - \zeta_{\mathbf{k}}} \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}'}} \quad (5.204)$$

$$= T \sum_{ik_n} T \sum_{q_n} \left[\frac{1}{ik_n - \zeta_{\mathbf{k}}} - \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}'}} \right] \frac{1}{iq_n - \zeta_{\mathbf{k}'} + \zeta_{\mathbf{k}}} \quad (5.205)$$

$$= T \sum_{q_n} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})}{iq_n - \zeta_{\mathbf{k}'} + \zeta_{\mathbf{k}}} = -[f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})] n_B(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}}) \quad (5.206)$$

where we used, with n_B the Bose function

$$T \sum_{q_n} \frac{1}{iq_n - a} = -n_B(a) \quad \text{or} \quad -n_B(a) - 1 \quad (5.207)$$

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

$$\begin{aligned} -[f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}'})] n_B(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}}) &= -\frac{e^{\beta\zeta_{\mathbf{k}'}} - e^{\beta\zeta_{\mathbf{k}}}}{(e^{\beta\zeta_{\mathbf{k}'}} + 1)(e^{\beta\zeta_{\mathbf{k}}} + 1)} \frac{1}{e^{\beta(\zeta_{\mathbf{k}'} - \zeta_{\mathbf{k}})} - 1} \\ &= -\frac{e^{\beta\zeta_{\mathbf{k}}}}{(e^{\beta\zeta_{\mathbf{k}'}} + 1)(e^{\beta\zeta_{\mathbf{k}}} + 1)} \quad (5.208) \\ &= -(1 - f(\zeta_{\mathbf{k}})) f(\zeta_{\mathbf{k}'}) \quad (5.209) \end{aligned}$$

Eq.(5.203) and the last equation are not strictly equal and that is why it is necessary to subtract n_0 in Eq.(5.203).

Fig.(5-25) 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.(5-26). Indeed, in such a case, multiplying Σ by \mathcal{G}

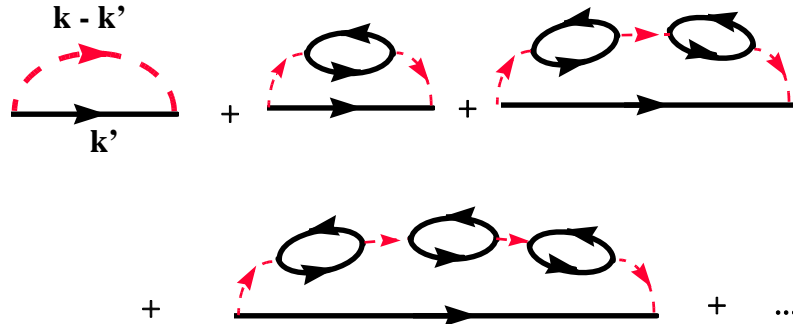


Figure 5-26 Diagrammatic expression for the self-energy in the RPA approximation.

gives a result, illustrated in Fig.(5-27) that does correspond to multiplying the RPA expression for the density Fig.(5-18) by $V_{\mathbf{q}}$ and summing over \mathbf{q} . These are the ring diagrams.

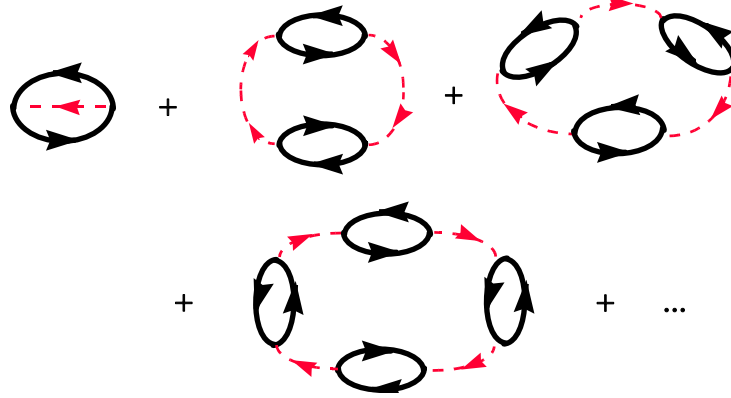


Figure 5-27 Ring diagrams for $\Sigma\mathcal{G}$ in the RPA approximation. The same diagrams are used for the free energy calculation.

Using Feynman's rules, the corresponding analytical expression is

$$\begin{aligned} \Sigma_{RPA}(\mathbf{k}, ik_n) &= \quad (5.210) \\ &= - \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{iq_n} \frac{V_{\mathbf{q}}}{1 + V_{\mathbf{q}}\chi_{nn}^0(\mathbf{q}, iq_n)} \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \\ &= - \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{iq_n} \frac{V_{\mathbf{q}}}{\varepsilon(\mathbf{q}, iq_n)} \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \end{aligned}$$

Comparing with the Hartree-Fock approximation Eq.(5.189) 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.(5-28) which is analogous

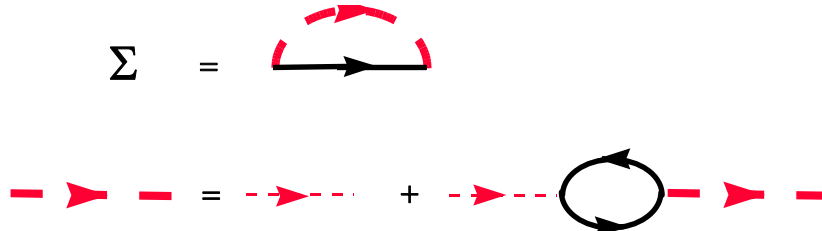


Figure 5-28 RPA self-energy written in terms of the screened interaction.

to the diagram for the Hartree-Fock approximation Fig.(5-24) but with a screened interaction and only the first rainbow diagram, without self-consistency.

Remark 111 *If, instead of summing the whole series in Fig.(5-26) 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.(5.210). 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.

Before we extract a few results analytically from this RPA self-energy, let us look at numerical evaluations of the corresponding integrals.

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.(5-29) 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. There are several points worth mentioning.

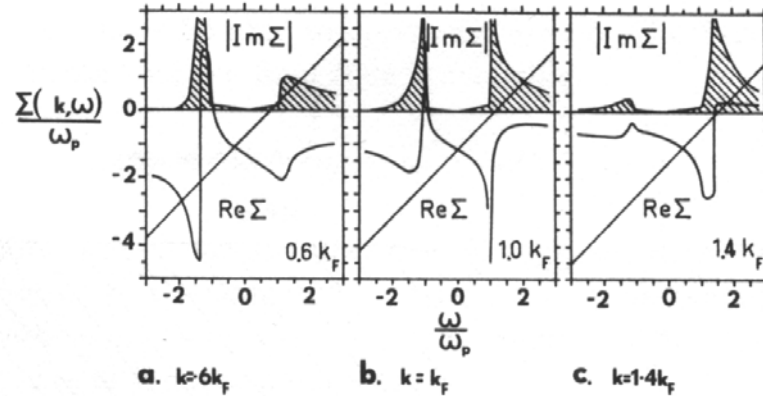


Figure 5-29 Real and imaginary part of the RPA self-energy for three wave vectors, in units of the plasma frequency. The chemical potential is included in $\text{Re}\Sigma$. The straight line that appears on the plots is $\omega - \epsilon_{\mathbf{k}}$. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7**, 117 (1968). $r_s = 5$?

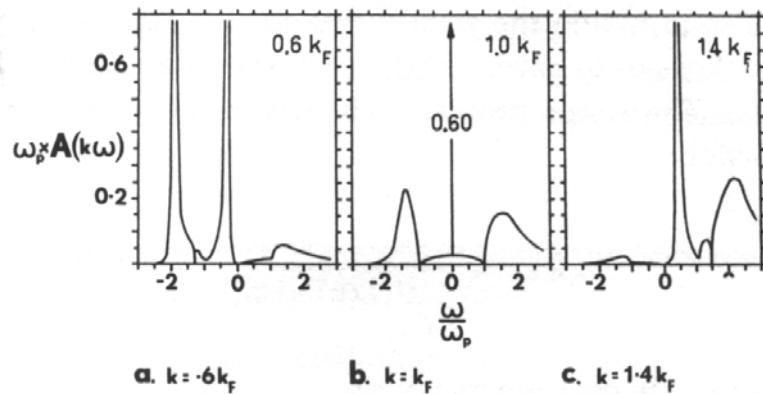


Figure 5-30 RPA spectral weight, in units of the inverse plasma frequency. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7**, 117 (1968).

