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

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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 practival 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 $\hbar/1\,\mathrm{eV} \sim 10^{-15}s$. If we take the characteristic macroscopic scale to be $1s$, the leap to go between the two scale is as big as that necessary to go from $1s$ to a sizeable fraction of 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.

Note that indifference to details about higher energy scales, or shorter distances if you wish, also occurs in purely classical mechanics. Ordinary hydrodynamics, as contained in the Navier-Stokes equation, is a theory that is valid for a very broad class of liquids. The specific atomic details will come in for example in determining the specific value of viscosity for example, but the concept of viscosity is a notion that emerges at long wave lengths and large time scales.

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 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 adiabiatically connected to the original Hamiltonian. At phase transitions, the free energy has mathematical singularities that cannot be treated by perturbation theory. These new phases can very often be connected to a new Hamiltonian, that must 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 cunjunction 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 hidding places, is part of what it means to understand the physics of a problem. We work part with images, part with formalism, but in quantum mechanics, often the images or physical intuitions are meaningless without the formalism.

This 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.

Part I

A refresher in statistical mechanics and quantum mechanics

This first part will contain some of the results you might have seen in earlier courses on statistical mechanics and quantum mechanics that do not use Green's functions. They will help set some of the notation but they are not necessarily a prerequisite for what follows.

2. STATISTICAL PHYSICS AND DENSITY MATRIX

2.1 Density matrix in ordinary quantum mechanics

Quantum mechanics tells us that the expectation value of an observable O in a *normalized* state $|\psi\rangle$ is given by $\langle\psi| O |\psi\rangle$. Expanding over complete sets of states, we obtain

$$\begin{aligned} \langle\psi| O |\psi\rangle &= \sum_{i,j} \langle\psi| i\rangle \langle i| O |j\rangle \langle j |\psi\rangle && (2.1) \\ &= \sum_{i,j} \langle j |\psi\rangle \langle\psi| i\rangle \langle i| O |j\rangle && (2.2) \\ &= \sum_{i,j} \langle j| \rho |i\rangle \langle i| O |j\rangle && (2.3) \\ &= \mathrm{Tr}\left[\rho O\right] && (2.4) \end{aligned}$$

where the *Density Matrix* ρ is defined, as an operator, by

$$\rho \equiv |\psi\rangle \langle\psi| \,. \tag{2.5}$$

This is when we have a *pure* state. If the state is prepared in a statistical superposition, in other words, if we have a certain probability p_n that the state that is prepared is $|\psi_n\rangle$, then the expectation value of an observable will be given by the weighted sum of the results in each state, in other words, in the above formula for the average we should use

$$\rho \equiv \sum_n p_n |\psi_n\rangle \langle\psi_n| \,. \tag{2.6}$$

This is the density matrix for a *mixed state.* Note that

$$\rho^2 = \sum_{n,m} p_n p_m |\psi_n\rangle \langle\psi_n| \psi_m\rangle \langle\psi_m| \,. \tag{2.7}$$

We have the property $\rho^2 = \rho$ only for a *pure* state.

When a system of interest is in contact with an environment, it is very useful to work with an effective density matrix obtained by taking the trace first over the degrees of freedom of the environment. This idea is common in particular in the field of quantum information. In this school, we will see that by considering part of a large system as the environment, we can greatly reduce the size of the Hilbert space that needs to be considered to diagonalize a Hamiltonian, especially in one dimension. The optimal way of doing this was found by Steve White and will be discussed in the context of the "Density Matrix Renormalization Group". Not so surprisingly, quantum information theory has helped to improve even further this approach. Uli Schollwöck will explain this.

2.2 Density Matrix in Statistical Physics

Statistical Physics tells us that conserved quantities play a special role. Indeed, at equilibrium, the density matrix cannot depend on time, so it depends only on conserved quantities. This means that generally, the density matrix is diagonal in the energy and number basis for example. All that is left to do is to specify p_n. The basic postulate of statistical physics is that in an isolated system, all mcroscopic states consistent with the value of the conserved quantities are equiprobable. This is the microcanonical ensemble where p_n is identical for all energy eigenstates $|\psi_n\rangle$. The other ensembles are derived in the usual way by considering the microcanonical system as including the system of interest and various reservoirs. In the canonical ensemble for example, $p_n = e^{-\beta E_n}/Z$ where Z is the partition function $\sum_n e^{-\beta E_n}$ and $\beta = (k_B T)^{-1}$.

Alternatively, the various ensembles are obtained by maximizing the entropy

$$S \equiv -k_B \mathrm{Tr}\left[\rho \ln \rho\right] \tag{2.8}$$

subject to constraints such as fixed average energy and normalization in the case of the canonical ensemble. Important properties of the entropy include extensivity and concavity. The entropy also plays a major role in quantum information.

2.3 Legendre transforms

Legendre transforms are encountered in mechanics when going from a Lagrangian to a Hamiltonian formulation. That transformation is extremely useful in statistical physics as well and it will be used for example by Gabi Kotliar at this School.

The important idea of statistical physics that we start with is that of potentials. If you know the entropy as a function of mechanical quantities, like energy volume and number of particles for example, then you know all the thermodynamics. Indeed,

$$\begin{aligned} dE &= TdS - pdV + \mu dN & (2.9)\\ dS &= \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dN & (2.10)\end{aligned}$$

so you can obtain temperature T, pressure p and chemical potential μ simply by taking partial derivatives of the entropy. $(1/T, S)$ $(p/T, V)$ $(-\mu/T, N)$ are pairs of conjugate variables. Instead of using E, V, N as independent variables, given the concavity of the entropy and the uniqueness of the equilibrium state, you can write S as a function of any three other variables. Nevertheless, the purely mechanical variables E, V, N are the most natural ones for the entropy. The entropy plays the role of a thermodynamic potential. As a function of all microscopic variables not fixed by E, V, N, it is maximum at equilibrium.

Remark 1 *When there are broken symmetries, additional variables must be added. For example, for a ferromagnet with magnetization* $\mathbf{M}$ *in a magnetic field* $\mathbf{H}$,

$$dE = TdS - pdV + \mu dN + \mathbf{M}\cdot d\mathbf{H} \tag{2.11}$$

There are other potentials. For example, if a system is in contact with a heat reservoir, the work that will be done at constant temperature will be modified by the presence of the reservoir. It is thus physically motivated to define for example the Helmholtz free energy

$$
\begin{aligned}
F &= E - TS && (2.12) \\
T &= \left(\frac{\partial E}{\partial S}\right)_{V,N} && (2.13)
\end{aligned}
$$

In this case

$$
dF = dE - SdT - TdS = -SdT - pdV + \mu dN. \tag{2.14}
$$

The Helmholtz free energy F can be written in terms of any three thermodynamical variables, but T, V, N are the most natural ones. At fixed T, V, N it is the free energy that is a minimum instead of the energy because we have to take into account the reservoir. The change from S to T as a natural variable has been done through the pair of equations (2.12,2.13). This is the general structure of a Legendre transform. F and E are potentials, and the subtraction of the product of the conjugate variables $-\left(\frac{\partial E}{\partial S}\right)_{V,N} S$ does the trick of relating the two potentials

Remark 2 *Note that* $\left(\partial^2 E/\partial S^2\right) = (\partial T/\partial S) = 1/\left(\partial S/\partial T\right) = -1/\left(\partial^2 F/\partial T^2\right).$

2.4 Legendre transform from the statistical mechanics point of view

Note that since

$$
\begin{aligned}
-\frac{F}{T} &= S - \frac{E}{T} && (2.15) \\
&= S - \left(\frac{\partial S}{\partial E}\right)_{V,N} E && (2.16)
\end{aligned}
$$

the quantity $-F/T$ can be seen as the Legendre transform of the microcanonical entropy. From the point of view of statistical mechanics, if we define $\Omega(E)$ as the number of microstate n corresponding to a given energy, then $p_n = 1/\Omega(E)$ for every microstate and

$$
\begin{aligned}
S(E) &= -k_B \mathrm{Tr}\left[\rho \ln \rho\right] = -k_B \sum_n \frac{1}{\Omega(E)} \ln \frac{1}{\Omega(E)} && (2.17) \\
&= k_B \ln \Omega(E) && (2.18)
\end{aligned}
$$

So, from the point of view of statistical mechanics, the Legendre transform of the entropy is obtained from

$$
\begin{aligned}
-\frac{F}{T} &= k_B \ln Z = k_B \ln \sum_n e^{-\beta E_n} && (2.19) \\
&= k_B \ln \sum_E \Omega(E) e^{-\beta E} && (2.20) \\
&= k_B \ln \sum_E e^{\ln \Omega(E)} e^{-\beta E} && (2.21) \\
&= k_B \ln \sum_E e^{(S(E) - E/T)/k_B} && (2.22)
\end{aligned}
$$

Whereas the microcanonical entropy is a function of the energy of microstates, its Legendre transform is summed over energy and is a function of $1/T$, the coefficient of E in both the thermodynamical expression of the Legendre transform Eq.(2.17) and the statistical one Eq.(2.22).

We know that

$$\begin{aligned} \langle E\rangle &= -\frac{\partial \ln Z}{\partial\beta} \\ &= -\frac{\partial\left(-F/T\right)}{\partial\left(1/T\right)} \end{aligned} \tag{2.23}$$

which clarifies the connection between the statistical mechanics and thermodynamical definitions of Legendre transform. E in the case of thermodynamics is really the average energy from the statistical mechanical point of view. The last equation could have been written down directly from the statistical expression for $-F/T$.

3. SECOND QUANTIZATION

3.1 Describing symmetrized or antisymmetrized states

States that describe identical particles must be either symmetrized, for bosons, or antisymmetrized, for fermions. To simplify the calculations, it is useful to use second quantization. As its name suggest, there is also an axiomatic way to introduce this method as a quantization of fields but here we will just introduce it as a calculational tool. The approach will be familiar already if you master ladder operators for the harmonic oscillator.

For definiteness, let us concentrate on fermions. This can be translated for bosons. Define the operator $\psi^\dagger(\mathbf{r})$ that creates a particle in a position eigenstate $|\mathbf{r}\rangle$ and antisymmetrizes the resulting wave function. Define also the vacuum state $|0\rangle$ that is destroyed by the adjoint, namely $\psi(\mathbf{r})|0\rangle = 0$. In this language

$$\begin{aligned}\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')|0\rangle &= \frac{1}{\sqrt{2}}\left(|\mathbf{r}\rangle|\mathbf{r}'\rangle - |\mathbf{r}'\rangle|\mathbf{r}\rangle\right) && (3.1)\\ &\equiv |\mathbf{r},\mathbf{r}'\rangle = -|\mathbf{r}',\mathbf{r}\rangle. && (3.2)\end{aligned}$$

The state to the right is clearly normalized and antisymmetric. There are two copies of the one-particle Hilbert space. In one component of the wave function, the particle in the first copy is at $|\mathbf{r}\rangle$, in the other component the particle in the first copy is at $|\mathbf{r}'\rangle$. Clearly, that can become quite complicated. The two body-wave function $\langle\mathbf{r},\mathbf{r}'|\varphi\rangle$ is antisymmetric and in the case where there are only two one-particle states occupied it is a Slater determinant. Clearly, that becomes a mess. In terms of the creation-annihilation operators however, all we need to know is that by definition of these operators,

$$\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}') + \psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r}) = 0. \tag{3.3}$$

We use the short-hand for anticommutation

$$\left\{\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\} = 0. \tag{3.4}$$

Taking the adjoint,

$$\{\psi(\mathbf{r}),\psi(\mathbf{r}')\} = 0. \tag{3.5}$$

The only thing missing is that

$$\left\{\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}'). \tag{3.6}$$

That is a bit more complicated to show, but let us take it for granted. It is clear that if $\psi^\dagger(\mathbf{r})$ creates a particle, then $\psi(\mathbf{r})$ removes one (or destroys it). If the particles are at different positions, that can be done in any order. If $\mathbf{r} = \mathbf{r}'$, then it will matter if we create a particle before destroying it. If the creation occurs before the destruction, there will be one more particle to destroy. The Dirac delta function comes from normalization in the continuum. For discrete basis, we would have unity on the right.

3.2 Change of basis

A key formula for the “field” operators $\psi^{\dagger}(\mathbf{r})$ is the formula for basis change. Suppose that one has a new complete basis of one-particle states $|\alpha\rangle$. Then, we can change basis as follows:

$$|\mathbf{r}\rangle = \sum_{\alpha} |\alpha\rangle \langle\alpha| \,\mathbf{r}\rangle \tag{3.7}$$

Given the definition of creation operators, the creation operator $\psi^{\dagger}(\mathbf{r})$ for a particle in state $|\mathbf{r}\rangle$ is related to the creation operator $c_{\alpha}^{\dagger}$ for a particle in state $|\alpha\rangle$ by the analogous formula, namely

$$\psi^{\dagger}(\mathbf{r}) = \sum_{\alpha} c_{\alpha}^{\dagger} \langle\alpha| \,\mathbf{r}\rangle\,. \tag{3.8a}$$

This formula is quite useful.

3.3 Second quantized version of operators

3.3.1 One-body operators

If we know the matrix elements of an operator in the one-particle basis, the calculation of any observable can be reduced to some algebra with the creation-annihilation operators. In other words, not only states, but also operators corresponding to observables can be written using creation-annihilation operators. The expression for these operators is independent of the number of particles and formally analogous to the calculation of averages of operators in first quantized notation.

To be more specific, consider the operator for the density of particles at position $|\mathbf{r}\rangle$. It can be written as $\psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})$ as we prove now. Since $ABC - CAB = ABC + ACB - ACB - CAB$ the commutator ot this operator with $\psi^{\dagger}(\mathbf{r}')$ is,

$$\begin{aligned}
\left[\psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})\,,\psi^{\dagger}(\mathbf{r}')\right] &= \psi^{\dagger}(\mathbf{r})\left\{\psi(\mathbf{r})\,,\psi^{\dagger}(\mathbf{r}')\right\} - \left\{\psi^{\dagger}(\mathbf{r})\,,\psi^{\dagger}(\mathbf{r}')\right\}\psi(\mathbf{r}) && (3.9)\\
&= \delta(\mathbf{r}-\mathbf{r}')\,\psi^{\dagger}(\mathbf{r}) && (3.10)
\end{aligned}$$

We can now use the following little “theorem” on commutator of ladder operators:

Theorem 1 *If* $[A,B] = \beta B$ *and* $|\alpha\rangle$ *is an eigenstate of* A *with eigenvalue* α, *then* $B|\alpha\rangle$ *is an eigenstate of* A *with eigenvalue* $\alpha+\beta$, *as follows from* $AB|\alpha\rangle - BA|\alpha\rangle = A(B|\alpha\rangle) - \alpha(B|\alpha\rangle) = \beta(B|\alpha\rangle)$.

Since $\psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})|0\rangle = 0$, the above implies that $\psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})\left(\psi^{\dagger}(\mathbf{r}_1)|0\rangle\right) = \delta(\mathbf{r}-\mathbf{r}_1)\left(\psi^{\dagger}(\mathbf{r}_1)|0\rangle\right)$, and generally a state $\psi^{\dagger}(\mathbf{r}_1)\,\psi^{\dagger}(\mathbf{r}_2)\ldots|0\rangle$ is an eigenstate of $\psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})$ with eigenvalue $\delta(\mathbf{r}-\mathbf{r}_1) + \delta(\mathbf{r}-\mathbf{r}_2) + \ldots$ Clearly, the potential energy of identical electrons in a potential $V(\mathbf{r})$ can ve written

$$\int \psi^{\dagger}(\mathbf{r})\,V(\mathbf{r})\,\psi(\mathbf{r})\,d^3\mathbf{r}. \tag{3.11}$$

The same reasoning leads to the kinetic energy in the momentum basis, where it is diagonal

$$\int c^{\dagger}(\mathbf{k})\frac{\hbar^2\mathbf{k}^2}{2m}c(\mathbf{k})\frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{3.12}$$

Returning to the position-space basis, we obtain

$$\int \psi^{\dagger}(\mathbf{r})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right)\psi(\mathbf{r})\,d^3\mathbf{r}. \tag{3.13}$$

In other words, for any one-body operator, we can always obtain its second-quantized form in the one-particle basis $|\alpha\rangle$ where it is diagonal:

$$\sum_{\alpha} c_{\alpha}^{\dagger}\langle\alpha|O|\alpha\rangle c_{\alpha} = \sum_{\alpha,\beta} c_{\alpha}^{\dagger}\langle\alpha|O|\beta\rangle c_{\beta}. \tag{3.14}$$

If we change to an arbitrary basis

$$|\alpha\rangle = \sum_i |i\rangle\langle i|\,\alpha\rangle \tag{3.15}$$

the operator takes the form

$$\sum_{\alpha,\beta} c_{\alpha}^{\dagger}\langle\alpha|O|\beta\rangle c_{\beta} = \sum_{\alpha,i,j} c_{\alpha}^{\dagger}\langle\alpha|\,i\rangle\langle i|O|j\rangle\langle j|\,\alpha\rangle c_{\alpha} = \sum_{i,j} c_{i}^{\dagger}\langle i|O|j\rangle c_{j}. \tag{3.16}$$

Exemple 2 *Let $\psi_{\alpha}^{\dagger}(\mathbf{r})$ be the creation operator for the position state $|\mathbf{r}\rangle$ with the spin $\alpha = \uparrow, \downarrow$. We know the matrix elements of all component of the spin operators in the basis where S_z is diagonal. Thus, from the last formula, we see that the three components of the spin operator are*

$$\int \psi_{\alpha}^{\dagger}(\mathbf{r})\left(\frac{\hbar}{2}\boldsymbol{\sigma}_{\alpha\beta}\right)\psi_{\beta}(\mathbf{r})\,d^3\mathbf{r} \tag{3.17}$$

where, as usual, the Pauli matrices are given by $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

3.3.2 Two-body operators

Let us now consider a two-body operator such as the potential energy. It is diagonal in position-space. The Coulomb interaction

$$V_c(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \tag{3.18}$$

is an example. The second quantized Coulomb energy takes the form

$$\int V_c(\mathbf{r}-\mathbf{r}')\frac{1}{2}\left(\rho(\mathbf{r})\rho(\mathbf{r}') - \delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})\right)d^3\mathbf{r}d^3\mathbf{r}' \tag{3.19}$$

where the $1/2$ comes from avoiding double-counting and $\delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})$ is necessary not to count the interaction of an electron with itself. Including spin, the density operator is

$$\rho(\mathbf{r}) = \sum_{\sigma}\psi_{\sigma}^{\dagger}(\mathbf{r})\psi_{\sigma}(\mathbf{r}). \tag{3.20}$$

Substituting in the expression for the Coulomb interaction and using anti-commutation relations, we obtain

$$\frac{1}{2}\sum_{\sigma,\sigma'}\int V_c\left(\mathbf{r}-\mathbf{r}'\right)\psi^\dagger_\sigma\left(\mathbf{r}\right)\psi^\dagger_{\sigma'}\left(\mathbf{r}'\right)\psi_{\sigma'}\left(\mathbf{r}'\right)\psi_\sigma\left(\mathbf{r}\right)d^3\mathbf{r}d^3\mathbf{r}'. \tag{3.21}$$

It is an interesting and not very long exercise to prove that formula (which happens to have the same form for bosons and fermions).

Let us change to some arbitrary basis. First notice that in terms of the potential energy operator $\hat{V}_c$

$$V_c\left(\mathbf{r}-\mathbf{r}'\right)=\left\langle\mathbf{r}\right|\left\langle\mathbf{r}'\right|\hat{V}_c\left|\mathbf{r}\right\rangle\left|\mathbf{r}'\right\rangle. \tag{3.22}$$

Then, the change of basis

$$\psi^\dagger_\sigma\left(\mathbf{r}\right)=\sum_i c^\dagger_{i\sigma}\left\langle i\right|\left.\mathbf{r}\right\rangle. \tag{3.23a}$$

leads to the following two-particle analog of the one-body operator Eq.(3.16) in an arbitrary basis

$$\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\left\langle i\right|\left\langle j\right|\hat{V}_c\left|k\right\rangle\left|l\right\rangle c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{l\sigma'}c_{k\sigma}. \tag{3.24}$$

4. HARTREE-FOCK APPROXIMATION

The Hartree-Fock approximation is the simplest approximation to the many-body problem. It is a mean-field theory of the full Hamiltonian, that we will call “The theory of everything”. We will begin by writing it explicitely then proceed with two theorems that form the basis of this approximation.

4.1 The theory of everything

Gathering the results of the previous section, an electron gas interacting with a *static* lattice takes the form

$$\begin{aligned} H_{toe} &= \sum_{\sigma}\int \psi_{\sigma}^{\dagger}(\mathbf{r})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+V_{c,e-i}(\mathbf{r})\right)\psi_{\sigma}(\mathbf{r})\,d^3\mathbf{r} \\ &+\frac{1}{2}\sum_{\sigma,\sigma'}\int V_c(\mathbf{r}-\mathbf{r}')\,\psi_{\sigma}^{\dagger}(\mathbf{r})\,\psi_{\sigma'}^{\dagger}(\mathbf{r}')\,\psi_{\sigma'}(\mathbf{r}')\,\psi_{\sigma}(\mathbf{r})\,d^3\mathbf{r}d^3\mathbf{r}' \end{aligned} \tag{4.1}$$

where $V_{c,e-i}(\mathbf{r})$ is the electron-ion Coulomb potential. The dynamics of the ions (phonons) can be added to this problem, but until the rest of these introductory notes, we shall take the lattice as static. We need the to allow the lattice to move to have the complete "theory of everything" we want to solve in this School. But the above is certainly a non-trivial start.

4.2 Variational theorem

The Ritz variational principle states that any normalized wave function satisfies

$$\langle\psi|\,H\,|\psi\rangle \geq \langle\psi_0|\,H\,|\psi_0\rangle \tag{4.2}$$

where $|\psi_0\rangle$ is the ground state wave function.
Proof. That follows easily by expanding $|\psi\rangle = \sum_i a_i\,|\psi_i\rangle$, where $H\,|\psi_i\rangle = E_i\,|\psi_i\rangle$, and using $E_0 \leq E_i$:

$$\begin{aligned} \langle\psi|\,H\,|\psi\rangle &= \sum_{i,j} a_j^* a_i \left\langle\psi_j\right|H\,|\psi_i\rangle = \sum_i |a_i|^2\,E_i \\ &\geq E_0\sum_i |a_i|^2 = \langle\psi_0|\,H\,|\psi_0\rangle \end{aligned} \tag{4.3}$$

■

In the Hartree Fock approximation, we use the variational principle to look for the best one-body Green function for H_{toe}. In other words, we use our formula for a change of basis (there is no sum on repeated spin index here)

$$\psi_{\sigma}^{\dagger}\left(\mathbf{r}\right) = \sum_i c_{i\sigma}^{\dagger}\left\langle i,\sigma\right|\left.\mathbf{r},\sigma\right\rangle = \sum_i c_{i\sigma}^{\dagger}\phi_{i\sigma}^{*}\left(\mathbf{r}\right) \tag{4.4}$$

$$c_{i\sigma}^{\dagger} = \int d^3\mathbf{r}\psi_{\sigma}^{\dagger}\left(\mathbf{r}\right)\left\langle \mathbf{r},\sigma\right|\left. i,\sigma\right\rangle = \int d^3\mathbf{r}\psi_{\sigma}^{\dagger}\left(\mathbf{r}\right)\phi_{i\sigma}\left(\mathbf{r}\right) \tag{4.5}$$

and write our ground state wave function as

$$\left|\psi_{HF}\right\rangle = c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}\ldots c_{N/2\uparrow}^{\dagger}c_{N/2\downarrow}^{\dagger}\left|0\right\rangle . \tag{4.6}$$

Our variational parameters are the one-particle Green functions $\phi_{\sigma}^{*}\left(\mathbf{r}\right)$. Note that the most general wave function would be a linear combination of wave functions of the type $\left|\psi_{HF}\right\rangle$, each with different one-particle states occupied.

4.3 Wick's theorem

To compute $\left\langle\psi_{HF}\right| H \left|\psi_{HF}\right\rangle$, we expand each of the creation-annihilation operators in the Hamiltonian Eq.(4.1) in the basis we are looking for, using the change of basis formula Eq.(4.4). Consider first the quadratic term and focus on the second quantized operators. We need to know

$$\left\langle\psi_{HF}\right| c_{i\uparrow}^{\dagger}c_{j\uparrow}\left|\psi_{HF}\right\rangle \tag{4.7}$$

The key to compute such matrix elements is to simply use the anticommutation relations for the creation-annihilation operators and the fact that annihilation operators acting on the vacuum give zero. Let us do this slowly.

The anticommutation relations for the operators $c_{i\sigma}^{(\dagger)}$ are as follows:

$$\left\{c_{i\sigma},c_{j\sigma'}^{\dagger}\right\} = \int d^3\mathbf{r}\int d^3\mathbf{r}'\phi_{i\sigma}^{*}\left(\mathbf{r}\right)\left\{\psi_{\sigma}\left(\mathbf{r}\right),\psi_{\sigma'}^{\dagger}\left(\mathbf{r}'\right)\right\}\phi_{j\sigma'}\left(\mathbf{r}'\right) \tag{4.8}$$

$$= \int d^3\mathbf{r}\phi_{i\sigma}^{*}\left(\mathbf{r}\right)\phi_{j\sigma'}\left(\mathbf{r}\right) = \delta_{i,j}\delta_{\sigma,\sigma'} \tag{4.9}$$

so

$$\left\langle 0\right| c_{i\uparrow}c_{i\uparrow}^{\dagger}\left|0\right\rangle = 1-\left\langle 0\right| c_{i\uparrow}^{\dagger}c_{i\uparrow}\left|0\right\rangle = 1. \tag{4.10}$$

Generalizing this reasoning, we see that $\left\langle\psi_{HF}\right|\left.\psi_{HF}\right\rangle = 1$. Now, $\left\langle\psi_{HF}\right| c_{i\uparrow}^{\dagger}c_{j\uparrow}\left|\psi_{HF}\right\rangle$ will vanish if either i or j are not in the list of occupied states in $\left|\psi_{HF}\right\rangle$ since $c_{i\uparrow}^{\dagger}$ also annihilates the vacuum in the bra. If i and j are both in the list of occupied states, $\left\langle\psi_{HF}\right| c_{i\uparrow}^{\dagger}c_{j\uparrow}\left|\psi_{HF}\right\rangle = \delta_{i,j}$ since $c_{j\uparrow}$ will remove a particle in state j in $\left|\psi_{HF}\right\rangle$ while $c_{i\uparrow}^{\dagger}$ will remove a particle in state i in $\left\langle\psi_{HF}\right|$. If the list of particles is not the same in the bra and in the ket, the annihilation operators can be anticommuted directly to the vacuum and will destroy it. With this, we have that

$$\left\langle\psi_{HF}\right|\sum_{\sigma}\int\psi_{\sigma}^{\dagger}\left(\mathbf{r}\right)\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+V_{c,e-i}\left(\mathbf{r}\right)\right)\psi_{\sigma}\left(\mathbf{r}\right)d^3\mathbf{r}\left|\psi_{HF}\right\rangle \tag{4.11}$$

$$= \sum_{\sigma}\sum_{i=1}^{N/2}\int\phi_{i\sigma}^{*}\left(\mathbf{r}\right)\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+V_{c,e-i}\left(\mathbf{r}\right)\right)\phi_{i\sigma}\left(\mathbf{r}\right)d^3\mathbf{r}. \tag{4.12}$$

To compute the expectation value of the interacting part of H_{toe} we need

$$\left\langle\psi_{HF}\right| c_{i\sigma}^{\dagger}c_{j\sigma'}^{\dagger}c_{k\sigma'}c_{l\sigma}\left|\psi_{HF}\right\rangle . \tag{4.13}$$

Since $|\psi_{HF}\rangle$ is a direct product of wave functions for up and down spins, if the spins are different, we obtain

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k}. \tag{4.14}$$

If the spins are identical, something new happens. If the conditions $k = l$ or $i = j$ are satisfied, the expectation value vanishes because of the anticommutation relations (Pauli principle). Consider k different from l. Since all we need is that the list of states created be the same as the list of states destroyed there are two possibilities

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma}c_{k\sigma}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l}. \tag{4.15}$$

The last contribution is known as the exchange contribution. The difference in sign comes from the anticommutation. All these results, including the cases $k = l$ or $i = j$ for same spin, can be summarized by

$$\langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l}\delta_{\sigma,\sigma'}. \tag{4.16}$$

The last result can be written as

$$\begin{aligned} \langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma'}c_{k\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle &= \langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c_{l\sigma}\,|\psi_{HF}\rangle \langle\psi_{HF}|\, c^{\dagger}_{j\sigma'}c_{k\sigma'}\,|\psi_{HF}\rangle \qquad (4.17)\\ &\quad - \langle\psi_{HF}|\, c^{\dagger}_{i\sigma}c_{k\sigma'}\,|\psi_{HF}\rangle \langle\psi_{HF}|\, c^{\dagger}_{j\sigma'}c_{l\sigma}\,|\psi_{HF}\rangle. \qquad (4.18) \end{aligned}$$

A four point correlation function has been factored into a product of two-point correlation functions. For states such as $|\psi_{HF}\rangle$ that are single-particle states, creation operators are "contracted" in all possible ways with the destruction operators. This elegant form is a special case of Wick's theorem. It applies to expectation values of any number of creation and annihilation operators. The signs follow from anticommutation.

4.4 Minimization and Hartree-Fock equations

Using Wick's theorem Eq.(4.16) and proceeding with the Coulomb interaction between electrons as we did with the one-body part of the Hamiltonian in Eq.(4.12) we obtain

$$\begin{aligned} \langle\psi_{HF}|\, H_{toe}\,|\psi_{HF}\rangle &= \sum_{\sigma}\sum_{i=1}^{N/2}\int \phi^{*}_{i\sigma}(\mathbf{r})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V_{c,e-i}(\mathbf{r})\right)\phi_{i\sigma}(\mathbf{r})\,d^3\mathbf{r} \\ &+ \sum_{\sigma,\sigma'}\sum_{i=1}^{N/2}\sum_{j=1}^{N/2}\frac{1}{2}\int V_c(\mathbf{r}-\mathbf{r}')\left[\phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r})\,\phi^{*}_{j\sigma'}(\mathbf{r}')\,\phi_{j\sigma'}(\mathbf{r}')\right. \qquad (4.19)\\ &\left. - \,\delta_{\sigma,\sigma'}\phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r}')\,\phi^{*}_{j\sigma'}(\mathbf{r}')\,\phi_{j\sigma'}(\mathbf{r})\right] d^3\mathbf{r}d^3\mathbf{r}'. \qquad (4.20) \end{aligned}$$

To find our variational parameters, namely the functions $\phi_{i\sigma}(\mathbf{r})$, we minimize the above, subject to the constraint that the wave functions must be orthonormalized. This means that we take partial derivatives with respect to all variables in the above expression. We satisfy the constraints

$$\int \phi^{*}_{i\sigma}(\mathbf{r})\,\phi_{j\sigma'}(\mathbf{r})\,d^3\mathbf{r} - \delta_{i,j}\delta_{\sigma,\sigma'} = 0 \tag{4.21}$$

using Lagrange multipliers. We have to think of $\phi^{*}_{i\sigma}(\mathbf{r})$ and $\phi_{i\sigma}(\mathbf{r})$ as independents variable defined at each different position $\mathbf{r}$ and for each index i, σ. To take the partial derivatives carefully, one should discretize space and take the limit but the final result is pretty obvious. All we need to know is that what replaces the partial derivative in the continuum version is the functional derivative

$$\begin{aligned}\frac{\delta\phi_{i\sigma}(\mathbf{r})}{\delta\phi_{j\sigma'}(\mathbf{r}')} &= \delta(\mathbf{r}-\mathbf{r}')\,\delta_{i,j}\delta_{\sigma,\sigma'} \qquad (4.22)\\ \frac{\delta\phi^*_{i\sigma}(\mathbf{r})}{\delta\phi_{j\sigma'}(\mathbf{r}')} &= 0. \qquad (4.23)\end{aligned}$$

The result of the minimization with respect of $\phi^*_{i\sigma}(\mathbf{r})$ is straightforward. One obtains

$$\begin{aligned}&\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}+V_{c,e-i}(\mathbf{r})\right)\phi_{i\sigma}(\mathbf{r})+V_H(\mathbf{r})\,\phi_{i\sigma}(\mathbf{r})-\int d^3\mathbf{r}'V_{ex}(\mathbf{r},\mathbf{r}')\,\phi_{i\sigma}(\mathbf{r}')\\ &= \sum_{i=1}^{N/2}\gamma_{ij}\phi_{j\sigma}(\mathbf{r}) \qquad (4.24)\\ V_H(\mathbf{r}) &= \int d^3\mathbf{r}'V_c(\mathbf{r}-\mathbf{r}')\sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r})\right|^2 \qquad (4.25)\\ V_{ex}(\mathbf{r},\mathbf{r}') &= V_c(\mathbf{r}-\mathbf{r}')\sum_{j=1}^{N/2}\phi^*_{j\sigma}(\mathbf{r}')\,\phi_{j\sigma}(\mathbf{r}). \qquad (4.26)\end{aligned}$$

The matrix γ_{ij} is a real symmetric matrix of Lagrange multipliers. Diagonalizing γ_{ij} and writing the eigenvalues ε_i, the above equation looks like a Schrödinger equation. The Hartree contribution $V_H(\mathbf{r})$ has the physical interpretation that each electron interacts with the average density of the other electrons

$$n(\mathbf{r})=\sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r})\right|^2. \qquad (4.27)$$

The exchange contribution $V_{ex}(\mathbf{r},\mathbf{r}')$ has no classical analog. It comes from the anticommutation of indistinguishible particles. The ε_i can be interpreted as single-particle excitation energies only if removing a particle does not modify too much the effective potentials.

5. MODEL HAMILTONIANS

Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. Nevertheless, it does not diagonalize the Hamiltonian. If the problem has been solved for a translationally invariant lattice, the one-particle states will be Bloch states indexed by crystal momentum $\mathbf{k}$ and band index n. If we expand the creation-annihilation operators in that basis using the general formulas for one-particle Eq.(3.16) and two-particle Eq.(3.24) parts of the Hamiltonian, clearly it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

Model Hamiltonians can now explicitly be constructed using cold atoms in optical traps. A laser interference pattern can be used to create an optical lattice potential using the AC Stark effect. One can control tunneling between potential minima as well as the interation of atoms between them.