- $\text{Im}\Sigma(\mathbf{k}, \omega = 0) = 0$ 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.
- The straight line that appears on the plots is $\omega - \epsilon_{\mathbf{k}}$. The intersection of this straight line with $\text{Re}\Sigma$, which is defined on the figure to contain the chemical potential, corresponds (in our notation) to the solution of the equation

$$\omega - \epsilon_{\mathbf{k}} = \text{Re}\Sigma(\mathbf{k}, \omega) - \mu \quad (5.211)$$

As we argued in the previous chapter Eq.(4.238), this determines the position of maxima in the spectral weight,

$$A(\mathbf{k},\omega) = -2 \operatorname{Im} G^R(\mathbf{k},\omega) \quad (5.212)$$

$$= \frac{-2 \operatorname{Im} \Sigma^R(\mathbf{k},\omega)}{\left(\omega - \zeta_{\mathbf{k}} - \operatorname{Re} \Sigma^R(\mathbf{k},\omega)\right)^2 + \left(\operatorname{Im} \Sigma^R(\mathbf{k},\omega)\right)^2} \quad (5.213)$$

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.(5-30). 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.(4.243),

$$A(\mathbf{k},\omega) \approx 2\pi Z_{\mathbf{k}} \left[\frac{1}{\pi} \frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega - E_{\mathbf{k}} + \mu)^2 + (\Gamma_{\mathbf{k}}(\omega))^2} \right] + inc \quad (5.214)$$

it is necessary that at the crossing point, the slope of $\operatorname{Re} \Sigma^R(\mathbf{k},\omega)$ be negative because it is necessary that

$$Z_{\mathbf{k}} = \frac{1}{1 - \left. \frac{\partial}{\partial \omega} \operatorname{Re} \Sigma^R(\mathbf{k},\omega) \right|_{\omega=E_{\mathbf{k}}-\mu}} \geq 0 \quad (5.215)$$

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. 5-29 there is a threshold-like feature at $\omega_p = \pm 1$ where $\operatorname{Im} \Sigma^R$ becomes large. This is when the one-particle excitations can emit or absorb real plasmons. This is discussed further in the Sec. 5.4.2 just 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 $\operatorname{Im} \Sigma^R$ that are large, but not too large compared with the value of $\omega - \zeta_{\mathbf{k}} - \operatorname{Re} \Sigma^R(\mathbf{k},\omega)$. At the threshold where $\operatorname{Im} \Sigma^R$ is really large, the spectral weight in fact vanishes because of the denominator in the general expression for the spectral weight Eq.(5.212). Note that the maxima away from $\omega = 0$ at $k = k_F$ are near the value of ω where the quasiparticle condition Eq. (5.211) 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 $\operatorname{Im} \Sigma^R$ is large and the quasiparticle condition Eq. (5.211) is almost satisfied.
- For $k = 0.6k_F$, there seems to be an additional quasiparticle solution, namely a solution where $\frac{\partial}{\partial \omega} \operatorname{Re} \Sigma^R$ is negative and $\operatorname{Im} \Sigma^R$ is not too large, located at an energy ω_p below the main quasiparticle energy. Since the free-electron band is bounded from below, $\operatorname{Im} \Sigma^R$ vanishes at sufficiently negative frequency, allowing a new solution to develop when interactions are sufficiently strong. This solution looks like a bound state.

Physical interpretation of 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 subsection. Here we want to first show that the imaginary part of the self-energy defined by

$$\Sigma^R(\mathbf{k}, \omega) = \Sigma'(\mathbf{k}, \omega) + i\Sigma''(\mathbf{k}, \omega) \quad (5.216)$$

may be written in the form

$$\Sigma''(\mathbf{k}, \omega) = -\frac{m}{2|k|} \int \frac{d^2 q_{\perp}}{(2\pi)^2} \int \frac{d\omega'}{\pi} [n_B(\omega') + f(\omega + \omega')] V_{\mathbf{q}}^2 \chi''_{nn}(q_{\perp}, q_{\parallel}, \omega') \quad (5.217)$$

where q_{\parallel} is the solution of the equation

$$\frac{|k|}{m} q_{\parallel} + \frac{q_{\parallel}^2}{2m} = - \left[\omega + \omega' - \left(\frac{k^2}{2m} - \mu + \frac{q_{\perp}^2}{2m} \right) \right] \quad (5.218)$$

Proof: It is preferable to first rewrite the RPA expression Eq.(5.210) in the following form

$$\Sigma_{RPA}(\mathbf{k}, ik_n) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} T \sum_{iq_n} V_{\mathbf{q}} \left[1 - \frac{V_{\mathbf{q}} \chi_{nn}^0(\mathbf{q}, iq_n)}{1 + V_{\mathbf{q}} \chi_{nn}^0(\mathbf{q}, iq_n)} \right] \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \quad (5.219)$$

$$= \Sigma_{HF}(\mathbf{k}) + \int \frac{d^3 \mathbf{q}}{(2\pi)^3} T \sum_{iq_n} [V_{\mathbf{q}} \chi_{nn}^{RPA}(\mathbf{q}, iq_n) V_{\mathbf{q}}] \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_n) \quad (5.220)$$

The first term at $T = 0$ is the Hartree-Fock contribution, as we can see from Eq.(5.194). 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

$$\Sigma_{RPA}(\mathbf{k}, ik_n) - \Sigma_{HF}(\mathbf{k}) = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} T \sum_{iq_n} \left[V_{\mathbf{q}} \frac{\chi''_{nn}(\mathbf{q}, \omega')}{\omega' - iq_n} V_{\mathbf{q}} \right] \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.221)$$

We cannot perform the analytical continuation $ik_n \rightarrow \omega + i\eta$ 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. To do the sum over bosonic Matsubara frequencies first, we do the partial fraction decomposition as usual

$$-T \sum_{iq_n} \frac{1}{iq_n - \omega'} \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.222)$$

$$= -T \sum_{iq_n} \left[\frac{1}{iq_n - \omega'} - \frac{1}{ik_n + iq_n - \zeta_{\mathbf{k}+\mathbf{q}}} \right] \frac{1}{ik_n + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.223)$$

$$= [n_B(\omega') + f(\zeta_{\mathbf{k}+\mathbf{q}})] \frac{1}{ik_n + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.224)$$

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 $ik_n \rightarrow \omega + i\eta$ can be done and we obtain

$$\Sigma^R(\mathbf{k}, \omega) - \Sigma_{HF}(\mathbf{k}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} [n_B(\omega') + f(\zeta_{\mathbf{k}+\mathbf{q}})] \frac{V_{\mathbf{q}} \chi''_{nn}(\mathbf{q}, \omega') V_{\mathbf{q}}}{\omega + i\eta + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}} \quad (5.225)$$

The imaginary part is thus

$$\Sigma''(\mathbf{k}, \omega) = -\pi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} [n_B(\omega') + f(\omega + \omega')] V_{\mathbf{q}}^2 \chi''_{nn}(\mathbf{q}, \omega') \delta(\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) \quad (5.226)$$

Defining q_{\parallel} by the direction parallel to the wave vector \mathbf{k} and calling q_{\perp} the other directions, the integral over q_{\parallel} can be performed, giving the condition in Eq.(5.218). We then obtain, assuming that we are in a region of frequency where the delta function has a solution, the desired result Eq.(5.217)

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.(5.217) 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.(5-29) 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 112 *Vanishing of Σ'' at zero temperature: Our general formula for the imaginary part Eq.(5.217) tells us that at zero temperature $\Sigma''(\mathbf{k}, \omega = 0) = 0$ for **all** wave vectors, as we have seen in Fig.(5-29). Mathematically, this is so because $\lim_{T \rightarrow 0} [n_B(\omega') + f(\omega')] = 0$ for all ω' . Physically, it is because phase space vanishes when we sit right at the chemical potential ($\omega = 0$).*

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 $\omega' \rightarrow -\omega'$. Then the integration window at $T = 0$ becomes $-\omega < -\omega' < 0$, or $\omega > \omega' > 0$. Using

$$n_B(-\omega') = -(1 + n_B(\omega')) \quad (5.227)$$

and $\chi''_{nn}(\mathbf{q}, -\omega') = -\chi''_{nn}(-\mathbf{q}, \omega')$, the imaginary part of the self-energy becomes

$$\begin{aligned} \Sigma''(\mathbf{k}, \omega) &= -\pi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} [(1 + n_B(\omega')) - f(\omega - \omega')] V_{\mathbf{q}}^2 \chi''_{nn}(\mathbf{q}, \omega') \delta(\omega - \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) \\ &= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} V_{\mathbf{q}}^2 \chi''_{nn}(-\mathbf{q}, \omega - \zeta_{\mathbf{k}+\mathbf{q}}) \\ &\quad [(1 + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}})) (1 - f(\zeta_{\mathbf{k}+\mathbf{q}})) + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}}) f(\zeta_{\mathbf{k}+\mathbf{q}})] \end{aligned}$$

The first term $(1 + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}})) (1 - f(\zeta_{\mathbf{k}+\mathbf{q}}))$ 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 $n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}}) f(\zeta_{\mathbf{k}+\mathbf{q}})$ represents the case where the incident state is a hole 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. “Scattering-in” terms that represent repopulation of the state \mathbf{k} occur in transport equations, or two-body response functions, not here.

Fermi liquid results

Perhaps the best known characteristic of a Fermi liquid is that at frequencies and temperatures much smaller than the Fermi energy, $\Sigma''^R(\mathbf{k}_F, \omega; T=0) \propto \omega^2$ and $\Sigma''^R(\mathbf{k}_F, \omega=0; T) \propto T^2$. To recover this result, valid far from phase transitions, we start from the above expression Eq.(5.217) for Σ'' but we evaluate it at $\mathbf{k} = \mathbf{k}_F$ and use $v_F \equiv k_F/m$ so that

$$\Sigma''(\mathbf{k}_F, \omega) = -\frac{1}{2v_F} \int \frac{d^2 q_{\perp}}{(2\pi)^2} \int \frac{d\omega'}{\pi} [n_B(\omega') + f(\omega + \omega')] V_{\mathbf{q}}^2 \chi''_{nn}(q_{\perp}, q_{\parallel}, \omega') \quad (5.228)$$

where q_{\parallel} is obtained from the solution of

$$v_F q_{\parallel} + \frac{q_{\parallel}^2}{2m} = - \left[\omega + \omega' - \frac{q_{\perp}^2}{2m} \right] \quad (5.229)$$

The key to understanding the Fermi liquid regime is in the relative width in frequency of $\chi''_{nn}(\mathbf{q}, \omega')/\omega'$ vs the width of the combined Bose and Fermi functions. In general, the function $n_B(\omega') + f(\omega + \omega')$ depends on ω' on a scale $\max(\omega, T)$ while far from a phase transition, $\chi''_{nn}(\mathbf{q}, \omega')/\omega'$ is independent of frequency at low frequency.