5.1 The Hubbard model

Restricting ourselves to a single band and expanding in the Wannier basis associated with the Bloch states, the Hamiltonian takes the form

$$H = \sum_{\sigma}\sum_{i,j} c^{\dagger}_{i\sigma} \langle i| \hat{K} |j\rangle c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl} \langle i| \langle j| \hat{V}_c |k\rangle |l\rangle c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} c_{l\sigma'} c_{k\sigma}. \tag{5.1}$$

where $\hat{K}$ contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. The operator $c^{(\dagger)}_{i\sigma}$ annihilate (create) a particle in a Wannier state centered at lattice site i and with spin σ. The one-body part by itself is essentially the DFT band structure. In 1964, Hubbard, Kanamori and Gutzwiller did the most dramatic of approximations, hoping to have a model simple enough to solve. They assumed that $\langle i| \langle j| \hat{V}_c |k\rangle |l\rangle$ would be much larger than all other interaction matrix elements when all lattice sites are equal. Defining $t_{ij} \equiv \langle i| \hat{K} |j\rangle$ and $U \equiv \langle i| \langle i| \hat{V}_c |i\rangle |i\rangle$, and using $c_{i\sigma}c_{i\sigma} = 0$ they were left with

$$\begin{aligned} H &= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{i} U c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} \\ &= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \qquad (5.2) \\ &= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow}. \qquad (5.3) \end{aligned}$$

Most of the time, one considers hopping only to nearest neighbors. The model can be solved exactly only in one dimension using the Bethe ansatz, and in infinite dimension. The latter solution is the basis for Dynamical Mean Field Theory (DMFT) that will be discussed at this School. Despite that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable. The laser intensity of the trapping potential and the magnetic field are the control parameters. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of cold atoms, one can find conditions where the Hubbard model description is very accurate. By the way, interesting physics occurs only in the nano Kelvin range. Discussing how such low temperatures are achieved would distract us to much.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a Mott insulator. The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe high-temperature superconductivity, depending on lattice and range of interaction parameters.

5.2 Heisenberg and t-J model

Suppose we are in the limit where U is much larger than the bandwidth. One expects that in low energy eigenstates, single-particle Wannier states will be either empty or occupied by a spin up or a spin down electron and that double occupation will be small. If we could write an effective Hamiltonian valid at low energy, that means that we would reduce the size of the Hilbert space from roughly 4^N to 3^N for an N site lattice. This is possible. The effective Hamiltonian that one obtains in this case is the $t-J$ model, which becomes the Heisenberg model at half-filling.

To obtain this model, one can use canonical transformations or equivalently degenerate perturbation theory. Although both approches are equivalent, the one that is most systematic is the canonical transformation approach. Nevertheless, we will see a simplified version of the degenerate perturbation theory approach since it is sufficient for our purpose and simpler to use.

We start from the point of view that the unperturbed part of the Hamiltonian is the potential energy. If there is no hopping, the ground state has no double occupancy and it is highly degenerate since the spins can take any orientation. Hopping will split this degeneracy. Let us write the eigenvalue problem for the Hubbard Hamiltonian in the block form

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E \begin{pmatrix} X \\ Y \end{pmatrix} \tag{5.4}$$

where H_{11} contains only terms that stay within the singly occupied subspace, H_{12} and H_{21} contains hopping that links the singly occupied subspace with the other ones and H_{22} contains terms that connect states where there is double occupancy. Formally, this separation can be achieved using projection operators. To project a state in the singly occupied subspace, one uses $H_{11} = PHP$ where the projector P is

$$P = \prod_{i=1}^{N} (1 - n_{i\uparrow} n_{i\downarrow}) \,. \tag{5.5}$$

Returning to the block form of the Hamiltonian, we can solve for $Y = (E - H_{22})^{-1} H_{21}X$ and write

$$\left(H_{11} + H_{12}\left(E - H_{22}\right)^{-1} H_{21}\right) X = EX. \tag{5.6}$$

What save us here is that the eigenstates we are looking for are near $E = 0$ whereas H_{22} will act on states where there is one singly occupied state since the hopping term in H_{12} can at most create one doubly occupied state from a state with no double occupation. The leading term in H_{22} will thus simbply give a contribution U which is large compared to E. We are left with the eigenvalue problem

$$\left(H_{11} - \frac{H_{12}H_{21}}{U}\right) X = EX. \tag{5.7}$$

The first part of the Hamiltonian H_{11} contains only hopping between states where no site is doubly occupied. The potential energy in those states vanishes.

The quantity $H_{12}H_{21}$ can be computed as follows. The only term of the original Hamiltonian that links singly and doubly occupied states is the hopping part. Let us consider only nearest neighbor hopping with $t_{ij} = -t$. Then

$$H_{12}H_{21} = t^2 \sum_{\langle ij\rangle\sigma} \sum_{\langle kl\rangle\sigma'} \left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right)\left(c^\dagger_{k\sigma'}c_{l\sigma'} + h.c.\right) \tag{5.8}$$

where each nearest-neighbor bond $\langle ij\rangle$ is counted only once in the sum. Since we leave from a state with singly occupied sites and return to a state with singly occupied sites, $\langle kl\rangle = \langle ij\rangle$ survives as well as cases such as $\langle kl\rangle = \langle il\rangle$ if one of the sites i is empty in the initial state. The latter contribution is called correlated hopping. It describes second-neighbor hopping through a doubly occupied state. In the $t-J$ model, this term is often neglected on the grounds that it is proportional to t^2/U whereas H_{11} is of order t. That is not necessarily a good reason to neglect this term.

Let us return to the contribution coming from $\langle kl\rangle = \langle ij\rangle$. Discarding terms that destroy two particles on the same site, we are left with only

$$-\frac{H_{12}H_{21}}{U} = -\frac{t^2}{U} \sum_{\langle ij\rangle\sigma\sigma'} \left(c^\dagger_{i\sigma}c_{j\sigma}Qc^\dagger_{j\sigma'}c_{i\sigma'} + i \leftrightarrow j\right) \tag{5.9}$$

where Q is the projection operator that makes sure that the intermediate state is doubly occupied. We have to consider four spin configurations for the neighboring sites i and j . The configurations $|i\uparrow\rangle\ \ |j\uparrow\rangle$ and $|i\downarrow\rangle\ \ |j\downarrow\rangle$ do not contribute since the intermediate state is prohibited by the Pauli principle. The configuration $|i\uparrow\rangle\ \ |j\downarrow\rangle$ when acted upon by the first term in the last equation Eq.(5.9) has non-zero matrix elements with two possible finite states, $\langle i\uparrow|\,\langle j\downarrow|$ and $\langle i\downarrow|\,\langle j\uparrow|$. The matrix element has the value $-t^2/U$ for the first case and t^2/U for the configuration where the spins have been exchanged because of the fermionic nature of the states. The configuration $|i\downarrow\rangle\ \ |j\uparrow\rangle$ has the corresponding possible final states. And the $i \leftrightarrow j$ term in Eq.(5.9) just doubles the previous results, in other words the magnitude of the non-zero matrix elements is $2t^2/U$. Since only spins are involved, all we need to do is to find spin operators that have exactly the same matrix elements.

What we are looking for is

$$\frac{4t^2}{U\hbar^2}\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{\hbar^2}{4}n_in_j\right) = J\sum_{\langle ij\rangle}\left(S^z_iS^z_j + \frac{1}{2}\left(S^+_iS^-_j + S^-_iS^+_j\right) - \frac{\hbar^2}{4}n_in_j\right) \tag{5.10}$$

where $J \equiv 4t^2/U\hbar^2$. Indeed, if the neighboring spins are parallel, the quantity $S^+_iS^-_j + S^-_iS^+_j$ has zero expectation value while the expectation of $S^z_iS^z_j$, namely

$\hbar^2/4$, is cancelled by the expectation of $-\hbar^2 n_i n_j/4$. For antiparallel spins, $S_i^z S_j^z - \hbar^2 n_i n_j/4$ has expectation value $-\hbar^2/2$ between configurations where the spins do not flip while $\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$ has vanishing matrix elements. In the case where the spins flip between the initial and final state, only$\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$ has non-zero expectation value and it is equal to $\hbar^2/2$. With the definition of J given, this corresponds to the matrix elements we found above.

This is the form of the Heisenberg Hamiltonian. Including the correlated hopping term, the $t - J$ Hamiltonian takes the following form

$$\begin{aligned} H &= P\left[\sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{\hbar^2}{4}n_i n_j\right)\right]P \qquad (5.11)\\ &+P\left[-\frac{J}{4}\sum_{i,k\neq k'}\left(c_{i,-\sigma}^\dagger c_{j,-\sigma} c_{j+k,\sigma}^\dagger c_{j+k',\sigma} + c_{j+k,-\sigma}^\dagger c_{i,-\sigma}^\dagger c_{j,-\sigma} c_{j+k',\sigma}\right)\right]P \end{aligned}$$

where the last term is the three-site hopping term that is usually neglected.

It is remarkable, but expected, that at half-filling the effective Hamiltonian is a spin-only Hamiltonian (The first term in the above equation does not contribute when there is no hole because of the projection operators). From the point of view of perturbation theory, the potential energy is the large term. We are in an insulating phase and hopping has split the spin degeneracy.

Classically, the ground state on a hypercubic lattice would be an antiferromagnet. This mechanism for antiferromagnetism is known as *superexchange*.

In closing, one should remember that to compute the expectation value of any operator in the singly occupied space, one must first write it in block form, in other words, one should not forget the contribution from the Y component of the wave function. *For example, the kinetic energy $\langle K\rangle$ of the Hubbard model calculated in the low energy subspace will be equal to minus twice the potential energy $\langle V\rangle$.* That can be seen from

$$\langle K\rangle = (X\ Y)\,K\begin{pmatrix} X \\ Y \end{pmatrix} = (XKY) + (YKX) = -\frac{2}{U}\,(X\ KK\ X) \qquad (5.12)$$

$$\langle V\rangle = (X\ Y)\,V\begin{pmatrix} X \\ Y \end{pmatrix} = (YVY) = +\frac{1}{U}\,(X\ KK\ X) \qquad (5.13)$$

since in the intermediate state, V gives the eigenvalue U in all intermediate states.

5.3 Anderson lattice model

In the Anderson lattice model, on purely phenomenological grounds one considers localized states $\left(f_{i\sigma}^\dagger\right)$ with a Hubbard U, hybridized with a conduction band $\left(c_{\mathbf{k}\sigma}^\dagger\right)$ of non-interacting electrons. This model is particularly useful for heavy fermions, for example, where one can think of the localized states as being f electrons:

$$H_A = H_f + H_c + H_{fc} \qquad (5.14)$$

$$H_f \equiv \sum_\sigma\sum_i \varepsilon f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U\left(f_{i\uparrow}^\dagger f_{i\uparrow}\right)\left(f_{i\downarrow}^\dagger f_{i\downarrow}\right) \qquad (5.15)$$

$$H_c \equiv \sum_\sigma\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \qquad (5.16)$$

$$H_{fc} \equiv \sum_\sigma\sum_i V_i c_{i\sigma}^\dagger f_{i\sigma} + h.c. \qquad (5.17)$$

In the case where there is only one site with f electrons, one speaks of the Anderson impurity model. When U is large, one can proceed as for the $t-J$ Hamiltonian and obtain an effective model where there is no double occupancy of the impurity and where the spin of the conduction electrons interacts with the spin of the impurity. The transformation is called the Schrieffer-Wolf transformation and the effective Hamiltonian is the Kondo Hamiltonian.

6. BROKEN SYMMETRY AND CANONICAL TRANSFORMATIONS

The occurence of broken symmetry can be obtained from mathematical arguments only in very few situations, such as the Ising model in two dimensions. A simple paramagnetic state and a state with broken symmetry are separated by a phase transition, in other words by singularities in the free energy. Hence, the broken symmetry state cannot be obtained perturbatively. One postulates a one-body Hamiltonian where the symmetry is broken its stability verified using variational arguments. In this and many other contexts, canonical transformations are key tools to understand and solve the problem. We have seen examples above. Basis changes obtained from unitary transformations preserve the (anti)commutation relations. Such transformations are called canonical. We will illustrate these concepts with the example of superconductivity.

6.1 The BCS Hamiltonian

The general idea of Cooper pairs is that $c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}$ almost plays the role of a boson $b^\dagger_{\mathbf{p}}$. Commutation relations are not the same, but we want to use the general idea that superconductivity will be described by a non-zero expectation value of $b^\dagger_{\mathbf{p}}$ by analogy to superfluidity. The expectation value $\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle$ occurs in the Ginzburg-Landau theory as a pair wave function. The mean-field state will be described by a coherent state.

We first write the general Hamiltonian in momentum space and, in the spirit of Weiss, the trial Hamiltonian for the mean-field takes the form

$$\begin{aligned} H_E-\mu N &= H_0-\mu N+\frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow} \\ &\quad +\frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle \\ &= H_0-\mu N+\sum_{\mathbf{p}}\left(\Delta^*_{\mathbf{p}}c_{-\mathbf{p}\downarrow}c_{\mathbf{p}\uparrow}+c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\Delta_{\mathbf{p}}\right) \qquad (6.1)\end{aligned}$$

where we defined

$$\Delta_{\mathbf{p}}=\frac{1}{V}\sum_{\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle. \qquad (6.2)$$

The potential $U\left(\mathbf{p}-\mathbf{p}'\right)$ is an effective attraction that comes from phonons in standard BCS theory. We take this for granted. The states within an energy shell of size $\hbar\omega_D$ around the Fermi level are those that are subject to that attraction.The kinetic part of the Hamiltonian is given by

$$\begin{aligned} H_0-\mu N &= \sum_{\mathbf{p},\boldsymbol{\sigma}}\left(\varepsilon_{\mathbf{p}}-\mu\right)c^\dagger_{\mathbf{p},\boldsymbol{\sigma}}c_{\mathbf{p},\boldsymbol{\sigma}} \qquad (6.3)\\ &\equiv \sum_{\mathbf{p},\boldsymbol{\sigma}}\zeta_{\mathbf{p}}c^\dagger_{\mathbf{p},\boldsymbol{\sigma}}c_{\mathbf{p},\boldsymbol{\sigma}}. \qquad (6.4)\end{aligned}$$

In the so-called jellium model, $\varepsilon_{\mathbf{p}} = \hbar^2\mathbf{p}^2/2m_e$ but one can take a more general dispersion relation. In matrix form, the combination of all these terms gives, within a constant

$$H_E - \mu N = \sum_{\mathbf{p}} \left(\begin{array}{cc} c^{\dagger}_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{array} \right) \left(\begin{array}{cc} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{-\mathbf{p}} \end{array} \right) \left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c^{\dagger}_{-\mathbf{p}\downarrow} \end{array} \right). \tag{6.5}$$

One is looking for a canonical transformation that diagonalize the Hamiltonian. When this will be done, the $c^{(\dagger)}_{-\mathbf{p}\downarrow}$ will be linear combinations of eigenoperators. These linear combinations will involve $\Delta_{\mathbf{p}}$. To find the value of $\Delta_{\mathbf{p}}$, it will suffice to substitute the eigenoperator expression for $c_{\mathbf{p}\boldsymbol{\sigma}}$ in the definition of $\Delta_{\mathbf{p}}$, Eq.(6.2). This will give a self-consistent expression for $\Delta_{\mathbf{p}}$.

Let us define the Nambu spinor

$$\Psi_{\mathbf{p}} = \left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c^{\dagger}_{-\mathbf{p}\downarrow} \end{array} \right) \tag{6.6}$$

whose anticommutator is

$$\left\{ \Psi_{\mathbf{p},i}, \Psi^{\dagger}_{\mathbf{p}'.j} \right\} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{i,j} \tag{6.7}$$

where i and j identiby the components of the Nambu spinor. Any unitary transformation of the Nambu spinors will satisfy the anticommutation relations, as one can easily check. Since the Hamiltonian matrix is Hermitian, it can be diagonalized by a unitary transformation.