Proof: As we can see from the explicit expression for the imaginary part of χ''_{nn} Eq.(5.119), and using the fact that $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, 0) = 0$,

$$\lim_{\omega \rightarrow 0} \text{Im} \chi_{nn}^R(\mathbf{q}, \omega)/\omega = \lim_{\omega \rightarrow 0} \frac{\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)/\omega}{(1 + V_{\mathbf{q}} \text{Re} \chi_{nn}^{0R}(\mathbf{q}, 0))^2} \quad (5.230)$$

it suffices that the Lindhard function $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ has the property that $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)/\omega$ is independent of frequency at low frequency. As expected from the fact that $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ is odd in frequency, it turns out that $\text{Im} \chi_{nn}^{0R}(\mathbf{q}, \omega)$ is indeed linear in frequency at low frequency, which proves our point. The linearity can be explicitly checked from our previous results Eqs.(5.115) and (5.112).

Hence, at low frequency, we can assume that $\chi''_{nn}(\mathbf{q}, \omega')/\omega'$ is independent of frequency in the frequency range over which $n(\omega') + f(\omega + \omega')$ differs from zero. Also, $V_{\mathbf{q}}^2 \chi''_{nn}(\mathbf{q}, \omega')/\omega'$ depends on wave vector over a scale that is of order q_F as we can see from Fig.(5-20). Hence, we can neglect the ω and ω' dependence of the solution for q_{\parallel} in Eq.(5.229) when we substitute it in our expression for Σ'' . One then finds

$$\Sigma''(\mathbf{k}_F, \omega) \simeq -\frac{A(\mathbf{k}_F)}{2v_F} \int \frac{d\omega'}{\pi} [n(\omega') + f(\omega + \omega')] \omega' = -\frac{A(\mathbf{k}_F)}{4v_F} \left[\omega^2 + (\pi T)^2 \right] \quad (5.231)$$

where the substitution $x = e^{\beta\omega}$ allowed the integral to be done exactly [15] and where

$$A(\mathbf{k}_F) \equiv \int \frac{d^2 q_{\perp}}{(2\pi)^2} \lim_{\omega' \rightarrow 0} \frac{V_{\mathbf{q}}^2 \chi''_{nn}(q_{\perp}, q_{\parallel}(q_{\perp}, v_F); \omega')}{\omega'} \quad (5.232)$$

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.(5.230). The above result Eq.(5.231) for Σ'' is the well known Fermi liquid result.

There are known corrections to the Fermi liquid self-energy that come from the non-analytic $\omega'/v_F q$ behavior of $\chi''_{nn}(\mathbf{q}, \omega')/\omega'$ near $\mathbf{q} = \mathbf{0}$. In three dimensions[16] 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.[17][18]

Remark 113 *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.*

We now just quote without proof some of the results of further calculations of Fermi liquid parameters. The solution of the quasiparticle equation Eq.(5.211) gives

$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - 0.17r_s (\ln r_s + 0.2) \frac{k_F k}{2m} + cst \quad (5.233)$$

The effective mass appearing in this expression is now obviously finite and given by

$$m^* = \frac{m}{1 - 0.08r_s (\ln r_s + 0.2)} \quad (5.234)$$

If we evaluate the scattering rate for $\omega = E_{\mathbf{k}} - \mu$ we find

$$\Gamma_{\mathbf{k}}(E_{\mathbf{k}} - \mu) = 0.25r_s^{1/2} \frac{(k - k_F)^2}{2m} \quad (5.235)$$

Quinn and Ferrell[19] write the following physically appealing form

$$\Gamma_{\mathbf{k}}(\zeta_{\mathbf{k}}) Z_{\mathbf{k}}^{-1} = \frac{\sqrt{3}\pi^2}{128} \omega_p \left(\frac{\zeta_{\mathbf{k}}}{E_F} \right)^2 \quad (5.236)$$

The scattering rate is proportional to the plasma frequency, but reduced by an important phase space factor.

Fig.(5-31) 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 114 *These results 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.*

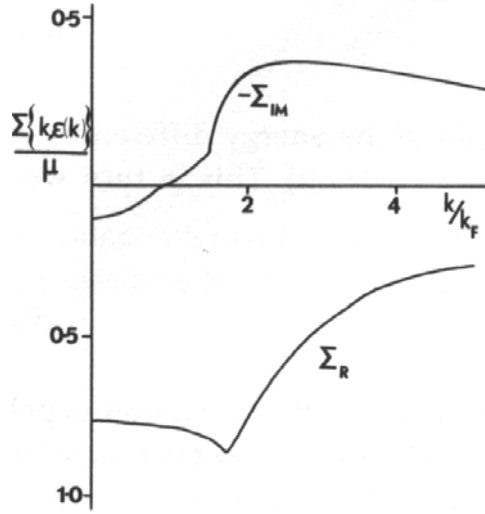


Figure 5-31 Real and imaginary parts of the self-energy of the causal Green's function in the zero-temperature formalism. From L. Hedin and S. Lundqvist, *Solid State Physics* **23**, 1 (1969).

Free energy

Finally, we use our coupling-constant integration formula Eq.(5.168). In the zero temperature limit, there will be no contribution from entropy and we will obtain the ground state energy in the RPA approximation

$$E_{Tot}^{RPA}(T=0) - \mu N = \lim_{T \rightarrow 0} \Omega = \lim_{T \rightarrow 0} \left\{ -T \ln \left[\prod_{\mathbf{k}, \sigma} (1 + e^{-\beta \zeta_{\mathbf{k}}}) \right] + \frac{\mathcal{V}}{2} \int_0^1 \frac{d\lambda}{\lambda} \lambda \int \frac{d^3 q}{(2\pi)^3} V_{\mathbf{q}} \left[T \sum_{iq_n} \chi_{nn}^{\lambda}(\mathbf{q}, iq_n) - n_0 \right] \right\} \quad (5.237)$$

We have for the sum over Matsubara frequencies

$$T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) = T \sum_{iq_n} \int \frac{d\omega'}{\pi} \frac{\chi''_{nn}(\mathbf{q}, \omega')}{\omega' - iq_n} \quad (5.238)$$

$$= \int \frac{d\omega'}{\pi} n_B(\omega') \chi''_{nn}(\mathbf{q}, \omega') \quad (5.239)$$

In the zero temperature limit,

$$\lim_{T \rightarrow 0} \int \frac{d\omega'}{\pi} n_B(\omega') \chi''_{nn}(\mathbf{q}, \omega') = - \int_{-\infty}^0 \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, \omega') \quad (5.240)$$

$$= \int_0^{\infty} \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, -\omega') \quad (5.241)$$

$$= - \int_0^{\infty} \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, \omega') \quad (5.242)$$

so that the expression for the ground state energy becomes

$$\begin{aligned}
& \frac{E_{Tot}^{RPA}(T=0) - \mu N}{\mathcal{V}} \tag{5.243} \\
&= 2 \int_{k < k_F} \frac{d^3 k}{(2\pi)^3} \left(\frac{k^2}{2m} - \mu \right) \\
&+ \frac{\mathcal{V}}{2} \int \frac{d^3 q}{(2\pi)^3} \int_0^1 \frac{d\lambda}{\lambda} \lambda V_{\mathbf{q}} \left[-\text{Im} \int_0^\infty \frac{d\omega'}{\pi} \frac{\chi_{nn}^{0R}(\mathbf{q}, \omega')}{1 + \lambda V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q}, \omega')} - n_0 \right] \tag{5.244}
\end{aligned}$$

Note that we have replaced everywhere $V_{\mathbf{q}}$ by $\lambda V_{\mathbf{q}}$ as prescribed in the coupling constant integration trick.

Remark 115 *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.(5-27) 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

$$\begin{aligned}
& \int_0^1 \frac{d\lambda}{\lambda} \lambda V_{\mathbf{q}} \left[-\text{Im} \int_0^\infty \frac{d\omega'}{\pi} \frac{\chi_{nn}^{0R}(\mathbf{q}, \omega')}{1 + \lambda V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q}, \omega')} - n_0 \right] \\
&= -V_{\mathbf{q}} n_0 - \int_0^\infty \frac{d\omega'}{\pi} \text{Im} \{ \ln [1 + V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q}, \omega')] \} \tag{5.245}
\end{aligned}$$

The rest of the calculation is tedious. One finds[20]

$$\frac{E_{Tot}^{RPA}(T=0)}{N} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622 \ln r_s - 0.142 + \mathcal{O}(r_s, r_s \ln r_s) \tag{5.246}$$

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.

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.[21].

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.(5-32) illustrates the prediction for sodium at $r_s = 3.96$. The following Table of expected jumps is from Hedin[13].

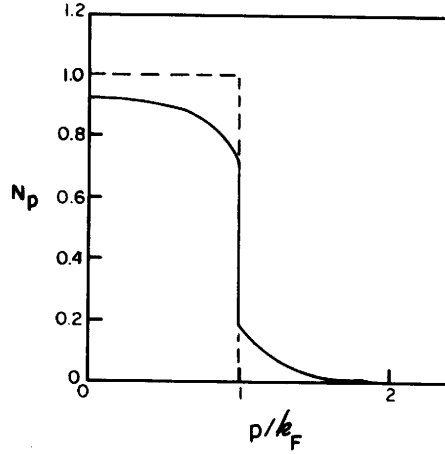


Figure 5-32 Momentum density in the RPA approximation for an electron gas with $r_s = 3.97$. From E. Daniel and S.H. Vosko, Phys. Rev. **120**, 2041 (1960).

r_s	Z_{RPA}
0	1
1	0.859
2	0.768
3	0.700
4	0.646
5	0.602
6	0.568

(5.247)

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, 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

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int d^3\mathbf{k} n_{\mathbf{k}} \delta(\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}) \quad (5.248)$$

where ω is the energy and \mathbf{q} the wave vector transferred by the photon. Changing to polar coordinates, we see that

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int k^2 dk d(\cos\theta) n_{\mathbf{k}} \delta\left(\omega - \varepsilon_{\mathbf{q}} - \frac{kq}{m} \cos\theta\right) \quad (5.249)$$

$$\propto \int k dk \frac{m}{q} n_k \theta(k - |Q|) \quad (5.250)$$

where

$$Q \equiv \frac{m}{q} (\varepsilon_q - \omega) \quad (5.251)$$

In terms of Q , we have

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \frac{1}{q} \int_{|Q|}^{\infty} n_k k dk \quad (5.252)$$

For free electrons, this gives

$$\frac{d^2\sigma}{d\omega d\Omega} \propto J(Q) \propto \frac{1}{2q} (k_F^2 - Q^2) \theta(k_F - Q) \quad (5.253)$$

In this case then, the slope is discontinuous at $k_F = Q$ as illustrated on the left of Fig.(5-33). 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.

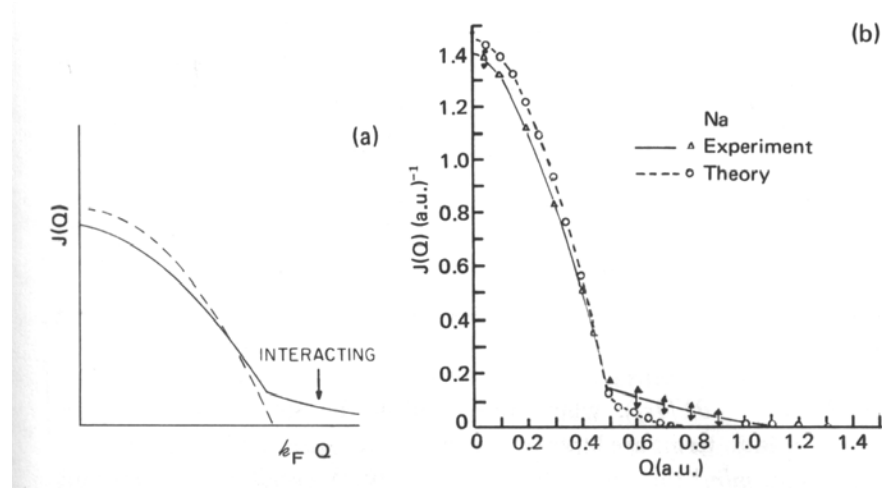


Figure 5-33 a) Dashed line shows the momentum distribution in Compton scattering for the non-interacting case while the solid line is for an interacting system. b) Experimental results in metallic sodium compared with theory, $r_s = 3.96$. Eisenberger *et al.* Phys. Rev. B **6**, 3671 (1972).

The experimental results for the mean free path are more satisfactory. Let the mean free path $\ell_{\mathbf{k}}$ be defined by

$$\frac{1}{\ell_{\mathbf{k}}} = \frac{\Gamma_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1}{\tau_{\mathbf{k}} v_{\mathbf{k}}} = -\frac{2}{v_{\mathbf{k}}} \text{Im} \Sigma(\mathbf{k}, \zeta_{\mathbf{k}}) \quad (5.254)$$

Remark 116 *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. We should discuss this in more detail in the section on Boltzmann transport.*

Fig.(5-34) 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. We do not show the cross section for inelastic electron scattering since, as expected from the fact that it is proportional to $\text{Im}(1/\epsilon^L)$, its only prominent feature at low momentum transfer is the plasma resonance that is much larger than the particle-hole continuum, as we saw in the theoretical plot of Fig.(5-21).

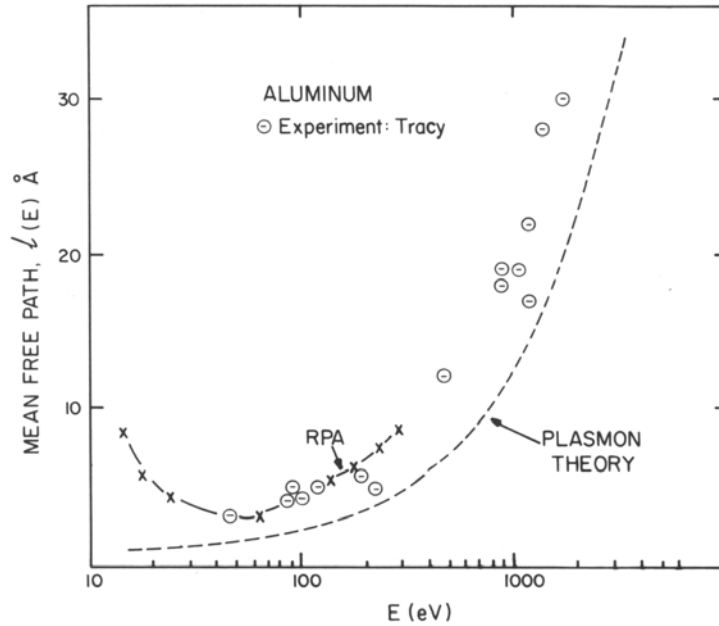


Figure 5-34 Mean free path of electrons in aluminum ($r_s = 2.07$) as a function of energy above the Fermi surface. Circles are experimental results of J.C. Tracy, *J. Vac. Sci. Technol.* **11**, 280 (1974). The dashed line with symbols X was obtained with RPA for $r_s = 2$ by B.I. Lundqvist *Phys. Status Solidi B* **63**, 453 (1974).

5.5 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.(5.246), the effective mass Eq.(5.234) or the scattering rate Eq.(5.235) 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.[24] is instructive of the nature of asymptotic expansions.

Suppose we want to evaluate the following integral

$$Z(g) = \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2} - \frac{g}{4}x^4} \quad (5.255)$$

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,

$$Z(g) = \sum_{n=0}^{\infty} g^n Z_n \quad (5.256)$$

where

$$Z_n = \frac{(-1)^n}{4^n n!} \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} x^{4n} \quad (5.257)$$

$$= \frac{(-1)^n (4n-1)!!}{4^n n! 2^n} \quad (5.258)$$

with

$$(4n-1)!! \equiv (4n-1)(4n-3)(4n-5)\dots 1 \quad (5.259)$$

$$= \frac{(4n)!}{(4n)(4n-2)(4n-4)\dots 2} \quad (5.260)$$

$$= \frac{(4n)!}{2^n (2n)!} \quad (5.261)$$

hence,

$$Z_n = \frac{(-1)^n (4n)!}{16^n n! (2n)!} \quad (5.262)$$

Using Stirling's formula,

$$n! \approx \sqrt{2\pi n} n^{n+1/2} e^{-n}$$

we are left with

$$Z_n \propto \frac{1}{\sqrt{n\pi}} \left(\frac{-4n}{e} \right)^n \quad (5.263)$$

The value of each successive term in the power series is illustrated in Fig.(5-35). Clearly, whatever the value of g , if n is sufficiently large, the higher order terms start to be larger than the low order ones. This is a characteristic of an asymptotic series.

Figure 5-35 Asymptotic expansion of $Z(g)$ for different values of g . The residual error R_n 's plotted for the half-integer values. From J.W. Negele and H. Orland, *op. cit.* p.56

We can even evaluate the error done when the series is stopped at order n . Let this error be

$$R_n = \left| Z(g) - \sum_{m=0}^n g^m Z_m \right| \quad (5.264)$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| e^{-\frac{g}{4}x^4} - \sum_{m=0}^n \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \quad (5.265)$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| \sum_{m=n+1}^{\infty} \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \quad (5.266)$$

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

$$a_{n+1} - (a_{n+2} - a_{n+3}) - (a_{n+4} - a_{n+5}) - \dots \leq a_{n+1} \quad (5.267)$$

Hence,

$$R_n \leq g^{n+1} |Z_{n+1}| \quad (5.268)$$

We also plot the error in Fig.(5-35). 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.(5.263) 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.

5.6 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.

To see this, we will show that the following consequence of charge conservation is violated[26]

$$\chi_{nn}(\mathbf{q} = \mathbf{0}, iq_n) = 0 \quad ; \quad \text{if} \quad iq_n \neq 0 \quad (5.269)$$

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 $\chi_{nn}(\mathbf{q} = \mathbf{0}, \tau)$ 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

$$\tilde{\chi}_0(\mathbf{q}, iq_n) = \frac{2}{N} \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega) A(\mathbf{k} + \mathbf{q}, \omega') \frac{(\omega - \omega')(f(\omega') - f(\omega))}{(\omega - \omega')^2 + q_n^2}. \quad (5.270)$$

When there are no interactions and $A(\mathbf{k}, \omega)$ is a delta function, it is clear that our exact result Eq.(5.269) is satisfied since only $\omega = \omega'$ will contribute. Otherwise, the integrand is positive definite so the result is different from zero. 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.(5-17). The diagrams on the bottom may be accounted for by using dressed propagators, but the diagrams on the first line cannot be. They enter the general category of vertex corrections, namely diagrams that cannot be included by simply dressing propagators. Also, the lesson we have just learned is that to satisfy conservation laws, the vertex has to do some non-trivial things since the dressed bubble by itself does not satisfy the conservation law expressed in the form of Eq.(5.269),

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

$$\frac{Z_{\mathbf{k}}}{ik_n - E_{\mathbf{k}} + \mu} \quad (5.271)$$

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 $1 - \frac{1}{4}V_{\mathbf{q}}GG$. 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.

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.

The first reformulation is illustrated in Fig.(5-36). 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 the so-called 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) 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. 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.