Eigenvalues $E_{\mathbf{p}}$ are obtained from the characteristic equation

$$\left(\lambda_{\mathbf{p}} - \zeta_{\mathbf{p}}\right)\left(\lambda_{\mathbf{p}} + \zeta_{\mathbf{p}}\right) - \left|\Delta_{\mathbf{p}}\right|^2 = 0 \tag{6.8}$$

where one used $\zeta_{\mathbf{p}} = \xi_{-\mathbf{p}}$ valid for a lattice with inversion symmetry. The solutions are

$$\lambda_{\mathbf{p}} = \pm E_{\mathbf{p}} = \pm\sqrt{\zeta^2_{\mathbf{p}} + \left|\Delta_{\mathbf{p}}\right|^2} \tag{6.9}$$

and the eigenvectors obey

$$\left(\begin{array}{cc} \pm E_{\mathbf{p}} - \zeta_{\mathbf{p}} & -\Delta_{\mathbf{p}} \\ -\Delta^*_{\mathbf{p}} & \pm E_{\mathbf{p}} + \zeta_{\mathbf{p}} \end{array} \right) \left(\begin{array}{c} a_{1\mathbf{p}} \\ a_{2\mathbf{p}} \end{array} \right) = 0. \tag{6.10}$$

whose solution is

$$\left(\pm E_{\mathbf{p}} - \zeta_{\mathbf{p}}\right) a_{1\mathbf{p}} = \Delta_{\mathbf{p}} a_{2\mathbf{p}} \tag{6.11}$$

The constraint of normalization for a unitary transformation is

$$\left|a_{1\mathbf{p}}\right|^2 + \left|a_{2\mathbf{p}}\right|^2 = 1. \tag{6.12}$$

The unitary transformation U

$$U = \left(\begin{array}{cc} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v^*_{\mathbf{p}} & u^*_{\mathbf{p}} \end{array} \right) \tag{6.13}$$

$$U^{\dagger} = \left(\begin{array}{cc} u^*_{\mathbf{p}} & v_{\mathbf{p}} \\ -v^*_{\mathbf{p}} & u_{\mathbf{p}} \end{array} \right) \tag{6.14}$$

where

$$\left(\begin{array}{c} u_{\mathbf{p}} \\ v^*_{\mathbf{p}} \end{array} \right) = \frac{1}{\sqrt{2}} \left(\begin{array}{c} \left(1 + \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{-i\phi_{1\mathbf{p}}} \\ \left(1 - \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{i\phi_{2\mathbf{p}}} \end{array} \right)$$

diagonalizes the Hamiltonian

$$\left(\begin{array}{cc} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{array}\right) = U^{\dagger}\left(\begin{array}{cc} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^{*} & -\zeta_{\mathbf{p}} \end{array}\right)U.$$

Using this result, we can write

$$\begin{aligned} H_E - \mu N &= \sum_{\mathbf{p}} \left(\begin{array}{cc} c_{\mathbf{p}\uparrow}^{\dagger} & c_{-\mathbf{p}\downarrow} \end{array}\right) UU^{\dagger}\left(\begin{array}{cc} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^{*} & -\zeta_{\mathbf{p}} \end{array}\right)UU^{\dagger}\left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) && (6.15)\\ &= \sum_{\mathbf{p}} \left(\begin{array}{cc} \alpha_{\mathbf{p}\uparrow}^{\dagger} & \alpha_{-\mathbf{p}\downarrow} \end{array}\right)\left(\begin{array}{cc} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{array}\right)\left(\begin{array}{c} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) && (6.16)\\ &= \sum_{\mathbf{p},\boldsymbol{\sigma}} E_{\mathbf{p}}\alpha_{\mathbf{p},\sigma}^{\dagger}\alpha_{\mathbf{p},\boldsymbol{\sigma}} + cte. && (6.17) \end{aligned}$$

where the new operators are related to the old by the Bogoliubov-Valentin (1958) transformation

$$\left(\begin{array}{c} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) = U^{\dagger}\left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) = \left(\begin{array}{cc} u_{\mathbf{p}}^{*} & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^{*} & u_{\mathbf{p}} \end{array}\right)\left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right). \quad (6.18)$$

The ground state is the state that is annihilated by these new operators

$$\alpha_{\mathbf{p}\boldsymbol{\sigma}}\left|BCS\right\rangle = 0.$$

The new operators are linear combination of creation-annihilation operators since the eigenstate is a linear combination of states having different numbers of particles. At zero temperature for example, one can check explicitely that the following state is indeed annihilated by $\alpha_{\mathbf{p}\boldsymbol{\sigma}}$

$$\left|BCS\right\rangle = \prod_{\mathbf{k}}\left(1 + \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^{*}}c_{-\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}^{\dagger}\right)\left|0\right\rangle.$$

The value of the gap $\Delta_{\mathbf{p}}$ is obtained from the self-consistency equation Eq.(6.2). It suffices to write the $c_{\mathbf{p}\uparrow}$ en as a function of the diagonal operators $\alpha_{\mathbf{p}\boldsymbol{\sigma}}$. Inverting the Bogoliubov transformation Eq.(6.18) gives

$$\left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) = \left(\begin{array}{cc} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v_{\mathbf{p}}^{*} & u_{\mathbf{p}}^{*} \end{array}\right)\left(\begin{array}{c} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^{\dagger} \end{array}\right) \quad (6.19)$$

whose adjoint is

$$\left(\begin{array}{cc} c_{\mathbf{p}\uparrow}^{\dagger} & c_{-\mathbf{p}\downarrow} \end{array}\right) = \left(\begin{array}{cc} \alpha_{\mathbf{p}\uparrow}^{\dagger} & \alpha_{-\mathbf{p}\downarrow} \end{array}\right)\left(\begin{array}{cc} u_{\mathbf{p}}^{*} & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^{*} & u_{\mathbf{p}} \end{array}\right). \quad (6.20)$$

We also note that

$$n\left(E_{\mathbf{p}}\right) \equiv \left\langle \alpha_{\mathbf{p}\uparrow}^{\dagger}\alpha_{\mathbf{p}\uparrow}\right\rangle = \frac{1}{e^{\sigma' E_{\mathbf{p}}} + 1}. \quad (6.21)$$

The Fermi-Dirac distribution arises from the fact the the Hamiltonian is diagonal and quadratic when written as a function of fermionic operators $\alpha_{\mathbf{p}}^{(\dagger)}$. We can now compute the mean value of the pair operator.

$$\begin{align}
\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\rangle &= \left\langle \left(v_{\mathbf{p}'}\alpha^{\dagger}_{\mathbf{p}'\uparrow}+u_{\mathbf{p}'}\alpha_{-\mathbf{p}'\downarrow}\right)\left(u_{\mathbf{p}'}\alpha_{\mathbf{p}'\uparrow}-v_{\mathbf{p}'}\alpha^{\dagger}_{-\mathbf{p}'\downarrow}\right)\right\rangle \tag{6.22}\\
&= v_{\mathbf{p}'}u_{\mathbf{p}'}\left\langle \alpha^{\dagger}_{\mathbf{p}'\uparrow}\alpha_{\mathbf{p}'\uparrow}-\alpha_{-\mathbf{p}'\downarrow}\alpha^{\dagger}_{-\mathbf{p}'\downarrow}\right\rangle \tag{6.23}\\
&= -v_{\mathbf{p}'}u_{\mathbf{p}'}\left(1-2n\left(E_{\mathbf{p}'}\right)\right) \tag{6.24}\\
&= -\frac{1}{2}\left(1-\frac{\zeta^{2}_{\mathbf{p}'}}{E^{2}_{\mathbf{p}'}}\right)^{1/2} e^{-i\phi_{1\mathbf{p}'}-i\phi_{2\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right) \tag{6.25}\\
&= -\frac{1}{2}\frac{|\Delta_{\mathbf{p}'}|}{E_{\mathbf{p}'}}e^{-i\phi_{1\mathbf{p}'}-i\phi_{2\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right). \tag{6.26}\\
&= -\frac{1}{2}\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right) \tag{6.27}
\end{align}$$

Substituting in self-consistency equation, we Eq.(6.2) on obtain

$$\Delta_{\mathbf{p}}=-\frac{1}{2V}\sum_{\mathbf{p}'}U\left(\mathbf{p}-\mathbf{p}'\right)\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right). \tag{6.28}$$

where $\Delta_{\mathbf{p}}$ is in general complex. This is known as the BCS equation.

Remark 3 *Even when the interaction depends on* $\mathbf{p}-\mathbf{p}'$*, the phase is necessarily independent of* $\mathbf{p}$*. Indeed, the gap equation can be rewritten in the form*

$$\left[C_{\mathbf{p}}\Delta_{\mathbf{p}}\right]=-\frac{1}{2V}\sum_{\mathbf{p}'}C_{\mathbf{p}}U\left(\mathbf{p}-\mathbf{p}'\right)C_{\mathbf{p}'}\left[C_{\mathbf{p}'}\Delta_{\mathbf{p}'}\right]. \tag{6.29}$$

where

$$C_{\mathbf{p}}=\left(\frac{\left(1-2n\left(E_{\mathbf{p}}\right)\right)}{E_{\mathbf{p}}}\right)^{1/2}. \tag{6.30}$$

The gap equation can then be reinterpreted as an eigenvalue equation. The eigenvectors are in brackets and the eigenvalue is unity. Since the matrix $-C_{\mathbf{p}}U\left(\mathbf{p}-\mathbf{p}'\right)C_{\mathbf{p}'}/\left(2V\right)$ *whose eigenvalues we are looking for is real and symmetric, the eigenvector is real within a global phase, i.e. a complex number* $e^{i\phi}$ *that multiplies all components of the eigenvector. This independence of* $\mathbf{p}$ *of the phase is known as "phase coherence". It is key to superconductivity, If the eigenvalue of the gap equation is degenerate, something new can happen. One obvious degeneracy is associated with time-reversal symmetry. When this symmetry is broken, there is still an overall* $\mathbf{p}$ *independent phase, but the order parameter is complex in a way that does not correspond to a global phase. This in general gives, for example, a non-trivial value of the orbital angular momentum.*

Remark 4 *Coherence: Since* $\phi_{1\mathbf{p}}+\phi_{2\mathbf{p}}=\phi$ *for all values of* $\mathbf{p}$*, all the pairs are added to the wave function with exactly the same phase. This can be seen from the BCS wave function at zero temperature*

$$\prod_{\mathbf{k}}\left(1+\frac{v_{\mathbf{k}}}{u^{*}_{\mathbf{k}}}c^{\dagger}_{-\mathbf{k}\downarrow}c^{\dagger}_{\mathbf{k}\uparrow}\right)|0\rangle\,.$$

It is the interactions that impose that phase coherence that is at the origin of the phenomenon of superconductivity. Only the overall $\mathbf{p}$ *independent phase of* Δ *is arbitrary. The global gauge symmetry is broken by fixing the phase since phase and number obey an uncertainty relation. Fixing the phase thus corresponds to making the total number of particles uncertain.*

7. ELEMENTARY QUANTUM MECHANICS AND PATH INTEGRALS

Chapter moved to the end of the introduction to Green's functions.

7.1 Coherent-state path integrals

In the many-body context, the amplitudes that are interesting are of the form

$$\mathrm{Tr}\left[\rho c_f\left(t\right)c_i^\dagger\right]. \tag{7.1}$$

In the special case where only the ground state contibutes and that state is the vacuum state (i.e. no particle present), the above reduces precisely to our previous definition since $c_i^\dagger\left|0\right\rangle = \left|x_i\right\rangle$ and $\left\langle 0\right| e^{-\beta H}c_f\left(t\right) = \left\langle 0\right| e^{-\beta H}e^{iHt}c_f e^{-iHt} = \left\langle 0\right| c_f e^{-iHt} = \left\langle x_f\right| e^{-iHt}$.

To derive a path integral formulation for that type of amplitude, we note that destruction operators in H always appear first on the right. Hence, if we replace the position eigenstates in the one-particle case by eigenstates of the destruction operator, we will be able to derive a path integral formulation in the many-body case by following an analogous route. We will not do the full derivation here. The final result is that both for bosons and fermions, the path integral also involves exponentials of the action. For fermions, one must introduce Grassmann algebra with non-commuting numbers to define coherent states. For bosons the situation is simpler.

Let us see how boson coherent states are constructed. Let $\left[a,a^\dagger\right]=1$, then define the coherent state $\left|z\right\rangle$ by

$$\left|z\right\rangle = e^{-\left|z\right|^2/2}e^{za^\dagger}\left|0\right\rangle. \tag{7.2}$$

To show that this is an eigenstate of a, note first that one can easily show by induction that

$$\left[a,\left(a^\dagger\right)^n\right] = n\left(a^\dagger\right)^{n-1} \tag{7.3}$$

which formally looks like

$$\left[a,\left(a^\dagger\right)^n\right] = \frac{\partial\left(a^\dagger\right)^n}{\partial a^\dagger} \tag{7.4}$$

and since the exponential is defined in terms of its power series

$$\left[a,e^{za^\dagger}\right] = \frac{\partial e^{za^\dagger}}{\partial a^\dagger} = ze^{za^\dagger} \tag{7.5}$$

Using our little theorem on commutators of ladder operators (3.2), we have that since $a\left|0\right\rangle = 0$ then $a\left(e^{za^\dagger}\left|0\right\rangle\right) = z\left(e^{za^\dagger}\left|0\right\rangle\right)$ and $\left|z\right\rangle$ is an eigenstate of a.

To show that $\left|z\right\rangle$ is normalized, consider

$$\begin{aligned}\left\langle z\,|z\right\rangle &= e^{-\left|z\right|^2}\left\langle 0\right| e^{z^*a}e^{za^\dagger}\left|0\right\rangle = e^{-\left|z\right|^2}e^{\left|z\right|^2}\left\langle 0\right| e^{za^\dagger}\left|0\right\rangle \\ &= 1\end{aligned} \tag{7.6}$$

In the last step, one has simply expanded the exponential in a power series and used the normalization of the vacuum.

Finally we the closure relation

$$I = \frac{1}{\pi} \int dz dz^* \left|z\right\rangle \left\langle z\right| \tag{7.7}$$

that can be proven by taking matrix elements with states with arbitrary number of bosons $\left|n\right\rangle = \left(a^\dagger\right)^n \left|0\right\rangle / \sqrt{n!}$ and doing the integral in polar coordinates.

Part II

Correlation functions, general properties

Whenever the N-body problem can be solved exactly in d dimensions, the result is a function of Nd coordinates and of time, $\Psi(x_1, y_1, ..., x_d, y_d, ...; t)$. Variational approaches, such as that used in the description of the fractional Quantum-Hall effect, start from such a wave-function. While all the Physics is in the wave-function, it is sometimes not easy to develop a physical intuition for the result. One case where it is possible is when the wave function has a simple fariational form with very few physically motivated parameters. We encounter this in the fractional Quantum Hall effect for example, or in BCS theory. In the cases where perturbation theory can be applied, Feynman diagrams help develop a physical intuition.

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

8. RELATION BETWEEN CORRELATION FUNCTIONS AND EXPERIMENTS

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

In this chapter, we want to first illustrate the fact that scattering experiments with weak probes usually measure various equilibrium correlation functions of a system. This is one of the reasons why we will be so concerned about correlation functions. The other reason will be that they also come out from linear response. 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 first figure in the next section illustrates what we have in mind. The plan is simply to use Fermi's Golden Rule to compute the differential cross section. We will obtain

$$\boxed{\frac{d\sigma}{d\epsilon_f d\Omega_f}=\left[\frac{m^2}{(2\pi)^3\hbar^5}\frac{k_f}{k_i}\left|V^c_{-\mathbf{q}}\right|^2\right]\int dt\;e^{i\omega t}\left\langle\rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)\right\rangle.} \tag{8.1}$$

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...

To illustrate the main ideas in a simple but sketchy manner, before entering the nitty gritty details, recall that the elements of the Hamiltonian involving the probe are

$$H_p=H_p^0+H_{ps} \tag{8.2}$$

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

$$H_{ps}=gA_sA_p \tag{8.3}$$

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

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

$$\boxed{P_{i\to f}=\tfrac{2\pi}{\hbar}\left|V_{fi}\right|^{2}\delta(E_f-E_i-\hbar\omega)} \tag{8.4}$$

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

$$\begin{aligned} V_{fi} &= \langle s_f|\otimes\langle p_f|\,H_{ps}\,|p_i\rangle\otimes|s_i\rangle = g\,\langle s_f|\otimes\langle p_f|\,A_sA_p\,|p_i\rangle\otimes|s_i\rangle \\ &= g\,\langle p_f|\,A_p\,|p_i\rangle\,\langle s_f|\,A_s\,|s_i\rangle \end{aligned} \tag{8.5}$$

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

$$P_{i\to f}=\frac{2\pi}{\hbar}\left[g^2\left|\langle p_f|\,A_p\,|p_i\rangle\right|^2\right]\left|\langle s_f|\,A_s\,|s_i\rangle\right|^2\delta(E_f-E_i-\hbar\omega). \tag{8.6}$$

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

What we are interested in is what the transition probability tells us about the system. Since the final state of the probe is measured but not that of the system, the correct transition probability for the probe must be computed by summing over all final states of the system. In other words, what we need is

$$\sum_{s_f}P_{i\to f}=\left[\frac{g^2}{\hbar^2}\left|\langle p_f|\,A_p\,|p_i\rangle\right|^2\right]2\pi\hbar\sum_{s_f}\left|\langle s_f|\,A_s\,|s_i\rangle\right|^2\delta(E_f-E_i-\hbar\omega). \tag{8.7}$$

The next elegant step in the derivation is due to van Hove. It takes advantage of the fact that there is as sum over final states that can allow us to take advantage of the completeness relation. Using the integral representation of the delta function, $A_s=A_s^\dagger$, and the Heisenberg equations of motion with H_s the system Hamiltonian, we find

$$\begin{aligned} 2\pi\hbar\sum_{s_f}\left|\langle s_f|\,A_s\,|s_i\rangle\right|^2\delta(E_f-E_i-\hbar\omega) &= \sum_{s_f}\langle s_i|\,A_s\,|s_f\rangle\,\langle s_f|\,A_s\,|s_i\rangle\int dt\;e^{i\omega t}e^{-i(E_f-E_i)t/\hbar} \\ &= \int dt\;e^{i\omega t}\sum_{s_f}\langle s_i|\,e^{iH_st/\hbar}A_se^{-iH_st/\hbar}\,|s_f\rangle\,\langle s_f|\,A_s\,|s_i\rangle \\ &= \int dt\;e^{i\omega t}\,\langle s_i|\,e^{iH_st/\hbar}A_se^{-iH_st/\hbar}A_s\,|s_i\rangle \qquad (8.8) \\ &= \int dt\;e^{i\omega t}\,\langle s_i|\,A_s\left(t\right)A_s\,|s_i\rangle \qquad (8.9) \end{aligned}$$

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

In general, when we work at finite temperature, we do not know the initial state. All we know is that the probability of each initial state is given by the

Boltzmann factor for a system in thermal equilibrium with a reservoir. In this case to compute the transition probability for the probe we will need the proper canonical average over the initial states of the system, namely it is the following expectation value that will enter the transition probability:

$$\frac{\sum_i e^{-\beta E_i} \int dt\, e^{i\omega t} \langle s_i | A_s(t) A_s | s_i \rangle}{\sum_i e^{-\beta E_i}} = \int dt\, e^{i\omega t} \frac{\mathrm{Tr}\left[e^{-\beta H_s} A_s(t) A_s\right]}{\mathrm{Tr}\left[e^{-\beta H_s}\right]} \tag{8.10}$$

$$\equiv \int dt\, e^{i\omega t} \langle A_s(t) A_s \rangle . \tag{8.11}$$

In the last line, we have defined what we mean by averages $\langle \rangle$. Correlation functions will essentially always be computed in thermal equilibrium, as above. There is no need to average over the initial state of the probe which is assumed to be in a pure state. We often define the density matrix by

$$\varrho = e^{-\beta H_s} / \mathrm{Tr}\left[e^{-\beta H_s}\right] . \tag{8.12}$$

Then, we can write

$$\langle A_s(t) A_s \rangle = \mathrm{Tr}\left[\varrho A_s(t) A_s\right] \tag{8.13}$$

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

Remark 5 *In quantum information, (or atomic physics) when a two-level system (a qubit) is in an excited state, this is not a stationnary state of the whole system. It can decay to the ground state because of its coupling to the electromagnetic field. In this case, the "probe" is the qubit and the "system" is the electromagnetic environment. With a coupling of the form* $\mathbf{j} \cdot \mathbf{A}$, *where* $\mathbf{j}$ *is the current and* $\mathbf{A}$ *the vector potential, we see that the decay rate depends on the correlation function between the vector potential at two different times, in other words, it depends on vacuum fluctuations of the electromagnetic field. More precisely, it is the size of the vacuum fluctuations at the transition frequency of the qubit that determines the transition rate.*

8.1 Details of the derivation for the specific case of electron scattering

Consider the experiment illustrated on figure (8-1). $\mathcal{V}$ 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

$$v(\mathbf{R}) = \sum_{\alpha=1}^{N} e_\alpha V^c(\mathbf{R} - \mathbf{r}_\alpha) = \int d^3 r \rho(\mathbf{r}) V^c(\mathbf{R} - \mathbf{r}) \tag{8.14}$$

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

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{N} e_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \tag{8.15}$$

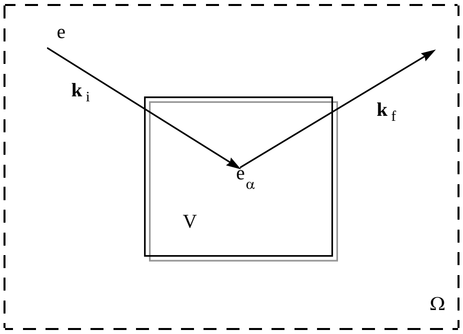

Figure 8-1 Electron scattering experiment. Ω is the quantization volume for the incoming and outgoing plane waves while V is the sample's volume. Each charge inside is labeled by e_α while the probe's charge is e and the incident and outgoing momenta are resprectively $\mathbf{k}_i$ and $\mathbf{k}_f$.