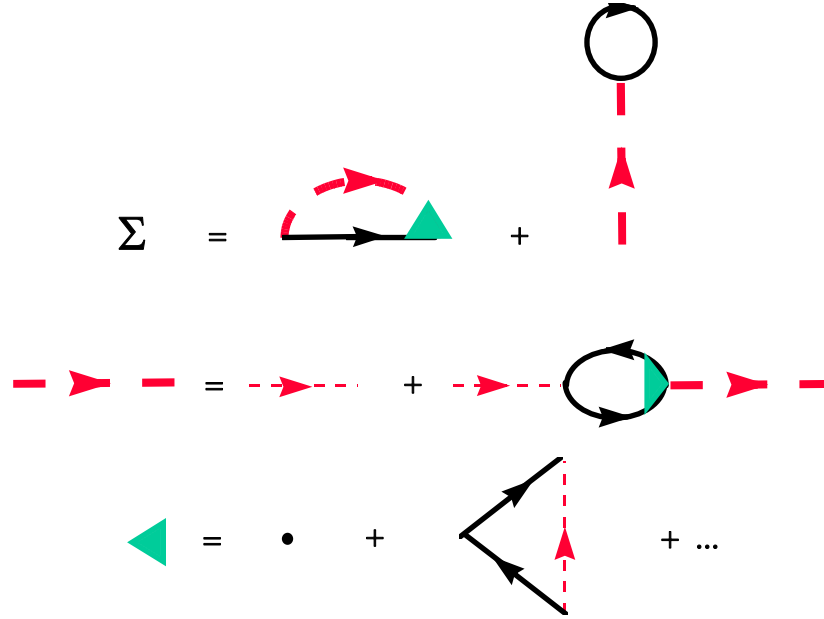


Figure 5-36 Exact resummation of the diagrammatic perturbation expansion. The dressed interaction on the second line involves the one-interaction irreducible polarisation propagator. The last line gives the first terms of the diagrammatic expansion for the vertex corrections.

We will see in a subsequent chapter that the theory for electron-phonon interactions may be written precisely in the form of Fig.(5-36) 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.(5-36) then form a closed set of equations. Migdal's theorem is behind the success of electron-phonon theories, in particular the theory of superconductivity 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[25], have proven more successful. We will show algebraically in a later chapter that perturbation theory for electron-electron interactions may also be formulated in a way that is diagrammatically equivalent to Fig.(5-37). That is our second exact reformulation of perturbation theory[26] (there are others). 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

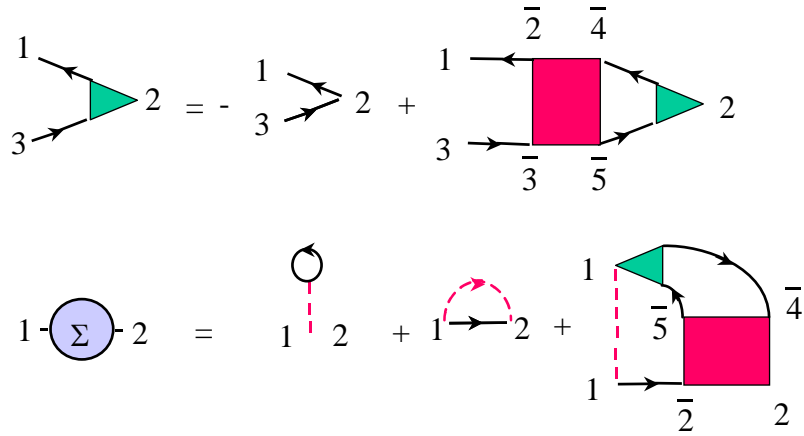


Figure 5-37 Exact representation of the full perturbation series. The triangle now represents the fully reducible vertex whereas the box represents all terms that are irreducible with respect to cutting a particle-hole pair of lines in the indicated channel.

many-body theory, such as the Pauli principle and conservation laws. This will be discussed in a later chapter.

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6. BROKEN SYMMETRY, FERRO- MAGNETISM AS AN EXAMPLE

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 by 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. 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. At the end of the chapter we will touch upon many problems of mean-field theories.

6.1 The Hubbard model

Suppose we consider the band closest to the Fermi energy for electrons moving on a lattice. We have seen that for energies not too far from the Fermi surface, the Coulomb interaction is screened, or short-ranged. Around 1964, Kanamori, Gutzwiller and Hubbard decided that it would be instructive to look at the limiting case where there is a non-zero Coulomb repulsion only when two electrons of opposite spins are in the same orbital. The simple-looking Hamiltonian reads

$$H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_{i,\sigma,\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} \quad (6.1)$$

$$= - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (6.2)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are creation and annihilation operators for electrons of spin σ in the Wannier orbital centered around site i , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ 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. 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 principle $c_{i\sigma}^\dagger c_{i\sigma}^\dagger = 0$.

Remark 117 *This last statement is important. To obtain the Hubbard model where up electrons interact only with down, we had to assume that the Pauli principle is satisfied exactly. So approximation methods that do not satisfy this constraint are suspicious.*

6.1.1 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

$$H_0 = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} \quad (6.3)$$

so that using

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma} \quad (6.4)$$

$$c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma}^\dagger \quad (6.5)$$

with \mathbf{r}_i the position of site i , and

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = N\delta_{\mathbf{k},0} \quad (6.6)$$

we find

$$\begin{aligned} H_0 &= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \\ \varepsilon_{\mathbf{k}} &= -2t(\cos k_x a + \cos k_y a) \end{aligned} \quad (6.7)$$

with a the lattice spacing. From now on, we take $a = 1$. The equal energy curves are drawn in Fig.(). 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

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a) \sim C + \frac{k_x^2 + k_y^2}{2m_b}. \quad (6.8)$$

6.1.2 The strongly interacting, atomic, limit $t = 0$

If there are no hoppings and only disconnected atomic sites,

$$H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (6.9)$$

there are two energy levels, corresponding 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

$$Z = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta(U-2\mu)}. \quad (6.10)$$

Already at this level we see that there are “correlations”. Z can be factored into $(1 + e^{\beta\mu})^2$ only if there are no interactions.

Things become more subtle when we consider the “dynamics”, as embodied for example in the Green function

$$G_{\sigma}(\tau) = -\langle T_{\tau} [c_{\sigma}(\tau) c_{\sigma}^{\dagger}] \rangle. \quad (6.11)$$

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 straightforward 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).

$$\frac{\partial G_{\sigma}(\tau)}{\partial \tau} = -\delta(\tau) - \langle T_{\tau} [[K, c_{\sigma}(\tau)] c_{\sigma}^{\dagger}] \rangle \quad (6.12)$$

$$= -\delta(\tau) + \mu G_{\sigma}(\tau) + U \langle T_{\tau} [c_{\sigma}(\tau) n_{-\sigma}(\tau) c_{\sigma}^{\dagger}] \rangle \quad (6.13)$$

This 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

$$G_{2,\sigma}(\tau) = \langle T_{\tau} [c_{\sigma}(\tau) n_{\sigma}(\tau) c_{\sigma}^{\dagger}] \rangle = \langle T_{\tau} [c_{\sigma} n_{-\sigma} c_{\sigma}^{\dagger}(-\tau)] \rangle. \quad (6.14)$$

Following the usual approach,

$$\frac{\partial G_{2,\sigma}(\tau)}{\partial \tau} = -\delta(\tau) \langle n_{-\sigma} \rangle + \mu G_{2,\sigma}(\tau) + U G_{2,\sigma}(\tau). \quad (6.15)$$

Instead of generating a higher order correlation function in the term coming from $[K, c_{\sigma}^{\dagger}(-\tau)]$, 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 (6.13) and (6.15) form a closed set of equations that is easy to solve in Matsubara frequencies where they become

$$(i\omega_n + \mu) G_{\sigma}(i\omega_n) = 1 + U G_{2,\sigma}(i\omega_n) \quad (6.16)$$

$$(i\omega_n + \mu) G_{2,\sigma}(i\omega_n) = \langle n_{-\sigma} \rangle + U G_{2,\sigma}(i\omega_n). \quad (6.17)$$

Substituting the second equation in the first

$$(i\omega_n + \mu) G_{\sigma}(i\omega_n) = 1 + \frac{U \langle n_{-\sigma} \rangle}{(i\omega_n + \mu - U)}. \quad (6.18)$$

Since

$$\frac{U \langle n_{-\sigma} \rangle}{(i\omega_n + \mu)(i\omega_n + \mu - U)} = \frac{U \langle n_{-\sigma} \rangle}{U} \left[\frac{1}{(i\omega_n + \mu - U)} - \frac{1}{(i\omega_n + \mu)} \right] \quad (6.19)$$

we are left with

$$G_{\sigma}(i\omega_n) = \frac{1 - \langle n_{-\sigma} \rangle}{i\omega_n + \mu} + \frac{\langle n_{-\sigma} \rangle}{i\omega_n + \mu - U} \quad (6.20)$$

$$G_{\sigma}^R(\omega) = \frac{1 - \langle n_{-\sigma} \rangle}{\omega + i\eta + \mu} + \frac{\langle n_{-\sigma} \rangle}{\omega + i\eta + \mu - U}.$$

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 affinity and ionization potential of the atom.

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,

$$G_{\sigma}^R(\omega) = \frac{1}{2} \left(\frac{1}{\omega + i\eta + U/2} + \frac{1}{\omega + i\eta - U/2} \right) = \frac{(\omega + i\eta)}{(\omega + i\eta)^2 - \left(\frac{U}{2}\right)^2} \quad (6.21)$$

$$= \frac{1}{(\omega + i\eta) - \frac{U^2}{4(\omega + i\eta)}} \quad (6.22)$$

so that clearly, the retarded self-energy $\frac{U^2}{4(\omega + i\eta)}$ is singular at low frequency.

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.

6.2 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. We will look at this result from many points of view. And then we will see that Stoner's argument has some problems and that ferromagnetism is much harder to find than what Stoner first thought.