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

$$\boxed{P_{i\to f} = \tfrac{2\pi}{\hbar}\left|V_{fi}\right|^2\delta(E_f - E_i - \hbar\omega)} \tag{8.16}$$

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

$$\begin{aligned}\epsilon_f &= \epsilon_i - \hbar\omega \\ \hbar\mathbf{k}_f &= \hbar\mathbf{k}_i - \hbar\mathbf{q}.\end{aligned} \tag{8.17}$$

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

$$V_{fi} = \langle f|\otimes\langle\mathbf{k}_f|\int d^3r\rho(\mathbf{r})V^c(\mathbf{R}-\mathbf{r})\;|\mathbf{k}_i\rangle\otimes|i\rangle \tag{8.18}$$

where the plane-wave matrix element can easily be evaluated

$$\int d^3R\,\langle\mathbf{k}_f|\,R\rangle\;V^c(\mathbf{R}-\mathbf{r})\;\langle R|\,\mathbf{k}_i\rangle = \Omega^{-1}\int d^3Re^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}}V^c(\mathbf{R}-\mathbf{r}) = \frac{V^c_{-\mathbf{q}}}{\Omega}e^{i\mathbf{q}\cdot\mathbf{r}} \tag{8.19}$$

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

$$V_{fi} = \frac{V^c_{-\mathbf{q}}}{\Omega}\int d^3r\quad\langle f|\,\rho(\mathbf{r})\,|i\rangle\,e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{V^c_{-\mathbf{q}}}{\Omega}\,\langle f|\,\rho_{-\mathbf{q}}\,|i\rangle\,. \tag{8.20}$$

Substituting back in Fermi's Golden rule (8.16), we obtain

$$P_{i\to f} = \frac{2\pi}{\hbar}\left|\frac{V^c_{-\mathbf{q}}}{\Omega}\right|^2\langle i|\,\rho_{\mathbf{q}}\,|f\rangle\,\langle f|\,\rho_{-\mathbf{q}}\,|i\rangle\,\delta(E_f - E_i - \hbar\omega). \tag{8.21}$$

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

Definition 3 *Note in passing that we use the following definitions for Fourier transforms in the continuum*

$$\boxed{f_{\mathbf{q}} = \int d^3r\ f(\mathbf{r})\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}} \tag{8.22}$$

$$\boxed{f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} f_{\mathbf{q}}\mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}} \tag{8.23}$$

$$\boxed{g_\omega = \int dt\ g(t)e^{i\omega t}} \tag{8.24}$$

$$\boxed{g(t) = \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t}} \tag{8.25}$$

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

$$\sigma = \frac{\text{Number of transitions per unit time}}{\text{Number of incident particles per unit time per unit surface}} \tag{8.26}$$

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

$$\Omega d^3k_f/(2\pi)^3 = \Omega k_f m d\epsilon_f d\Omega_f \hbar^{-2}/(2\pi)^3. \tag{8.27}$$

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

$$\begin{aligned}\frac{d\sigma}{d\epsilon_f d\Omega_f} &= \frac{\text{Number of transitions per unit time in given solid angle and energy interval}}{\text{Number of incident particules per unit time per unit surface}}. \qquad (8.28)\\ &= \left[\frac{\Omega k_f m\hbar^{-2}/(2\pi)^3}{\hbar k_i/(m\Omega)}\right] \frac{\sum_i e^{-\beta E_i}\sum_f P_{i\rightarrow f}}{\sum_i e^{-\beta E_i}}\end{aligned}$$

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

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

$$\mathcal{O}(t) = e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar} \tag{8.29}$$

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

$$2\pi\hbar\langle i|\rho_{\mathbf{q}}|f\rangle\,\delta(E_f - E_i - \hbar\omega) = \int dt\ e^{i\omega t}\langle i|\rho_{\mathbf{q}}|f\rangle\,e^{-i(E_f-E_i)t/\hbar} \tag{8.30}$$

$$= \int dt\, e^{i\omega t} \langle i | e^{iHt/\hbar} \rho_{\mathbf{q}} e^{-iHt/\hbar} | f \rangle = \int dt\, e^{i\omega t} \langle i | \rho_{\mathbf{q}}(t) | f \rangle . \tag{8.31}$$

Substituting this expression in the equation for the transition probability, (8.21)

$$\sum_f P_{i \to f} = \left| \frac{V^c_{-\mathbf{q}}}{\Omega \hbar} \right|^2 \int dt\, e^{i\omega t} \langle i | \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) | i \rangle \tag{8.32}$$

the cross section is proportional to

$$\frac{\sum_i e^{-\beta E_i} \int dt\, e^{i\omega t} \langle i | \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) | i \rangle}{\sum_i e^{-\beta E_i}} = \frac{\sum_i \int dt\, e^{i\omega t} \langle i | e^{-\beta H} \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) | i \rangle}{\sum_i e^{-\beta E_i}} \tag{8.33}$$

$$= \int dt\, e^{i\omega t} \frac{Tr\left[e^{-\beta H} \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \right]}{Tr\left[e^{-\beta H} \right]} = \int dt\, e^{i\omega t} \left\langle \rho_{\mathbf{q}}(t) \rho_{-\mathbf{q}}(0) \right\rangle . \tag{8.34}$$

More explicitly, we find Eq.(8.1) 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 4 *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* $e^{-\beta H} \to e^{-\beta(H-\mu N)}$. *Note also that the quantity*

$$\boxed{\varrho \equiv \frac{e^{-\beta H}}{\mathrm{Tr}\left[e^{-\beta H}\right]}} \tag{8.35}$$

is often called the density matrix. The fact that thermal averages are traces is an important fact that we will often use later. In the grand canonical ensemble, we would use instead

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

9. TIME-DEPENDENT PERTURBATION THEORY

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

9.1 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,

$$i\hbar\frac{\partial\psi_S}{\partial t}=\mathcal{H}(t)\psi_S. \tag{9.1}$$

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

$$\psi_S(t)=U(t,t_0)\psi_S(t_0) \tag{9.2}$$

where $U(t,t_0)$ is a unitary operator, not simply equal to an exponential as we will discuss later, that satisfies

$$U(t_0,t_0)=1 \tag{9.3}$$

while by time-reversal symmetry

$$U(t_0,t)U(t,t_0)=1. \tag{9.4a}$$

Conservation of probability gives

$$U(t,t_0)^{\dagger}U(t,t_0)=1 \tag{9.5}$$

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

$$U(t,t_0)^{-1}=U(t,t_0)^{\dagger}. \tag{9.6}$$

Furthermore, when we can use time-reversal invariance, Eq.(9.4a), we also have

$$U(t,t_0)^{-1}=U(t,t_0)^{\dagger}=U(t_0,t). \tag{9.7}$$

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

$$\boxed{\left\langle\psi_S(t)\right|\mathcal{O}_S\left|\psi_S(t)\right\rangle=\left\langle\psi_H\right|\mathcal{O}_H(t)\left|\psi_H\right\rangle.} \tag{9.8}$$

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

$$\mathcal{O}_S(t=0) = \mathcal{O}_H(t=0) \equiv \mathcal{O}_S \tag{9.9}$$

$$\psi_S\,(t=0) = \psi_H\,(t=0) \equiv \psi_S \tag{9.10}$$

Using the expression for the time-dependent wave function, and the equality of matrix elements Eq.(9.8), we obtain

$$\mathcal{O}_H(t) = U^\dagger(t,0)\mathcal{O}_S U(t,0). \tag{9.11}$$

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

$$\boxed{U(t,t_0) = e^{-i\mathcal{H}(t-t_0)/\hbar}.} \tag{9.12}$$

Remark 6 *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.(9.11) becomes*

$$\mathcal{O}_H(t) = U(0,t)\mathcal{O}_S U(t,0). \tag{9.13}$$

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.(9.11) but in much of the later chapters, the above representation will be used. Aharonov and others have been proponents of this time symmetric formulation of quantum mechanics (Physics Today, Novembre 2010).

9.2 Interaction picture and perturbation theory

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

$$\boxed{\mathcal{H}\,(t) = H_0 + \delta\mathcal{H}(t)} \tag{9.14}$$

where H_0 is time-independent as above, but the proof can be generalized to time-dependent H_0 simply by replacing $e^{iH_0t/\hbar}$ everywhere below by the appropriate evolution operator.

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

$$U(t,0) \equiv e^{-iH_0t/\hbar}U_I(t,0). \tag{9.15}$$

and, as follows from $U(t,0)U(0,t) = I$,

$$U(0,t) \equiv U_I(0,t)e^{iH_0t/\hbar}. \tag{9.16}$$

so that for example

$$\boxed{U(t,t_0) \equiv e^{-iH_0t/\hbar}U_I(t,t_0)e^{iH_0t_0/\hbar}} \tag{9.17}$$

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

$$\langle\psi_S(t)|\,\mathcal{O}_S\,|\psi_S(t)\rangle = \langle\psi_S|\,U^\dagger(t,0)\mathcal{O}_S U(t,0)\,|\psi_S\rangle \tag{9.18}$$

$$= \langle\psi_S|\,U_I^\dagger(t,0)e^{iH_0t/\hbar}\mathcal{O}_S e^{-iH_0t/\hbar}U_I(t,0)\,|\psi_S\rangle \tag{9.19}$$

$$= \langle\psi_S|\,U_I^\dagger(t,0)\mathcal{O}_I(t)\,U_I(t,0)\,|\psi_S\rangle \tag{9.20}$$

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

$$\boxed{\mathcal{O}_I(t) = e^{iH_0t/\hbar}\mathcal{O}_S e^{-iH_0t/\hbar}} \tag{9.21}$$

while the wave functions obey

$$\boxed{|\psi_I(t)\rangle = U_I(t,0)\,|\psi_S\rangle} \tag{9.22}$$

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,

$$i\hbar\frac{\partial U(t,t_0)}{\partial t} = \mathcal{H}(t)U(t,t_0) \tag{9.23}$$

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

$$H_0e^{-iH_0t/\hbar}U_I(t,0) + e^{-iH_0t/\hbar}i\hbar\frac{\partial}{\partial t}U_I(t,0) = \mathcal{H}(t)e^{-iH_0t/\hbar}U_I(t,0) \tag{9.24}$$

$$i\hbar\frac{\partial}{\partial t}U_I(t,0) = e^{iH_0t/\hbar}\delta\mathcal{H}(t)e^{-iH_0t/\hbar}U_I(t,0). \tag{9.25}$$

so that using the definition of time evolution of an arbitrary operator in the interaction representation as above (9.21), the equation for the time evolution operator $U_I(t,0)$ in the interaction representation may be written,

$$i\hbar\frac{\partial}{\partial t}U_I(t,0) = \delta\mathcal{H}_I(t)U_I(t,0) \tag{9.26}$$

with the initial condition

$$U_I(0,0) = 1. \tag{9.27}$$

As expected, Eq.(9.26) 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

$$\boxed{i\hbar\tfrac{\partial}{\partial t}U_I(t,t_0) = \delta\mathcal{H}_I(t)U_I(t,t_0)} \tag{9.28}$$

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 (9.28) and using the initial condition, $U_I(t_0,t_0) = 1$ we have

$$\boxed{U_I(t,t_0) = 1 - \tfrac{i}{\hbar}\int_{t_0}^{t} dt'\ \delta\mathcal{H}_I(t')U_I(t',t_0)} \tag{9.29}$$

which, iterated to first order, gives,

$$U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \; \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \tag{9.30}$$

and correspondingly

$$U_I^\dagger(t, t_0) = 1 + \frac{i}{\hbar} \int_{t_0}^{t} dt' \; \delta\mathcal{H}_I(t') + \mathcal{O}(\delta\mathcal{H}_I^2) \tag{9.31}$$

10. LINEAR-RESPONSE THEORY

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

Let

$$\mathcal{H}(t) = H + \delta\mathcal{H}(t) \tag{10.1}$$

where H is the Hamiltonian of the system under study (that we called H_s in the example of system interacting wih probe above) and $\delta\mathcal{H}(t)$ is the perturbation given by the time-dependent Hamiltonian

$$\boxed{\delta\mathcal{H}(t) = -\int d^3r A_i(\mathbf{r}) a_i(\mathbf{r},t).} \tag{10.2}$$

In this expression, A_i is some observable of the system (excluding external perturbation) in the Schrödinger representation, while $a_i(\mathbf{r},t)$ is 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, by contrast again with the scattering of probe with system discussed above.

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

$$\boxed{\delta\mathcal{H}_I(t) = -\int d^3r A_i(\mathbf{r},t) a_i(\mathbf{r},t)} \tag{10.3}$$

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

$$A_i(\mathbf{r},t) = e^{iHt/\hbar} A_i(\mathbf{r}) e^{-iHt/\hbar}. \tag{10.4}$$

Suppose we want the expectation value of the observable B in the presence of the external perturbation turned on at time t_0. Then, starting from a thermal equilibrium state $\widehat{\varrho} = e^{-\beta H}/\mathrm{Tr}\left[e^{-\beta H}\right]$ at time t_0, it suffices to evolve the operator $B(\mathbf{r})$ defined in the Schrödinger picture with the full evolution operator, including the external perturbation [1]

$$\langle B(\mathbf{r},t)_{n.e.}\rangle = \left\langle U^{\dagger}(t,t_0)B(\mathbf{r})U(t,t_0)\right\rangle . \tag{10.5}$$

In this expression, the subscript $n.e.$ on the left reminds us that the time dependence includes that from the external perturbation. Using the interaction representation Eq.(9.17), with H now playing the role of H_0 in the previous section, the last equation becomes

$$\begin{aligned} \langle B(\mathbf{r},t)_{n.e.}\rangle &= \left\langle e^{-iHt_0/\hbar}U_I^{\dagger}(t,t_0)e^{iHt/\hbar}B(\mathbf{r})e^{-iHt/\hbar}U_I(t,t_0)e^{iHt_0/\hbar}\right\rangle \qquad (10.6)\\ \langle B(\mathbf{r},t)_{n.e.}\rangle &= \left\langle U_I^{\dagger}(t,t_0)B(\mathbf{r},t)U_I(t,t_0)\right\rangle . \qquad (10.7)\end{aligned}$$

In this last expression, $B(\mathbf{r},t)$ on the right-hand side is now in the system's Heisenberg representation *without the external perturbation*. In the previous section, this Hamiltonian was called H_0. To cancel the extra $e^{-iHt_0/\hbar}$ and $e^{iHt_0/\hbar}$ appearing in the equation for the evolution operator in Eq.(9.17), we used the facts that the trace has the cyclic property and that the density matrix Eq. 8.12, namely $\widehat{\varrho} = e^{-\beta H}/\mathrm{Tr}\left[e^{-\beta H}\right]$ commutes with $e^{iHt_0/\hbar}$. This expression for the density matrix is justified by the fact that initially the external probe is absent.

Using the explicit expression Eq.(10.3) for the external perturbation in the equation for the evolution operator in the interaction representation (9.30), we have that the term linear in applied field

$$\delta\left\langle B(\mathbf{r},t)\right\rangle = \langle B(\mathbf{r},t)_{n.e.}\rangle - \langle B(\mathbf{r},t)\rangle \tag{10.8}$$

is then given by,

$$\delta\left\langle B(\mathbf{r},t)\right\rangle = \frac{i}{\hbar}\int_{t_0}^{t}dt'\int d^3r'\left\langle\left[B(\mathbf{r},t),A_i(\mathbf{r}',t')\right]\right\rangle a_i(\mathbf{r}',t'). \tag{10.9}$$

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

$$\boxed{\delta\left\langle B(\mathbf{r},t)\right\rangle = \int_{-\infty}^{\infty}dt'\int d^3r'\ \chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')a_i(\mathbf{r}',t')} \tag{10.10}$$

with,

$$\boxed{\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t') = \tfrac{i}{\hbar}\left\langle\left[B(\mathbf{r},t),A_i(\mathbf{r}',t')\right]\right\rangle\theta(t-t').} \tag{10.11}$$

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. We notice that the linear response is given by an equilibrium correlation function where everything is determined by the Hamiltonian H without the external probe.