6.2.1 Simple arguments, the Stoner model

In the Hartree Fock approximation,

$$\tilde{\epsilon}_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle \quad (6.23)$$

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 practical 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

$$\varepsilon_{\mathbf{k}_{F\uparrow}} - \varepsilon_{\mathbf{k}_{F\downarrow}} = U (\langle n_{\downarrow} \rangle - \langle n_{F\uparrow} \rangle). \quad (6.24)$$

Expanding the left-hand side in powers of $\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle$ we have, using that $\frac{\partial \varepsilon_{\mathbf{k}_{F\sigma}}}{\partial k_{F\sigma}} \frac{\partial k_{F\sigma}}{\partial n_{\sigma}}$ is independent of spin,

$$\frac{\partial \varepsilon_{k_F}}{\partial k_F} \frac{\partial k_F}{\partial n} (\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle) = U (\langle n_{\downarrow} \rangle - \langle n_{F\uparrow} \rangle) \quad (6.25)$$

$$\frac{\partial \varepsilon_{k_F}}{\partial n} = U \quad (6.26)$$

$$1 = U \frac{\partial n}{\partial \varepsilon_{k_F}} = U \frac{\partial}{\partial \varepsilon_{k_F}} \int^{\varepsilon_{k_F}} N(\varepsilon) d\varepsilon \quad (6.27)$$

$$1 = UN(\varepsilon_{k_F}) \quad (6.28)$$

where $N(E)$ is the density of states for a given spin species. The last formula is the celebrated Stoner criterion for antiferromagnetism.

6.2.2 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

$$|\Psi\rangle = \prod_{\mathbf{k}_{\uparrow}} \theta(k_{F\uparrow} - |\mathbf{k}|) \prod_{\mathbf{k}_{\downarrow}} \theta(k_{F\downarrow} - |\mathbf{k}|) c_{\mathbf{k}_{\uparrow}}^{\dagger} c_{\mathbf{k}_{\downarrow}}^{\dagger} |0\rangle. \quad (6.29)$$

Using Ritz's variational principle, we need to minimize

$$\langle \Psi | H - \mu N | \Psi \rangle = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} - \mu) \langle n_{\mathbf{k}, \sigma} \rangle + NU \langle n_{-\sigma} \rangle \langle n_{\sigma} \rangle. \quad (6.30)$$

We will not proceed further since this is a special case ($T = 0$) of the more general equations treated in the following section.

6.2.3 Feynman's variational principle for variational Hamiltonian. Order parameter and ordered state

Anticipating that there will be a broken symmetry, it is tempting to choose as a trial Hamiltonian

$$\tilde{H}_0 = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + U \sum_i (\langle n_{i\uparrow} \rangle n_{i\downarrow} + \langle n_{i\downarrow} \rangle n_{i\uparrow}) \quad (6.31)$$

$$= \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{k}} \left(\langle n_{\uparrow} \rangle c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow} + \langle n_{\downarrow} \rangle c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} \right) \quad (6.32)$$

In other words, it is as if we had written in the interaction term $n_{i\uparrow} \rightarrow \langle n_{i\uparrow} \rangle + \delta n_{i\uparrow}$ and neglected the terms quadratic in δn_i (with at the end $\delta n_{i\uparrow} \rightarrow n_{i\uparrow}$).

The calculation then proceeds as usual by using Feynman's variational principle

$$-T \ln Z \leq -T \ln Z_{\tilde{0}} + \left\langle (H - \tilde{H}_0) \right\rangle_{\tilde{0}} \quad (6.33)$$

to minimize the right-hand side, which can be written, using the usual definition $\zeta_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$

$$-T \ln \left[\prod_{\mathbf{k}} \left(1 + e^{-\beta(\zeta_{\mathbf{k}} + U \langle n_{\uparrow} \rangle)} \right) \left(1 + e^{-\beta(\zeta_{\mathbf{k}} + U \langle n_{\downarrow} \rangle)} \right) \right] + UN \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle - 2UN \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle. \quad (6.34)$$

Defining

$$n = \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle \quad (6.35)$$

and the “order parameter”

$$m = \langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle \quad (6.36)$$

that measures the magnetization, or spin polarization, we set the derivative with respect of m equal to zero to obtain the extremum. This leads to

$$\sum_{\sigma} \left\{ \left[-T \sum_{\mathbf{k}} \frac{e^{-\beta(\zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle)}}{1 + e^{-\beta(\zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle)}} \left(\beta U \frac{\partial \langle n_{-\sigma} \rangle}{\partial m} \right) \right] - UN \left(\frac{\partial \langle n_{\sigma} \rangle}{\partial m} \langle n_{-\sigma} \rangle \right) \right\} = 0 \quad (6.37)$$

which, using the definition of the magnetization Eq.(6.36) and of the Fermi function, can be written

$$- \sum_{\mathbf{k}} f(\zeta_{\mathbf{k}} + U \langle n_{\downarrow} \rangle) + \sum_{\mathbf{k}} f(\zeta_{\mathbf{k}} + U \langle n_{\uparrow} \rangle) - N \langle n_{\downarrow} \rangle + N \langle n_{\uparrow} \rangle = 0. \quad (6.38)$$

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

$$\langle n_{\downarrow} \rangle + \langle n_{\uparrow} \rangle = \frac{1}{N} \sum_{\mathbf{k}} (f(\zeta_{\mathbf{k}} + U \langle n_{\uparrow} \rangle) + f(\zeta_{\mathbf{k}} + U \langle n_{\downarrow} \rangle)). \quad (6.39)$$

6.2.4 The gap equation and Landau theory in the ordered state

Using our definition of the magnetization Eq.(6.36) and the equation for the minimum Eq.(6.38), we obtain an equation (also called the gap equation) for the order parameter m ,

$$m = \frac{1}{N} \sum_{\mathbf{k}} \left(f \left(\zeta_{\mathbf{k}} + U \frac{n}{2} - U \frac{m}{2} \right) + f \left(\zeta_{\mathbf{k}} + U \frac{n}{2} + U \frac{m}{2} \right) \right). \quad (6.40)$$

Suppose we are close to the transition where m is small. Expanding the right-hand side, we have

$$m = \frac{1}{N} \sum_{\mathbf{k}} \frac{\partial f(\zeta_{\mathbf{k}})}{\partial \zeta_{\mathbf{k}}} (-Um) + O(m^3) \quad (6.41)$$

$$= UN(\varepsilon_{k_F}) m + O(m^3), \quad (6.42)$$

where we have used that as $T \rightarrow 0$ the derivative of the Fermi function becomes minus a delta function.

The last equation may also be written

$$(1 - UN(\varepsilon_{k_F})) m = bm^3 \quad (6.43)$$

where a more detailed calculation gives that

$$b = \frac{N''(\varepsilon_{k_F})}{24} - \frac{(N'(\varepsilon_{k_F}))^2}{8N(\varepsilon_{k_F})}. \quad (6.44)$$

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.(6.43) 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.(6.43)? First of all we recover the Stoner criterion, $m = 0$ when $1 = UN(E_F)$ and takes a finite value $m^2 = b/(1 - UN(E_F))$ 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 118 *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.(6.41) is temperature dependent. In Eq.(6.42) we have taken the zero temperature limit.*

6.2.5 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 \tilde{H}_0 is spin dependent

$$\tilde{H}_0 = \sum_{\mathbf{k}, \sigma} \tilde{\varepsilon}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \quad (6.45)$$

Starting from the diagrams in Fig.(5-23) 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

$$\tilde{\Sigma}_\sigma = U \langle n_{-\sigma} \rangle + \varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_{\mathbf{k}\sigma} = 0 \quad (6.46)$$

so that we recover the Stoner result $\tilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle$. The gap equation is obtained from

$$G_\sigma(\mathbf{k}, ik_n) = \frac{1}{ik_n - \tilde{\varepsilon}_{\mathbf{k}\sigma} + \mu} \quad (6.47)$$

from which we extract the spin-dependent density

$$\langle n_\sigma \rangle = T \sum_n e^{ik_n \eta} \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{ik_n - \tilde{\varepsilon}_{\mathbf{k}\sigma} + \mu} \quad (6.48)$$

$$= \frac{1}{N} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle - \mu). \quad (6.49)$$

Adding the previous equations to $\langle n_\downarrow \rangle + \langle n_\uparrow \rangle$, we recover all the previous results for the magnetization etc.

6.2.6 Instability of the normal state

In this section, we will see 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

$$\left. \frac{\partial \langle S_z \rangle}{\beta \partial h} \right|_{h=0} = \left. \frac{\partial}{\beta \partial h} \frac{\text{Tr} [e^{-\beta(K-hS_z)} S_z]}{\text{Tr} [e^{-\beta(K-hS_z)}]} \right|_{h=0} \quad (6.50)$$

$$= \langle S_z S_z \rangle - \langle S_z \rangle \langle S_z \rangle \equiv \langle S_z S_z \rangle_c. \quad (6.51)$$

The noninteracting limit

The spin susceptibility is obtained from the spin-spin correlation function. Very schematically, consider the connected part of the time-ordered product,

$$\langle T_\tau S_z S_z \rangle_c = \langle T_\tau (n_\uparrow - n_\downarrow) (n_\uparrow - n_\downarrow) \rangle_c \quad (6.52)$$

$$= \langle T_\tau n_\uparrow n_\uparrow \rangle_c + \langle T_\tau n_\downarrow n_\downarrow \rangle_c - \langle T_\tau n_\uparrow n_\downarrow \rangle_c - \langle T_\tau n_\downarrow n_\uparrow \rangle_c \quad (6.53)$$

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

$$\langle T_\tau \rho \rho \rangle_c = \langle T_\tau (n_\uparrow + n_\downarrow) (n_\uparrow + n_\downarrow) \rangle_c \quad (6.54)$$

$$= \langle T_\tau n_\uparrow n_\uparrow \rangle_c + \langle T_\tau n_\downarrow n_\downarrow \rangle_c + \langle T_\tau n_\uparrow n_\downarrow \rangle_c + \langle T_\tau n_\downarrow n_\uparrow \rangle_c. \quad (6.55)$$

Since the last two terms do not contribute, we are left for both spin and charge with

$$\chi_0(\mathbf{q}, iq_n) = -\frac{1}{N} \sum_{\mathbf{p}, \sigma} T \sum_n G_\sigma^0(\mathbf{p} + \mathbf{q}, ip_n + iq_n) G_\sigma^0(\mathbf{p}, ip_n) \quad (6.56)$$

$$= -\frac{2}{N} \sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{iq_n + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}. \quad (6.57)$$

Rotational invariance should give us

$$\langle T_\tau S^+ S^- \rangle_c + \langle T_\tau S^- S^+ \rangle_c = \frac{1}{4} \langle T_\tau (S_x + iS_y) (S_x - iS_y) \rangle_c \quad (6.58)$$

$$+ \frac{1}{4} \langle T_\tau (S_x - iS_y) (S_x + iS_y) \rangle_c \quad (6.59)$$

$$= \frac{1}{2} (\langle T_\tau S_x S_x \rangle_c + \langle T_\tau S_y S_y \rangle_c) \\ = \langle T_\tau S_z S_z \rangle_c. \quad (6.60)$$

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 $S^+ S^-$.