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

Remark 7 *Translationally invariant case: Since we compute equilibrium averages, the susceptibility* $\chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')$ *can depend only on the time difference. In*

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

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 (10.10), we obtain from the convolution theorem in this case,*

$$\boxed{\delta \left\langle B(\mathbf{q},\omega)\right\rangle = \chi^R_{BA_i}(\mathbf{q},\omega)a_i(\mathbf{q},\omega).} \tag{10.12}$$

Remark 8 *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 9 *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". The classic example is the relation between the Seebeck and Peltier coefficients. In the first case a thermal gradient causes a voltage difference whereas in the other case a voltage difference causes a thermal gradient.*

Remark 10 *Validity of linear response and heating: Finally, we can ask whether it is really justified to linearize the response. Not always since the external perturbation can be large. But certain arguments suggest that it is basically never correct in practice to linearize the response. Indeed, assume we apply an external electric field* E*. As long as the energy gained by the action of the field is smaller than* k_BT*, the linearization should be correct. In other words, linear response theory should be valid for a time*

$$t < \frac{k_BT}{eEv}. \tag{10.13}$$

This is unfortunately a ridiculously small time. Taking $v \approx \sqrt{k_BT/m}$ *the condition becomes* $t < \sqrt{mk_BT}/eE$ *with* $E = 1V/cm$, $\sqrt{mk_BT}/eE \approx \sqrt{10^{-30}10^{-23}10^2}/10^{-19} \approx 10^{-6}s$*. 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 11 *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.*

10.1 Exercices

10.1.1 Autre dérivation de la réponse linéaire.

Redérivez la théorie de la réponse linéaire mais cette fois-ci en laissant l'Hamiltonien exterieur n'influencer que la matrice densité plutôt que l'operateur dont on veut calculer la réponse.

11. GENERAL PROPERTIES OF CORRELATION FUNCTIONS

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

11.1 Notations and definition of χ''

To start with, recall the definition

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') = \frac{i}{\hbar}\left\langle [B(\mathbf{r},t),A(\mathbf{r}',t')]\right\rangle \theta(t-t'). \tag{11.1}$$

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

$$\boxed{\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \tfrac{1}{2\hbar}\left\langle [B(\mathbf{r},t),A(\mathbf{r}',t')]\right\rangle.} \tag{11.2}$$

The factor of 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

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') = 2i\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t')\theta(t-t'). \tag{11.3}$$

The quantity χ''_{BA} has symmetry properties, discussed below, that suffice to find those of the retarded response. It also contains all the physics, except causality that is represented by the θ function.

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

$$\boxed{\chi^R_{A_iA_j}(t-t') = \tfrac{i}{\hbar}\left\langle [A_i(t),A_j(t')]\right\rangle \theta(t-t').} \tag{11.4}$$

where we include in the indices i and j the positions as well as any other label of the operator such as vector or spin component. In this notation, we have not assumed translational invariance. We did however assume time-translation invariance. Since we are working with equilibrium averages above, this is always true.

Exercise 11.1.1 *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

$$\boxed{\chi''_{A_iA_j}(t-t') \equiv \frac{1}{2\hbar}\left\langle [A_i(t), A_j(t')]\right\rangle}. \tag{11.5}$$

$$\boxed{\chi^R_{A_iA_j}(t-t') = 2i\chi''_{A_iA_j}(t-t')\theta(t-t').} \tag{11.6}$$

11.2 Symmetry properties of H and symmetry of the response functions

The quantity $\chi''_{A_iA_j}(t-t')$ contains all the non-trivial information on the response. Indeed, the causal response is simply obtained by multiplying by a trivial $\theta(t-t')$ function. Certain symmetries of this response function depend on the particular symmetry of the Hamiltonian, others are quite general. We begin with properties that depend on the symmetry of H. [1]

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

$$[H, S] = 0 \tag{11.7}$$

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

$$[\varrho, S] = 0 \tag{11.8}$$

In other words, $S^{-1}\varrho S = \varrho$ 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

$$\boxed{\left\langle S^{-1}\mathcal{O}S\right\rangle = \langle\mathcal{O}\rangle} \tag{11.9}$$

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 $\mathbf{r}_\alpha \rightarrow -\mathbf{r}_\alpha$.

11.2.1 Translational invariance

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

$$\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA}(\mathbf{r}+\mathbf{R},t;\mathbf{r}'+\mathbf{R},t') \tag{11.10}$$

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

$$\boxed{\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA}(\mathbf{r}-\mathbf{r}';t-t')} \tag{11.11}$$

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).

11.2.2 Parity

Under a parity transformation, operators transform as follows

$$P^{-1}\mathcal{O}\left(\mathbf{r}\right)P = \varepsilon^{P}\mathcal{O}\left(-\mathbf{r}\right) \tag{11.12}$$

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

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{N} e_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{11.13}$$

we find

$$P^{-1}\rho(\mathbf{r})P = \sum_{\alpha=1}^{N} e_\alpha \delta(\mathbf{r}+\mathbf{r}_\alpha) = \sum_{\alpha=1}^{N} e_\alpha \delta(-\mathbf{r}-\mathbf{r}_\alpha) = \rho(-\mathbf{r}) \tag{11.14}$$

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

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^{N} \frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{11.15}$$

$$P^{-1}\mathbf{p}(\mathbf{r})P = \sum_{\alpha=1}^{N} -\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta(\mathbf{r}+\mathbf{r}_\alpha) = -\sum_{\alpha=1}^{N} \frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta(-\mathbf{r}-\mathbf{r}_\alpha) = -\mathbf{p}(-\mathbf{r}) \tag{11.16}$$

In general then, this implies that

$$\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \varepsilon^P_B\varepsilon^P_A\chi''_{BA}(-\mathbf{r},t;-\mathbf{r}',t') \tag{11.17}$$

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

$$\boxed{\chi''_{BA}(\mathbf{q};t-t') = \varepsilon^P_B \varepsilon^P_A \chi''_{BA}(-\mathbf{q};t-t')} \tag{11.18}$$

Remark 12 *To clarify the meaning of the operators above, recall that for example to obtain the charge density of a two-particle wave function, you need to compute*

$$\begin{aligned} \langle\psi|\,\rho(\mathbf{r})\,|\psi\rangle &= e\int d^3\mathbf{r}_1 \int d\mathbf{r}_2 \psi^*(\mathbf{r}_1,\mathbf{r}_2)\,\rho(\mathbf{r})\,\psi(\mathbf{r}_1,\mathbf{r}_2) \\ &= e\int d^3\mathbf{r}_2 \psi^*(\mathbf{r},\mathbf{r}_2)\,\psi(\mathbf{r},\mathbf{r}_2) + e\int d^3\mathbf{r}_1 \psi^*(\mathbf{r}_1,\mathbf{r})\,\psi(\mathbf{r}_1,\mathbf{r}) \end{aligned} \tag{11.19}$$

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

11.2.3 Time-reversal symmetry in the absence of spin

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

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^{N} \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{11.20}$$

it appears that complex conjugation suffices. Does this mean that for the wave function, the operation of time reversal is simply complex conjugation? The answer is yes, except that in the most general case, there can be an additional unitary operation. We will encounter the latter in the case of spin in the following subsection. What we cannot guess from the classical limit is what happens to the wave function under time reversal. But inspired by the case of momentum, it is natural to suggest that in the simplest case, time reversal corresponds to complex conjugation. Inverting time again would mean taking complex the conjugate again and hence returning to the original state. That is reassuring. If we accept that time reversing an operator is taking its complex conjugate, then H^*should correspond to time inversion of H.

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

$$\psi_S(t) = e^{-iHt/\hbar}\psi_S(0)\,. \tag{11.21}$$

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

$$\widetilde{\psi}_S(-t) = e^{iHt/\hbar}\widetilde{\psi}_S(0)\,. \tag{11.22}$$

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

$$\psi^*_S(t) = e^{iHt/\hbar}\widetilde{\psi}^*_S(0)\,. \tag{11.23}$$

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

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

A system in equilibrium obeys time-inversion symmetry, unless an external magnetic field is applied. This means that equilibrium averages evaluated with time-reversed states are equal to equilibrium averages evaluated with the original bases. In fact time-inversion symmetry is a very subtle subject. A very complete discussion may be found in Gottfried [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 it that it is unlike any other operator in quantum mechanics. In particular, the Dirac notation must be used with extreme care. Indeed, for standard operators, say X, we have the associative axiom

$$\langle\alpha| X |\beta\rangle = \langle\alpha| \quad (X|\beta\rangle) = (\langle\alpha| X) \quad |\beta\rangle \tag{11.24}$$

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 $\underset{\rightarrow}{K}$ when we want to take the complex conjugate of a ket, and $\underset{\leftarrow}{K}$ to take the complex conjugate of a bra.

- **Remark 13** *Antiunitary operators: Time reversal is an antiunitary operation. The key property that differentiates an anti-unitary operator from a unitary one is its action on a linear combination*

  $$T_t\left(a_1|\psi_1\rangle + a_2|\psi_2\rangle\right) = a_1^*T_t|\psi_1\rangle + a_2^*T_t|\psi_2\rangle \tag{11.25}$$

  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 $\langle\psi_1|\underset{\leftarrow}{K}\underset{\rightarrow}{K}|\psi_2\rangle = \langle\psi_2|\psi_1\rangle \neq \langle\psi_1|\psi_2\rangle$ *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 14 *The adjoint is not the inverse. Note that* $T_t^\dagger T_t = \underset{\leftarrow}{K}\,\underset{\rightarrow}{K}$*, 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

$$\langle i|\,\underset{\leftarrow}{K}\mathcal{O}\underset{\rightarrow}{K}\,|j\rangle = \Big(\langle i|\,\underset{\leftarrow}{K}\Big)\Big(\underset{\rightarrow}{K}\mathcal{O}^*\,|j\rangle\Big) = \left(\langle i|\,\mathcal{O}^*\,|j\rangle\right)^* = \langle j|\,\mathcal{O}^{\dagger *}\,|i\rangle\,. \tag{11.26}$$

In the above expression, we used one of the properties of the hermitian product, namely $\langle k\,|l\rangle^* = \langle l\,|k\rangle$, as well as the definition of the adjoint of an operator $\mathcal{A}$: $\langle k|\,\mathcal{A}l\rangle = \left\langle \mathcal{A}^\dagger k\right|\,l\rangle$ which implies, that $\langle k|\,\mathcal{A}\,|l\rangle^* = \langle l|\,\mathcal{A}^\dagger\,|k\rangle$. Applying this expression Eq.(11.26) for diagonal expectation values, and recalling that the density matrix is real, we find for equilibrium averages,

$$\boxed{\left\langle \underset{\leftarrow}{K}\mathcal{O}\underset{\rightarrow}{K}\right\rangle = \left\langle \mathcal{O}^{\dagger *}\right\rangle = \varepsilon^t \left\langle \mathcal{O}^\dagger\right\rangle}. \tag{11.27}$$

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.(11.27) gives, when A and B are *self-adjoint* operators, and in addition the Hamiltonian is real ($\underset{\rightarrow}{K}H = H\underset{\rightarrow}{K}$)

$$\begin{aligned}
\left\langle \underset{\leftarrow}{K}A(t)B\underset{\rightarrow}{K}\right\rangle &= \left\langle B^* e^{-iHt/\hbar}A^* e^{iHt/\hbar}\right\rangle \\
&= \epsilon^t_A \epsilon^t_B \left\langle BA(-t)\right\rangle
\end{aligned} \tag{11.28}$$

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

$$\chi''_{A_iA_j}(t-t') = \epsilon^t_i \epsilon^t_j \chi''_{A_jA_i}(-t'-(-t)) \tag{11.29}$$

and for the corresponding Fourier transform in frequency,

$$\boxed{\chi''_{A_iA_j}(\omega) = \epsilon^t_i \epsilon^t_j \chi''_{A_jA_i}(\omega)}. \tag{11.30}$$

- **Remark 15** *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.(11.9),*
  $$\left\langle T_t^{-1}\mathcal{O}T_t\right\rangle = \langle \mathcal{O}\rangle\,. \tag{11.31}$$
  Hence as expected, Eqs.(11.27) and (11.31) together imply that Hermitian operators that have an odd signature with respect to time reversal symmetry have a vanishing expectation value in equilibrium.

11.2.4 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

$$T_t = \underrightarrow{K}U \tag{11.32}$$

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

$$U^\dagger \underleftarrow{K} \tag{11.33}$$

Let us first repeat the steps of calculating expectation values in time-reversed states, as in Eq.(11.26), but for the more general case

$$\langle i|\, U^\dagger \underleftarrow{K}\mathcal{O}\underrightarrow{K}U\,|j\rangle = \left(\langle i|\, U^\dagger \underleftarrow{K}\right)\left(\underrightarrow{K}\mathcal{O}^* U\,|j\rangle\right) = \left(\langle i|\, U^\dagger\mathcal{O}^* U\,|j\rangle\right)^* = \langle j|\, U^\dagger\mathcal{O}^{\dagger *} U\,|i\rangle \tag{11.34}$$

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

$$U^\dagger\boldsymbol{\sigma}^{\dagger *}U = -\boldsymbol{\sigma} \tag{11.35}$$

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

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad ; \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad ; \quad \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{11.36}$$

we have $\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$, and $\sigma_x^* = \sigma_x$, $\sigma_y^* = -\sigma_y$, $\sigma_z^* = \sigma_z$ so that Eq.(11.35) for time reversal gives us the following set of equations for the unitary operator U

$$U^\dagger\sigma_x U = -\sigma_x \tag{11.37}$$

$$U^\dagger\sigma_y U = \sigma_y \tag{11.38}$$

$$U^\dagger\sigma_z U = -\sigma_z \tag{11.39}$$

Given the fundamental properties of Pauli matrices

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

$$\sigma_i^2 = 1 \tag{11.40}$$

$$\sigma_i\sigma_j = i\sigma_k \tag{11.41}$$

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

$$U = e^{i\delta}\sigma_y \tag{11.42}$$

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

$$T_t = \underrightarrow{K}e^{i\delta}\sigma_y \tag{11.43}$$

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

$$T_t \left|\uparrow\right\rangle = -ie^{-i\delta} \left|\downarrow\right\rangle \tag{11.44}$$

$$T_t \left|\downarrow\right\rangle = ie^{-i\delta} \left|\uparrow\right\rangle \tag{11.45}$$

The time reversal operator thus transforms up into down and vice versa but with a phase. Even if we can choose $e^{i\delta} = i$ to make the phase real, the prefactor cannot be $+1$ for both of the above equations. In particular, note that $T_t T_t \left|\uparrow\right\rangle = -\left|\uparrow\right\rangle$, another strange property of spinors. The application of two time reversal operations on spinors is like a 2π rotation around y so that it changes the phase of the spinor. It can be proven that this result is independent of the choice of quantization axis, as we can expect.[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 $\chi''_{A_iA_j}(\omega)$ is real, the properties of being a commutator (11.47) and of Hermiticity (11.49) allow us to further show that $\chi''_{A_iA_i}(\omega)$ is also an odd function of frequency, an important result that we show in the following section.

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

Let us thus write down the general symmetry properties of $\chi''_{A_iA_j}(t-t')$ that simply follow from its definition (11.5). These properties are independent of the specific form of the Hamiltonian. It only needs to be Hermitian.

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

$$\chi''_{A_iA_j}(t-t') = -\chi''_{A_jA_i}(t'-t) \tag{11.46}$$

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

$$\boxed{\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)}. \tag{11.47}$$

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

$$\chi''_{A_iA_j}(t-t') = \left[\chi''_{A_jA_i}(t'-t)\right]^*. \tag{11.48}$$

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

In Fourier space, this becomes,

$$\boxed{\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^*}. \tag{11.49}$$

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

Remark 16 *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.*

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

$$\boxed{\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega) = \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^*} \tag{11.50}$$

To prove this, we first use Hermiticity Eq.(11.49) in the form

$$\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* \tag{11.51}$$

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

$$\begin{aligned}
\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) &= \int d^3\mathbf{r} \int d^3\mathbf{r}' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) && (11.52) \\
&= \left[\int d^3\mathbf{r} \int d^3\mathbf{r}' e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* && (11.53) \\
&= \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^* && (11.54)
\end{aligned}$$

The commutator property Eq.(11.47), $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega)$ and symmetry under parity transformation Eq.(11.18), $\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega) = \chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$ 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.(11.30) $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)$ and the commutator property Eq.(11.47) $\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega) = -\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(-\omega)$ which imply $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega)$ to show that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ is odd, namely $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$.

Quite generally, using the commutator property Eq.(11.47) and time reversal symmetry Eq.11.30, we see that for operators that have the same signature under time reversal

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_iA_j}(-\omega) \tag{11.55}$$

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

11.4 Kramers-Kronig relations and causality

You are familiar with optical conductivity for example, or with frequency dependent impedance. Generally one can measure the real and imaginary parts of frequency-dependent response functions, namely the dissipative and reactive parts of the response. Those are not independent. In reality, all the information on the system is in $\chi''_{A_iA_j}(\omega)$. That is the single function containing the physics.

Since the physics is in a single function, there are relations between real and imaginary parts of response functions. These are the Kramers-Kronig relation. These are by far the best known and most useful properties for response functions. The Kramers-Kronig relation follows simply from causality. Causality is insured by the presence of the θ function in the expression for the response functions

Eq.(11.6). Causality simply states that the response to an applied field at time t' occurs only at time t later. This is satisfied in general in our formalism, as can be seen by looking back at the formula for the linear response Eq.(10.10). 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:

$$\boxed{\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = \mathcal{P}\int \tfrac{d\omega'}{\pi}\tfrac{\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}} \tag{11.56}$$

$$\boxed{\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = -\mathcal{P}\int \tfrac{d\omega'}{\pi}\tfrac{\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}.} \tag{11.57}$$

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

11.4.1 The straightforward manner:

Let us first derive the relations the easy way. Suppose that we know the Fourier transform in frequency $\chi^R_{A_iA_j}(\omega)$ 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 $\chi^R_{A_iA_j}(t-t')$ contains $\theta(t-t')$ is to have $\chi^R_{A_iA_j}(\omega)$ 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

$$\chi^R_{A_iA_j}(t-t') = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\chi^R_{A_iA_j}(\omega). \tag{11.58}$$

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 $\chi^R_{A_iA_j}(\omega)$ is analytic in that half-plane, the result will be zero, which is just another way to say that $\chi^R_{A_iA_j}(t-t')$ 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 $\chi^R_{A_iA_j}(\omega)$ is analytic in the upper half plane, it is then easy to derive the Kramers-Kronig relations. It now suffices to use

$$\lim_{\eta\to 0}\int\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\eta}\chi^R_{A_iA_j}(\omega') = 2i\lim_{\eta\to 0}\chi^R_{A_iA_j}(\omega+i\eta) \tag{11.59}$$

which is easy to prove by applying the residue theorem on a contour closed in the upper half plane where $\chi^R_{A_iA_j}(\omega)$ is analytic. Here and from now on, it is assumed that η is a positive infinitesimal. The last formula also assumes that $\chi^R_{A_iA_j}(\omega')$ falls off at least like a small power of $1/\omega'$ so that there is no contribution from the part at ∞. Otherwise, if there is a term that does not decay, we need to subtract it before we use the residue theorem.

We then need the following all important identity,

$$\boxed{\lim_{\eta\to 0}\tfrac{1}{\omega\mp i\eta} = \lim_{\eta\to 0}\tfrac{\omega\pm i\eta}{\omega^2+\eta^2} = \lim_{\eta\to 0}\left[\tfrac{\omega}{\omega^2+\eta^2}\pm\tfrac{i\eta}{\omega^2+\eta^2}\right] = \mathcal{P}\tfrac{1}{\omega}\pm i\pi\delta\left(\omega\right)} \tag{11.60}$$

where δ is Dirac's delta function and $\mathcal{P}$ means principal part integral. — Suppose the factor $1/\left(\omega+i\eta\right)$ 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 (11.59) we obtain, upon taking the lim $\eta \to 0$,

$$\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega} - \mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = -2\,\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega)\right] \tag{11.61}$$

while from the imaginary part,

$$\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega} + \mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = 2\,\mathrm{Re}\left[\chi^R_{A_iA_j}(\omega)\right]. \tag{11.62}$$

This is precisely what we mean by the Kramers-Kronig relations, namely we recover the results Eqs.(11.56)(11.57) at the beginning of this section. From the proof just given, Kramers-Kronig relations will apply if

- $\chi^R_{A_iA_j}(\omega)$ is analytic, as a function of complex frequency, in the upper half-plane.
- $\chi^R_{A_iA_j}(\omega)$ falls off at least as a small power of ω at infinity. If there is a term that does not decay, it needs to be subtracted off before we can apply Kramers-Kronig relations.

11.5 Spectral representation

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 later 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, (11.6)

$$\chi^R_{A_iA_j}(\omega) = 2i\int \frac{d\omega'}{2\pi}\chi''_{A_iA_j}(\omega')\theta(\omega-\omega'). \tag{11.63}$$

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,

$$\int_{-\infty}^{\infty} dt e^{i\omega t}\theta(t) = \frac{e^{i\omega t}}{i\omega}|_0^\infty \tag{11.64}$$

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 (10.10). 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 $t\to\infty$ by using a factor $e^{-\eta t}$.The equation for the response in time (11.6) 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, $\int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}$, 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 (11.6) now reads,

$$\chi^R_{A_iA_j}(t-t')e^{-\eta(t-t')} = 2i\chi''_{A_iA_j}(t-t')\theta(t-t')e^{-\eta(t-t')} \tag{11.65}$$

so that in the calculation of the response (11.63) we have,

$$\int_{-\infty}^{\infty} d(t-t')e^{i(\omega+i\eta-\omega')(t-t')}\theta(t-t') = \frac{e^{i(\omega+i\eta-\omega')(t-t')}}{i(\omega+i\eta-\omega')}|_0^\infty = \frac{1}{i(\omega'-\omega-i\eta)}. \tag{11.66}$$

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

$$\chi^R_{A_iA_j}(\omega+i\eta) = 2i\int\frac{d\omega'}{2\pi}\chi''_{A_iA_j}(\omega')\theta(\omega+i\eta-\omega') \tag{11.67}$$

$$= \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-(\omega+i\eta)}. \tag{11.68}$$

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

$$\boxed{\chi_{A_iA_j}(z) = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-z}} \tag{11.69}$$

we can write for the retarded response,

$$\boxed{\chi^R_{A_iA_j}(\omega) = \lim_{\eta\to0}\chi_{A_iA_j}(z)|_{z=\omega+i\eta}} \tag{11.70}$$

and for the advanced one, which we hereby define,

$$\boxed{\chi^A_{A_iA_j}(\omega) = \lim_{\eta\to0}\chi_{A_iA_j}(z)|_{z=\omega-i\eta}.} \tag{11.71}$$

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

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

$$\left[\chi_{A_iA_j}(\omega+i\eta)-\chi_{A_iA_j}(\omega-i\eta)\right] = 2i\chi''_{A_iA_j}(\omega). \tag{11.72}$$

Definition 5 *Equations such as (11.69) are called spectral representations.*

So much for taking the Fourier transform of a response which is so simple looking in its ordinary time version Eq.(11.6). Time-reversal invariance (11.30) and Hermiticity in Eq.(11.49) imply, for two operators with the same signature under time-reversal, that $\chi''_{A_iA_j}(\omega')$ is a real function. Hence, from the mathematical identity for principal part Eq.(11.60) and from the spectral representation (11.69) we have, *for two hermitian operators* A_i, A_j *with the same signature under time reversal,* that

$$\boxed{\text{Im}\left[\chi^R_{A_iA_j}(\omega)\right] = \chi''_{A_iA_j}(\omega)} \tag{11.73}$$

so that from the spectral representation we recover the first of the Kramers-Krönig relation (11.56). 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.(11.30) and (11.49) imply that $\chi''_{A_iA_j}(\omega')$ is purely imaginary. In this case,

$$\boxed{\text{Re}\left[\chi^R_{A_iA_j}(\omega)\right] = i\chi''_{A_iA_j}(\omega)}. \tag{11.74}$$

Remark 17 *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.(11.73) 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* $\chi''_{A_iA_j}(\omega)$.

11.6 Lehmann representation and spectral representation

Definition 6 *The function that contains the information,* $\chi''_{A_iA_j}(\omega')$ *is called the spectral function.*

The reason for this name is that, as we discuss in the next section below, $\chi''_{A_iA_j}(\omega')$ contains information on dissipation or, alternatively, on the spectrum of excitations. Hence, in that kind of equations, the response is expressed in terms of the spectrum of excitations. We will also have spectral representations for Green's functions.

To see the connection with the spectrum of excitations and develop physical intuition, it is useful to express $\chi''_{A_iA_j}(\omega')$ in terms of matrix elements and excitation energies. We begin with the definition and use the Heisenberg equations of motion and insert a complete set of energy eigenstates so that we find

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\text{Tr}\left[\varrho\left(A_i(t)A_j(0) - A_j(0)A_i(t)\right)\right] \tag{11.75}$$

$$= \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\Big[\langle n|\, e^{iE_nt/\hbar}A_ie^{-iE_mt/\hbar}\,|m\rangle\langle m|\,A_j\,|n\rangle - \langle n|\,A_j\,|m\rangle\langle m|\,e^{iE_mt/\hbar}A_ie^{-iE_nt/\hbar}\,|n\rangle\Big] \tag{11.76}$$

Changing dummy summation indices m and n in the last term, we have

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta Em}}{Z}\langle n|\,A_i\,|m\rangle\langle m|\,A_j\,|n\rangle\, e^{i(E_n-E_m)t/\hbar} \tag{11.77}$$

so that the Fourier transform is

$$\chi''_{A_iA_j}(\omega) = \sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta Em}}{Z}\langle n|\,A_i\,|m\rangle\langle m|\,A_j\,|n\rangle\;\pi\,\delta\left(\hbar\omega-(E_m-E_n)\right). \tag{11.78}$$

Substituting in the spectral representation Eq.(11.69), we find

$$\chi_{A_iA_j}(z) = \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta Em}}{Z} \frac{\langle n| A_i |m\rangle \langle m| A_j |n\rangle}{(E_m - E_n) - \hbar z} \tag{11.79}$$

From this, one trivially deduces, by letting $z \to \omega + i\eta$, the so-called Lehmann representation for the retarded response function. The poles or the integrand are indeed in the lower-half frequency plane, as we wanted to prove. They are just below the real axis, a distance η along the imaginary direction. The position of the poles carries information on the excitation energies of the system. The residue at a given pole will depend on the value of $\chi''_{A_iA_j}$ at the corresponding value of the real coordinate of the pole. The residues tell us how strongly the external probe and system connect the two states. The Lehmann representation reminds us of low order perturbation theory in the external probe.

To refine our physical understanding of $\chi''_{A_iA_j}(\omega)$ let us go back to the original form we found in the time domain, Eq.(11.76), before we changed dummy indices. Taking Fourier transforms directly on this function, we find

$$\begin{aligned}\chi''_{A_iA_j}(\omega) \quad &= \quad \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \left[\langle n| A_i |m\rangle \langle m| A_j |n\rangle \; \pi\,\delta\left(\hbar\omega - (E_m - E_n)\right)\right. \\ &\quad \left. - \langle n| A_j |m\rangle \langle m| A_i |n\rangle \; \pi\,\delta\left(\hbar\omega - (E_n - E_m)\right)\right]. \end{aligned} \tag{11.80}$$

If we take the zero temperature limit, $\beta \to \infty$, we are left with $Z = e^{-\beta E_0}$ where E_0 is the ground state energy and the above formula reduces to

$$\begin{aligned}\lim_{\beta\to\infty} \chi''_{A_iA_j}(\omega) \quad &= \quad \sum_{m} \left[\langle 0| A_i |m\rangle \langle m| A_j |0\rangle \; \pi\,\delta\left(\hbar\omega - (E_m - E_0)\right)\right. \\ &\quad \left. - \langle 0| A_j |m\rangle \langle m| A_i |0\rangle \; \pi\,\delta\left(\hbar\omega - (E_0 - E_m)\right)\right]. \end{aligned} \tag{11.81}$$

For $m = 0$, $\chi''_{A_iA_j}(\omega)$ vanishes. Then, only excited states contribute and $E_m - E_0 > 0$. For positive frequencies only the first term contributes and it contributes only if $\hbar\omega$ is equal to the energy of an excitation in the system, namely $E_m - E_0$, and if the external probe through A_j, and the measured operator A_i, have a non-vanishing matrix element that connects the excited and ground state. Clearly then, $\chi''_{A_iA_j}(\omega)$ is related to absorption. The second term contributes only for negative frequencies. External probes that are in $\cos(\omega t) = \left(e^{i\omega t} + e^{-i\omega t}\right)/2$ couple to both positive and negative frequencies. It is not surprising that both positive and negative frequencies enter $\chi''_{A_iA_j}(\omega)$. At finite temperature, contributions to positive frequencies can also come from the second term and contributions to negative frequencies can also come from the first term. If $A_i = A_j$ it is easy to verify that at any temperature, $\chi''_{A_iA_i}(\omega) = -\chi''_{A_iA_i}(-\omega)$.

Remark 18 *In an infinite system, if $\chi''_{A_iA_j}(\omega')$ is a continuous function and then the poles of $\chi_{A_iA_j}(z)$ are below the real axis, but not ncessarily close to it. The passage from a series of poles to a continuous function is what introduces irreversibility in many-body systems.*

Remark 19 *In a system with time reversal symmetry, applying the time-reversal operator to all states should leave $\chi''_{A_iA_j}$ invariant. Then, using $\langle i| \underleftarrow{K}\mathcal{O}\underrightarrow{K} |j\rangle = \langle j| \mathcal{O}^{\dagger *} |i\rangle$ found in Eq.(11.26) we see that show that $\chi''_{A_iA_j}(\omega)$ is pure imaginary if A_i and A_j are hermitian and have different signatures under time-reversal. Otherwise it is real.*

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

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

Since the change in the energy of the system due to the external perturbation is given by the perturbation Hamiltonian Eq.(10.2), this means that the power dissipated by the external world is

$$\frac{dW}{dt} = \frac{d\delta\mathcal{H}(t)}{dt} = -\int d^3r A_i(\mathbf{r})\frac{da_i(\mathbf{r},t)}{dt} = -A_i\frac{da_i(t)}{dt}. \tag{11.82}$$

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

$$\frac{dW}{dt} = -\left[\langle A_i\rangle + \langle\delta A_i\rangle\right]\frac{da_i(t)}{dt} \tag{11.83}$$

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

$$\overline{W} = -\int_{-T/2}^{T/2} dt \quad \langle\delta A_i(t)\rangle\frac{da_i(t)}{dt} > 0. \tag{11.84}$$

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

$$-\int\frac{d\omega}{2\pi}\langle\delta A_i(\omega)\rangle\, i\omega a_i(-\omega) > 0. \tag{11.85}$$

Finally, linear response theory gives

$$-\int\frac{d\omega}{2\pi}a_i(-\omega)\chi^R_{A_iA_j}(\omega)i\omega a_j(\omega) > 0 \tag{11.86}$$

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

$$\overline{W} = -\frac{1}{2}\int\frac{d\omega}{2\pi}a_i(-\omega)\left[\chi^R_{A_iA_j}(\omega)-\chi^R_{A_jA_i}(-\omega)\right]i\omega a_j(\omega) > 0. \tag{11.87}$$

Calling the spectral representation (11.70) to the rescue, we can write

$$\left[\chi^R_{A_iA_j}(\omega)-\chi^R_{A_jA_i}(-\omega)\right] = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-(\omega+i\eta)} - \int\frac{d\omega'}{\pi}\frac{\chi''_{A_jA_i}(\omega')}{\omega'-(-\omega+i\eta)}. \tag{11.88}$$

We know from the fact that $\chi''_{A_iA_j}$ is a commutator that (11.47) $\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)$. Using this identity and the change of variables $\omega'\to-\omega'$ in the last integral, we immediately have that

$$\left[\chi^R_{A_iA_j}(\omega)-\chi^R_{A_jA_i}(-\omega)\right] = \int\frac{d\omega'}{\pi}\chi''_{A_iA_j}(\omega')\left[\frac{1}{\omega'-\omega-i\eta}+\frac{1}{-\omega'+\omega-i\eta}\right] \tag{11.89}$$

$$= 2i\chi''_{A_iA_j}(\omega). \tag{11.90}$$

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

$$\int \frac{d\omega}{2\pi} a_i^*(\omega) \left[\chi''_{A_iA_j}(\omega)\omega\right] a_j(\omega) > 0. \tag{11.91}$$

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

$$\boxed{a_i^*(\omega) \left[\chi''_{A_iA_j}(\omega)\omega\right] a_j(\omega) > 0} \tag{11.92}$$

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

$$\boxed{\chi''_{A_iA_i}(\omega)\omega > 0.} \tag{11.93}$$

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

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

Remark 20 *For Hermitian operators A_i, A_j, the matrix $\chi''_{A_iA_i}(\omega)$ is Hermitian, hence its eigenvalues are real, even if off-diagonal matrix elements between operators that do not have the same signature under time reversal are purely imaginary.*

11.8 Fluctuation-dissipation theorem

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

$$\boxed{S_{A_iA_j}(\omega) = \tfrac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega) = 2\hbar(1+n_B(\omega))\chi''_{A_iA_j}(\omega)} \tag{11.94}$$

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

$$S_{A_iA_j}(t) \equiv \langle A_i(t)A_j\rangle - \langle A_i\rangle\langle A_j\rangle = \langle (A_i(t) - \langle A_i\rangle)(A_j(0) - \langle A_j\rangle)\rangle \tag{11.95}$$

$$\equiv \langle \delta A_i(t)\delta A_j\rangle . \tag{11.96}$$

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.(C.10) is a correlation function 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,

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\left\langle [A_i(t), A_j]\right\rangle = \frac{1}{2\hbar}\left\langle [\delta A_i(t), \delta A_j]\right\rangle \tag{11.97}$$

$$= \frac{1}{2\hbar}\left\langle \delta A_i(t)\delta A_j - \delta A_j \delta A_i(t)\right\rangle \tag{11.98}$$

$$= \frac{1}{2\hbar}\left(S_{A_iA_j}(t) - S_{A_jA_i}(-t)\right) \tag{11.99}$$

then to use the key following identity that we set to prove,

$$\boxed{S_{A_jA_i}(-t) = S_{A_iA_j}(t - i\hbar\beta)}. \tag{11.100}$$

This kind of periodicity of equilibrium correlation functions will be used over and over in the context of Green's functions. It will allow to define Fourier expansions in terms of so-called Matsubara frequencies. The proof of the identity simply uses the definition of the time evolution operator and the cyclic property of the trace. More specifically using the cyclic property of the trace, we havewe start with,

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}\delta A_j \delta A_i(t)\right] = Z^{-1}Tr\left[\delta A_i(t) e^{-\beta H}\delta A_j\right]. \tag{11.101}$$

Using $e^{-\beta H}e^{\beta H} = 1$ to recover the density matrix on the left, simple manipulations and Heisenberg's representation for the time-evolution of the operators gives,

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}e^{\beta H}\delta A_i(t) e^{-\beta H}\delta A_j\right] \tag{11.102}$$

$$= Z^{-1}Tr\left[e^{-\beta H}\delta A_i(t - i\hbar\beta)\delta A_j\right] = S_{A_iA_j}(t - i\hbar\beta). \tag{11.103}$$

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

$$\int dt e^{i\omega t} S_{A_iA_j}(t - i\hbar\beta) = \int dt e^{i\omega(t+i\hbar\beta)} S_{A_iA_j}(t) = e^{-\beta\hbar\omega} S_{A_iA_j}(\omega). \tag{11.104}$$

To prove the last result, we had to move the integration contour from t to $t + i\hbar\beta$, in other words in the imaginary time direction. Because of the convergence factor $e^{-\beta H}$ in the traces, expectations of any number of operators of the type $e^{iHt}Ae^{-iHt}$ are analytic in the imaginary time direction for $-i\hbar\beta < t < i\hbar\beta$, hence it is permissible to displace the integration contour as we did. Fourier transforming the relation between $\chi''_{A_iA_j}(t)$ and susceptibility Eq.(11.97), one then recovers the fluctuation-dissipation theorem (C.10).