Effect of interactions

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 $\langle T_\tau S_z S_z \rangle_c$ is given in Fig.(?). It is different from the set of diagrams that contributes to $\langle T_\tau S^+ S^- \rangle_c + \langle T_\tau S^- S^+ \rangle_c$ but the final answer is the same in the paramagnetic state with no broken symmetry. Bubbles only contribute to $\langle T_\tau S_z S_z \rangle_c$ but the odd terms have one extra minus sign because the minus sign in $-\langle T_\tau n_\uparrow n_\downarrow \rangle_c - \langle T_\tau n_\downarrow n_\uparrow \rangle_c$. Hence, the result is exactly the same as for $\langle T_\tau S^+ S^- \rangle_c + \langle T_\tau S^- S^+ \rangle_c$ that we compute with the ladder sum in Fig.(?). Consider for example $\langle T_\tau S^+ S^- \rangle_c$. 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

$$\langle T_\tau S^+ S^- \rangle_c = \frac{\chi_0}{2} + \frac{\chi_0}{2} (-U) \left(-\frac{\chi_0}{2} \right) + \frac{\chi_0}{2} (-U)^2 \left(-\frac{\chi_0}{2} \right)^2 + \dots \quad (6.61)$$

$$= \frac{\chi_0/2}{1 - \frac{U}{2}\chi_0}. \quad (6.62)$$

We thus obtain in Fourier space where the above equation is algebraic,

$$\chi = \langle T_\tau S^+ S^- \rangle_c + \langle T_\tau S^- S^+ \rangle_c = \langle T_\tau S_z S_z \rangle_c = \frac{\chi_0}{1 - \frac{U}{2}\chi_0}. \quad (6.63)$$

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

$$\chi(\mathbf{q}, iq_n) = \int \frac{d\omega}{\pi} \frac{\chi''(\mathbf{q}, \omega)}{\omega - iq_n} \\ = \int \frac{d\omega}{\pi} \frac{\omega \chi''(\mathbf{q}, \omega)}{(\omega)^2 + (q_n)^2} \quad (6.64)$$

hence *a fortiori* $\chi(\mathbf{q}, 0)$ is positive. Hence, the RPA result Eq.(6.63) is non-physical when $1 < \frac{U}{2}\chi_0(\mathbf{q}, 0)$. There is a phase transition when the generalized

Stoner criterion

$$\boxed{1 = \frac{U}{2} \chi_0(\mathbf{q}, 0)} \quad (6.65)$$

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

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \chi_0(\mathbf{q}, 0) = \lim_{\mathbf{q} \rightarrow \mathbf{0}} -\frac{2}{N} \sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} = -\frac{2}{N} \sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \quad (6.66)$$

which reduces to $2N(\varepsilon_{k_F})$ in the zero temperature limit. So we recover the simple special case found previously for example in Eq.(6.28).

6.2.7 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. 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

$$\chi(\mathbf{q}, 0) \approx \frac{\chi_0(\mathbf{0}, 0)}{1 - \frac{U}{2} \chi_0(\mathbf{q}, 0) - \left(\frac{U}{2}\right)^2 \frac{\partial^2 \chi_0(\mathbf{q}, 0)}{\partial^2 q^2} q^2} \sim \frac{A}{\xi^{-2} + q^2} \quad (6.67)$$

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

$$S_{\perp}(\mathbf{q}, \omega) = \frac{2}{1 - e^{-\beta\omega}} \chi_{\perp}''(\mathbf{q}, \omega). \quad (6.68)$$

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,

$$S_{\perp}(\mathbf{q}, \omega) = 2 \text{Im} \left[\frac{\chi_0^R}{1 - \frac{U}{2} \chi_0^R} \right] = \frac{2\chi_0''(\mathbf{q}, \omega)}{\left(1 - \frac{U}{2} \chi_0'(\mathbf{q}, \omega)\right)^2 + \left(\frac{U}{2} \chi_0''(\mathbf{q}, \omega)\right)^2} \quad (6.69)$$

$$\approx \frac{2\chi_0''(\mathbf{q}, \omega)}{\left(1 - UN(\varepsilon_{k_F})\right)^2 + \left(\frac{U}{2} \chi_0''(\mathbf{q}, \omega)\right)^2}. \quad (6.70)$$

To evaluate $\chi_0''(\mathbf{q}, \omega)$, it suffices to analytically continue our general result for the non-interacting spin susceptibility Eq.(6.57) in the small \mathbf{q} limit

$$\chi_0^R(\mathbf{q}, \omega) = -\frac{2}{N} \sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} \quad (6.71)$$

$$\approx -\frac{2}{N} \sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \frac{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} \quad (6.72)$$

and to use

$$\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}} = -\frac{\mathbf{p} \cdot \mathbf{q}}{m} - \frac{q^2}{2m}$$

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 $\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}} \approx -\mathbf{v}_F \cdot \mathbf{q}$

$$\chi_0^R(\mathbf{q}, \omega) = 2 \int d\varepsilon N(\varepsilon) \int_{-1}^1 \frac{d(\cos \theta)}{2} \frac{\partial f(\varepsilon - \mu)}{\partial \varepsilon} \frac{v_F q \cos \theta}{\omega + i\eta - v_F q \cos \theta} \quad (6.73)$$

$$\begin{aligned} \chi_0''(\mathbf{q}, \omega) &= -2\pi \int d\varepsilon N(\varepsilon) \int_{-1}^1 \frac{d(\cos \theta)}{2} \frac{\partial f(\varepsilon - \mu)}{\partial \varepsilon} v_F q \cos(\theta) \delta(\omega - v_F q \cos \theta) \\ &= \pi N(\varepsilon_{k_F}) \frac{\omega}{v_F q} \equiv C \frac{\omega}{v_F q} \end{aligned} \quad (6.75)$$

Substituting in the RPA expression Eq.(6.69) we find

$$S_{\perp}(\mathbf{q}, \omega) = 2\chi_{\perp}''(\mathbf{q}, \omega) = \frac{2C \frac{\omega}{v_F q}}{(1 - UN(\varepsilon_{k_F}))^2 + \left(C \frac{\omega}{v_F q}\right)^2}. \quad (6.76)$$

This function is plotted in Fig.(?) as a function of ω for two small values of \mathbf{q} and for $U = 0$ and $UN(\varepsilon_{k_F}) = 0.8$ 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 $\xi^{-2} \approx 1 - UN(\varepsilon_{k_F})$ 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

$$\chi_{\perp}(\mathbf{q}, \omega) = \frac{A}{\xi^{-2} + aq^2 + bh^{2/3} - c \frac{i\omega}{v_F q}}. \quad (6.77)$$

6.2.8 Collective Goldstone mode, stability and the Mermin-Wagner theorem

What do the collective modes look like in the ordered state? The energy to make a particle-hole excitation by creating say a hole of up spin and a particle of down spin, as can be done for example by scattering a neutron that flips its spin, is $\varepsilon_{\mathbf{k}_{F\downarrow}} - \varepsilon_{\mathbf{k}_{F\uparrow}} = U(\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle) = Um$. This tells us, with $m > 0$, that there is a gap

$$\Delta = Um$$

in the particle-hole continuum in the ordered state. 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 the collective modes. 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 will be very small by continuity.

Transverse 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.(6.63). 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,

$$\chi_{\perp}^{R-+}(\mathbf{q}, \omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)} \quad (6.78)$$

with, given the new excitation spectrum in the ordered state, a new definition of the “non-interacting” susceptibility $\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)$

$$\chi_{0\perp}^{R-+}(\mathbf{q}, \omega) = -\frac{1}{N} \sum_{\mathbf{p}} \frac{f(\tilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\tilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta + \tilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \tilde{\zeta}_{\mathbf{p}\downarrow}}. \quad (6.79)$$

that corresponds to the diagram in Fig.(?). Expanding as before in the small \mathbf{q} limit, we have for small wave vector

$$\tilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \tilde{\zeta}_{\mathbf{p}\downarrow} \approx \mathbf{v}_F \cdot \mathbf{q} + U(\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle) = \mathbf{v}_F \cdot \mathbf{q} - \Delta \quad (6.80)$$

so that for $\mathbf{v}_F \cdot \mathbf{q} \ll \Delta$ we can expand,

$$\begin{aligned} \chi_{0\perp}^{R-+}(\mathbf{q}, \omega) &\approx -\frac{1}{N} \sum_{\mathbf{p}} \frac{f(\tilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\tilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta - \Delta} \\ &\times \left[1 - \frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta} \right)^2 + \dots \right] \\ &\approx -(\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle) \left(\frac{1}{\omega + i\eta - \Delta} + O(q^2) \right) = \frac{-\Delta/U}{\omega + i\eta - \Delta} + O(q^2) \end{aligned} \quad (6.81)$$

The above formula immediately gives that at $q = 0$ imaginary part is non 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 $|\omega| < \Delta$

$$\chi_{\perp}^{R-+}(\mathbf{q}, \omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)} \approx \frac{\frac{-\Delta/U}{\omega + i\eta - \Delta}}{1 - \frac{-\Delta}{\omega + i\eta - \Delta} + UCq^2} \quad (6.83)$$

$$\approx \frac{-\Delta/U}{\omega + i\eta - Dq^2}. \quad (6.84)$$

The complete transverse spin susceptibility is obtained by combining the two results

$$\begin{aligned} \chi_{\perp}^{R-+}(\mathbf{q}, \omega) + \chi_{\perp}^{R+-}(\mathbf{q}, \omega) &= \frac{-\Delta/U}{\omega + i\eta - Dq^2} + \frac{\Delta/U}{\omega + i\eta + Dq^2} \\ &= -\frac{\Delta}{U} \frac{2Dq^2}{(\omega + i\eta)^2 - (Dq^2)^2}. \end{aligned} \quad (6.85)$$

In these expressions we have used that the calculation of $\chi_{0\perp}^{R-+}(\mathbf{q}, \omega)$ amounts to changing $\Delta \rightarrow -\Delta$ 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 $\omega = \pm Dq^2$ where $D = \Delta \frac{U}{2} C$. We did not evaluate the constant C .

This mode, a Goldstone mode, appears in the particle-hole continuum gap. We can also see this from the imaginary part

$$\text{Im}(\chi_{\perp}^{R-+}(\mathbf{q}, \omega) + \chi_{\perp}^{R+-}(\mathbf{q}, \omega)) = \pi \frac{\Delta}{U} \delta(\omega - Dq^2) - \pi \frac{\Delta}{U} \delta(\omega + Dq^2). \quad (6.86)$$

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 $\text{Im}(\chi_{\perp}^{R-+}(\mathbf{q}, \omega) + \chi_{\perp}^{R+-}(\mathbf{q}, \omega)) \omega > 0$ is violated.

Thermodynamics and the Mermin-Wagner theorem

The thermodynamic transverse susceptibility is obtained from the usual thermodynamic sum rule (Note that $\text{Im}(\chi_{\perp}^{R-+}(\mathbf{q}, \omega') + \chi_{\perp}^{R+-}(\mathbf{q}, \omega'))$ is odd but not each of the terms individually).

$$\chi_{\perp}^{R-+}(\mathbf{q}, \omega = 0) + \chi_{\perp}^{R+-}(\mathbf{q}, \omega = 0) = \int \frac{d\omega'}{\pi} \frac{\text{Im}(\chi_{\perp}^{R-+}(\mathbf{q}, \omega') + \chi_{\perp}^{R+-}(\mathbf{q}, \omega'))}{\omega'} \quad (6.87)$$

The contribution of the Goldstone mode to that susceptibility is easy to obtain from our previous results

$$\chi_{\perp}^{R-+}(\mathbf{q}, \omega = 0) + \chi_{\perp}^{R+-}(\mathbf{q}, \omega = 0) = \frac{\Delta}{U} \frac{2}{Dq^2}. \quad (6.88)$$

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. The $1/q^2$ dependence of the last result is very general. It is a consequence of so-called Bogoliubov inequalities (Foster). 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 $\langle S_x S_y \rangle = 0$. This means that the following quantity

$$T \sum_{iq_n} \frac{1}{N} \sum_{\mathbf{q}} \chi_{\perp}^{-+}(\mathbf{q}, iq_n) e^{\pm iq_n \eta} \quad (6.89)$$

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.(6.84) that the spin-wave contribution to that susceptibility is

$$\chi_{\perp}^{-+}(\mathbf{q}, iq_n) = \frac{-\Delta/U}{iq_n - Dq^2}. \quad (6.90)$$

Substituting this in our previous condition and using the usual result

$$\lim_{\eta \rightarrow 0} T \sum_n \frac{e^{iq_n \eta}}{iq_n - x} = \frac{-1}{e^{\beta x} - 1} \quad (6.91)$$

for performing the sum over bosonic Matsubara frequencies, we obtain in the long wavelength limit

$$T \sum_{i q_n} \frac{1}{N} \sum_{\mathbf{q}} \frac{-\Delta/U}{i q_n - D q^2} e^{i q_n \eta} = \frac{\Delta}{U} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^{\beta D q^2} - 1} \quad (6.92)$$

$$\sim \frac{\Delta}{U} \int \frac{d^d q}{(2\pi)^d} \frac{T}{D q^2} \quad (6.93)$$

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 119 *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 $q^2 C S_{x\mathbf{q}} S_{x-\mathbf{q}}$, so that by the equipartition theorem, $q^2 C \langle S_{x\mathbf{q}} S_{x-\mathbf{q}} \rangle \propto T$. Since the local value of $\langle S_x^2 \rangle$ is obtained from $\int \frac{d^d q}{(2\pi)^d} \langle S_{x\mathbf{q}} S_{x-\mathbf{q}} \rangle$ we recover the previous result Eq.(6.93) concerning the divergence of local fluctuations in two dimensions.*

6.2.9 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 susceptibiloity, we should instead use

$$U_{eff}(\mathbf{Q}, i Q_n) = \frac{U}{1 + U \Lambda(\mathbf{Q}, i Q_n)} \quad (6.94)$$

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 $i Q_n = 0$ 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 $1/\Lambda(\mathbf{Q}, 0)$. 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 node in the two-body wave function. 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

$N(\varepsilon_{k_F})$ is proportional to $1/W$. So at best the product $U_{eff}N(\varepsilon_{k_F})$ 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 discussed in the next section.

6.3 Two-Particle Self-Consistent Approach, motivation

The RPA in two dimensions has some desirable features (it satisfies conservation laws) and many undesirable features - it violates the Mermin-Wagner theorem and the Pauli principle. The Mermin-Wagner theorem says that there is no continuous symmetry breaking in two dimension at finite temperature. (Proof later) But we just saw above, that RPA predicts a finite-temperature phase transition in two dimensions. The Pauli principle on the other hand implies for example that $\langle n_{\uparrow}^2 \rangle = \langle n_{\uparrow} \rangle$ since in the one-band model, n_{\uparrow} is either 1 or 0. To see that the Pauli principle is violated, one can check that in the set of diagrams that are summed by RPA, not all exchanges of lines are included. Fig.() shows a very simple example with three bubbles where we do not include the diagram to the right, which corresponds to the exchange of two of the lines of the diagram to the left that is included in RPA.

A more direct way to see that the Pauli principle is violated is as follows. Consider the following two sum rules for the spin and charge susceptibilities, with q standing for (\mathbf{q}, iq_n) so that the corresponding sum includes also a sum over Matsubara frequencies,

$$\frac{T}{N} \sum_q \chi_{zz}(q) = \langle (n_{\uparrow} - n_{\downarrow})^2 \rangle = n - 2\langle n_{\uparrow}n_{\downarrow} \rangle \quad (6.95)$$

$$\frac{T}{N} \sum_q \chi_{\rho\rho}(q) = \langle (n_{\uparrow} + n_{\downarrow})^2 \rangle - n^2 = n + 2\langle n_{\uparrow}n_{\downarrow} \rangle - n^2.$$

On the right-hand side we have also used $\langle n_{\uparrow}^2 \rangle = \langle n_{\uparrow} \rangle$ (and the analog for down spin). Adding both equations we obtain

$$\frac{T}{N} \sum_q [\chi_{zz}(q) + \chi_{\rho\rho}(q)] = 2n - n^2. \quad (6.96)$$

In the RPA approximation this would mean

$$\frac{T}{N} \sum_q \left[\frac{\chi^0(q)}{1 - \frac{U}{2}\chi^0(q)} + \frac{\chi^0(q)}{1 + \frac{U}{2}\chi^0(q)} \right] = 2n - n^2. \quad (6.97)$$

But the above equation is not satisfied, as one can see by recalling that without interactions $\frac{T}{N} \sum_q 2\chi^0(q) = 2n - n^2$ which implies by expanding the denominators that the identity is violated to second order in U already.

Rest of TPSC some other time.

6.4 Antiferromagnetism close to half-filling, nesting

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

$$\zeta_{\mathbf{p}+\mathbf{Q}} = -2t(\cos(k_x + \pi) + \cos(k_y + \pi)) = -\zeta_{\mathbf{p}}. \quad (6.98)$$

Using this result we find that the zero-frequency susceptibility at that wave vector \mathbf{Q} is

$$\begin{aligned} \chi_0^R(\mathbf{Q}, 0) &= -\frac{2}{N} \sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{Q}})}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{Q}}} = -\frac{2}{N} \sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(-\zeta_{\mathbf{p}})}{2\zeta_{\mathbf{p}}} \quad (6.99) \\ &= \frac{1}{N} \sum_{\mathbf{p}} \frac{1 - 2f(\zeta_{\mathbf{p}})}{\zeta_{\mathbf{p}}} = \frac{1}{2} \int d\varepsilon N(\varepsilon) \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{2\varepsilon}. \quad (6.100) \end{aligned}$$

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 $\ln(W/T)$ where W is the bandwidth. This means that at sufficiently low temperature, the criterion $1 - \frac{U}{2}\chi_0^R(\mathbf{Q}, 0) = 0$ 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 $N(\varepsilon)$ so that in fact $\chi_0^R(\mathbf{Q}, 0)$ scales like $\ln^2(W/T)$, 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.

6.5 Additional remarks: Hubbard-Stratonovich transformation and critical phenomena