A few remarks before concluding.

Remark 21 *Alternate derivation: Formally, the Fourier transform gives the same result as what we found above if we use the exponential representation of the Taylor series,*

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

Remark 22 *Relation to detailed balance: The Fourier-space version of the periodicity condition (11.100) is a statement of detailed balance:*

$$\boxed{S_{A_jA_i}(-\omega) = e^{-\beta\hbar\omega} S_{A_iA_j}(\omega)}. \tag{11.105}$$

Indeed, in one case the energy $\hbar\omega$ is absorbed in the process, while in the other case it has the opposite sign (is emitted). In Raman spectroscopy, when the photon comes out with less energy than it had, we have Stokes scattering. In the reverse *process, with a frequency transfer ω of opposite sign, it comes out with more energy. This is called anti-Stokes scattering. The cross section for Stokes scattering say, will be proportional to $S_{A_iA_j}(\omega)$ as we saw with our golden rule calculation. The ratio of the anti-Stokes and the Stokes cross sections will be given by the Boltzmann factor $e^{-\beta\hbar\omega}$, which is a statement of detailed balance. This is one way of seeing the basic physical reason for the existence of the fluctuation-dissipation theorem: Even though the response apparently had two different orders for the operators, the order of the operators in thermal equilibrium can be reversed using the cyclic property of the trace, or equivalently the principle of detailled balance.*

Remark 23 *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.*

11.9 Imaginary time and Matsubara frequencies, a preview

Recall that all the information that we need is in the spectral function χ''. To do actual calculations of correlation functions at finite temperature, whether by numerical or analytical means, it turns out that it is much easier to compute a function that is different from the retarded response function. That function is defined as follows

$$\chi_{A_iA_j}(\tau) = \frac{1}{\hbar}\langle A_i(\tau)A_j\rangle\theta(\tau) + \frac{1}{\hbar}\langle A_jA_i(\tau)\rangle\theta(-\tau) \tag{11.106}$$

where θ is the step function and by definition,

$$A_i(\tau) = e^{\tau H/\hbar}A_ie^{-\tau H/\hbar}. \tag{11.107}$$

In other words, if in this last equation we replace τ, a real number, by the purely imaginary number it, we recover that the operator evolves with the Heisenberg equations of motion. This definition is motivated by the fact that the operator $e^{-\beta H}$ in the density matrix really looks like evolution $e^{-iHt/\hbar}$ in imaginary time. It is also customary to define the time ordering operator T_τ in such a way that operators are ordered by from right to left by increasing order of time:

$$\chi_{A_iA_j}(\tau) = \frac{1}{\hbar}\langle T_\tau A_i(\tau)A_j\rangle. \tag{11.108}$$

That will be very useful in cunjunction with perturbation theory. As long as we can extract the spectral function χ'' from $\chi_{A_iA_j}(\tau)$ above, we are in good shape to obtain all we need.

To see how to do this, we first note that we can define $\chi_{A_iA_j}(\tau)$ on the interval $-\beta\hbar \leq \tau \leq \beta\hbar$, and that if we do that, this function *on this interval only* has some periodicity properties that can be put to use. More specifically, assume that

$-\beta\hbar < \tau < 0$,then from the definition of the function, we have that

$$\begin{aligned}
\chi_{A_iA_j}(\tau) &= \frac{1}{\hbar}\langle A_jA_i(\tau)\rangle = \frac{1}{\hbar}\mathrm{Tr}\left[e^{-\beta H}A_jA_i(\tau)\right]/Z \\
&= \frac{1}{\hbar}\mathrm{Tr}\left[A_i(\tau)e^{-\beta H}A_j\right]/Z \\
&= \frac{1}{\hbar}\mathrm{Tr}\left[e^{-\beta H}e^{\beta H}A_i(\tau)e^{-\beta H}A_j\right]/Z \\
&= \chi_{A_iA_j}(\tau+\beta\hbar)
\end{aligned} \tag{11.109}$$

since now $\tau+\beta\hbar>0$.We have a periodic function on a finite interval. Hence we can represent it by a Fourier series

$$\boxed{\chi_{A_iA_j}(\tau) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\chi_{A_iA_j}(i\omega_n)} \tag{11.110}$$

where the so-called bosonic Matsubara frequencies are defined by

$$\omega_n = \frac{2n\pi k_BT}{\hbar} = \frac{2n\pi}{\beta\hbar} \quad ; \quad n \quad \text{integer} \tag{11.111}$$

The periodicity property will be automatically fulfilled because $e^{-i\hbar\omega_n\beta} = e^{-i2n\pi} = 1$. The expansion coefficients are obtained as usual for Fourier series of periodic functions from

$$\boxed{\chi_{A_iA_j}(i\omega_n) = \int_0^{\beta\hbar} d\tau e^{i\omega_n\tau}\chi_{A_iA_j}(\tau)} \tag{11.112}$$

By using the Lehman representation, we can find a spectral representation for the latter function

$$\begin{aligned}
\chi_{A_iA_j}(i\omega_n) &= \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau e^{i\omega_n\tau}\langle A_i(\tau)A_j\rangle \\
&= \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau e^{i\omega_n\tau}\frac{1}{Z}\sum_{m,n}e^{-\beta E_n}\langle n| e^{E_n\tau/\hbar}A_ie^{-E_m\tau/\hbar}|m\rangle\langle m|A_j|n\rangle \qquad (11.113) \\
&= \frac{1}{Z}\sum_{m,n}\frac{e^{-\beta E_n}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\left(e^{i\omega_n\beta\hbar+\beta E_n-\beta E_m}-1\right)}{i\hbar\omega_n-(E_m-E_n)} \qquad (11.114) \\
&= \frac{1}{Z}\sum_{m,n}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{(E_m-E_n)-i\hbar\omega_n}\langle n|A_i|m\rangle\langle m|A_j|n\rangle \qquad (11.115)
\end{aligned}$$

where we used $e^{i\omega_n\beta\hbar}=1$. Using the Lehman representation for $\chi''_{A_iA_j}(\omega')$ Eq.(11.78) that we recopy here,

$$\chi''_{A_iA_j}(\omega) = \sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta Em}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\ \pi\,\delta\left(\hbar\omega-(E_m-E_n)\right).$$

we can write

$$\chi_{A_iA_j}(i\omega_n) = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-i\omega_n} \tag{11.116}$$

which is clearly a special case of our general spectral representation Eq.(11.69). This the response function in Matsubara frequency may be obtained from $\chi_{A_iA_j}(i\omega_n) = \chi_{A_iA_j}(z\to i\omega_n)$ whereas for the retarded function $\chi^R_{A_iA_j}(\omega) = \chi_{A_iA_j}(z\to\omega+i\eta)$.

Remark 24 *Once we write the expansion in Matsubara frequencies, the function $\chi_{A_iA_j}(\tau)$ in Eq.(11.110) is defined by its periodic extension outside the interval of definition $-\beta\hbar\le\tau\le\beta\hbar$. That follows the standard procedure for Fourier series. Outside the interval of definition however, it does not coincide with the original $\chi_{A_iA_j}(\tau)$ Eq.(11.106). Indeed, take $\chi_{A_iA_j}(\tau+2\beta\hbar) = \mathrm{Tr}\left[e^{-\beta H}e^{2\beta H}A_i(\tau)e^{-2\beta H}A_j\right]/(Z\hbar)$.There is no way this can become equal to $\chi_{A_iA_j}(\tau)$.*

11.10 Sum rules

All the many-body Physics of the response or scattering experiments is in the calculation of unequal-time commutators. These commutators in general involve the time evolution of the systems and thus they are non-trivial to evaluate. However, equal-time commutators are easy to evaluate in general using the usual commutation relations. Equal-time corresponds to integral over frequency as seen from Fourier space. Hence the name sum rules. We will not in general be able to satisfy all possible sum-rules since this would mean basically an exact solution to the problem, or computing infinite-order high-frequency expansion. In brief, sum-rules are useful to

- Relate different experiments to each other.
- Establish high frequency limits of correlation functions.
- Provide constraints on phenomenological parameters or on approximate theories.

11.10.1 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,

$$\delta \langle A_i(\omega = 0)\rangle = \chi^R_{A_iA_j}(\omega = 0)a_j(\omega = 0). \qquad (11.117)$$

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

$$\delta \langle A_i(\mathbf{q},\omega = 0)\rangle = \chi^R_{A_iA_j}(\mathbf{q},\omega = 0)a_j(\mathbf{q},\omega = 0). \qquad (11.118)$$

Using the spectral representation (11.69) and the usual relation between $i\eta$ and principal parts, Eq.(11.60), we also have,

$$\chi^R_{A_iA_j}(\mathbf{q},\omega = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega - i\eta} = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega}. \qquad (11.119)$$

There is no contribution from the imaginary part on the grounds that there can be no 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 $\chi''_{A_iA_j}(\mathbf{q},\omega)$ is odd, as proven at the end of the section on symmetry properties, so that $\chi''_{A_iA_j}(\mathbf{q},\omega = 0) = 0$. Note that in practice, the principal part in the above equation is not necessary since $\chi''_{A_iA_j}(\mathbf{q},\omega)$ usually vanishes linearly in ω for small ω. To be completly 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,

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{A_iA_j}(\mathbf{q},\omega = 0) = \frac{\partial A_i}{\partial a_j} \equiv \chi_{A_iA_j}. \qquad (11.120)$$

$$\boxed{\chi_{A_iA_j} = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega}}. \tag{11.121}$$

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

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{nn}(\mathbf{q},\omega=0) = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} = \left(\frac{\partial N}{\partial \mu}\right)_{T,V}. \tag{11.122}$$

As usual, a few remarks are in order:

Remark 25 *Thermodynamic sum-rule and moments: Thermodynamic sum-rules are in a sense the inverse first moment over frequency of $\chi''_{A_iA_j}(\mathbf{q},\omega)$ (the latter being analogous to the weight). Other sum-rules are over positive moments, as we now demonstrate.*

Remark 26 *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 where*

$$\langle N \rangle = Tr\left[e^{-\beta(H-\mu N)}N\right]/Z$$

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,

$$\langle NN \rangle - \langle N \rangle^2 = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega) \tag{11.123}$$

Using the general fluctuation-dissipation theorem, we now relate this quantity to $\chi''_{nn}(\mathbf{q},\omega)$ 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, at small $\mathbf{q}$ all the weight will be near zero frequency so the fluctuation-dissipation theorem Eq.(C.10) becomes

$$S_{nn}(\mathbf{q},\omega) = \lim_{\omega\to 0} \frac{2\hbar}{1-e^{-\beta\hbar\omega}} \chi''_{nn}(\mathbf{q},\omega) = \frac{2}{\beta\omega}\chi''_{nn}(\mathbf{q},\omega) \tag{11.124}$$

from which we obtain what is basically the thermodynamic sum-rule Eq.(11.122)

$$\langle NN \rangle - \langle N \rangle^2 = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega) \tag{11.125}$$

$$= \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\beta\omega} = \frac{1}{\beta}\left(\frac{\partial N}{\partial \mu}\right)_{T,V} \tag{11.126}$$

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).

11.10.2 Order of limits

It is extremely important to note that for thermodynamic sume rules, the $\omega \to 0$ limit is taken first, before the $\mathbf{q} \to 0$ limit. The other limit describes transport properties as we shall see. Take as an example of a $\mathbf{q} = \mathbf{0}$ quantity the total number of particles. Then

$$\chi''_{NN}(t) = \frac{1}{2\hbar} \langle [N(t), N] \rangle = 0 \tag{11.127}$$

This quantity vanishes for all times because N being a conserved quantity it is independent of time, and it commutes with itself. Taking Fourier transforms, $\chi''_{NN}(\omega) = 0$ for all frequencies. Hence, we must take the $\mathbf{q} \to \mathbf{0}$ limit after the $\omega = 0$.

Another important question is that of the principal part integral. If we take the $\mathbf{q} \to \mathbf{0}$ limit at the end, as suggested above, we do not run into problems. *As follows from a problem 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.(11.122). If we take the limit $\mathbf{q} \to \mathbf{0}$ before doing the integral however, $\lim_{\mathbf{q}\to\mathbf{0}} \chi''_{nn}(\mathbf{q},\omega)$ is proportionnal to $\omega\delta(\omega)$ so it is important NOT to take the principal part integral to get the correct result (in other words, under the integral sign the $\eta \to 0$ limit must be taken before the $\mathbf{q} \to \mathbf{0}$ limit). We also see this as follows. If we return to the original form $\lim_{\eta\to 0} 1/(\omega - i\eta) = \lim_{\eta\to 0} \omega/(\omega^2+\eta^2) + i\eta/(\omega^2+\eta^2)$, and then do the integral of the first term (real part), we can check that we have to take the $\eta \to 0$ limit under the integral sign before the $\mathbf{q} \to \mathbf{0}$ limit to recover the result obtained by doing the integral at finite $\mathbf{q}$ and then taking the $\mathbf{q} \to \mathbf{0}$ limit (the latter is unambiguous and does not depend on the presence of the principal part in the integral). Physically, this means that the adiabatic turning-on time must be longer than the diffusion time to allow the conserved quantity to relax. This is summarized by the following set of equations

$$\begin{aligned}
\lim_{\mathbf{q}\to\mathbf{0}} \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} &= \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} && (11.128)\\
&= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q}\to\mathbf{0}} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} && (11.129)\\
&\neq \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q}\to\mathbf{0}} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega}. && (11.130)
\end{aligned}$$

11.10.3 Moments, sum rules, and high-frequency expansions.

The n'th moment of a probability distribution is defined as the average of the random variable to the power n. By analogy, we define the n'th moment of the spectral function by $\int_{-\infty}^{\infty} \frac{d\omega}{\pi}\omega^n \chi''_{A_iA_j}(\omega)$. For operators with the same signature under time reversal, even moments vanish while odd moments of $\chi''_{A_iA_j}$ are related to equal-time commutators that are easy to compute:

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi}\omega^n \chi''_{A_iA_j}(\omega) = \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\left(i\frac{\partial}{\partial t}\right)^n e^{-i\omega t} 2\chi''_{A_iA_j}(\omega)\right]_{t=0} \tag{11.131}$$

$$= \frac{1}{\hbar}\left\langle\left[\left(i\frac{\partial}{\partial t}\right)^n A_i(t), A_j(0)\right]\right\rangle_{t=0} = \frac{1}{\hbar}\left\langle\left[\left[\left[A_i(t),\frac{H}{\hbar}\right],\frac{H}{\hbar}\right]...,A_j(0)\right]\right\rangle_{t=0} \tag{11.132}$$

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

These moments determine the high frequency behavior of response functions. One does expect that high frequencies are related to short times, and if time is short enough it is natural that commutators be involved. Let us see this. Suppose the spectrum of excitations is bounded, as usually happens when the input momentum $\mathbf{q}$ is finite. Then, $\chi''_{A_iA_j}(\omega') = 0$ for $\omega' > D$ 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,

$$\boxed{\chi^R_{A_iA_j}(\mathbf{q},\omega) = \int_{-\infty}^{\infty}\tfrac{d\omega'}{\pi}\tfrac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'-\omega-i\eta}} \tag{11.133}$$

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

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$$\boxed{\chi^R_{A_iA_j}(\mathbf{q},\omega) = \int_{-\infty}^{\infty}\tfrac{d\omega'}{\pi}\tfrac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'-\omega-i\eta}} \tag{11.134}$$

$$\boxed{\approx \sum_{n=1}^{\infty}\tfrac{-1}{\omega^{2n}}\int_{-\infty}^{\infty}\tfrac{d\omega'}{\pi}\left(\omega'\right)^{2n-1}\chi''_{A_iA_j}(\mathbf{q},\omega')} \tag{11.135}$$

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

11.10.4 The f-sum rule as an example

The f-sum rule is one of the most widely used moment of a correlation function, particularly in the context of optical conductivity experiments. It is quite remarkable that this sum rule does not depend on interactions, so it should be valid independently of many details of the system. The sum rule is

$$\boxed{\int_{-\infty}^{\infty}\tfrac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \tfrac{n\mathbf{q}^2}{m}} \tag{11.136}$$

If we return to our high-frequency expansion in terms of moments, Eq.(11.135), we see that

$$\chi^R_{nn}(\mathbf{q},\omega) \approx \frac{-1}{\omega^2}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\omega'\chi''_{nn}(\mathbf{q},\omega') + \ldots = -\frac{n\mathbf{q}^2}{m\omega^2} + \ldots. \tag{11.137}$$

This is equivalent to saying that at very high frequency the system reacts as if it was composed of free particles. It is the inertia that determines the response, like for a harmonic oscillator well above the resonance frequency.

Let us derive that sum rule, which is basically a consequence of particle conservation. When the potential-energy part of the Hamiltonian commutes with the density operator, while the kinetic-energy part is that of free electrons (not true for tight-binding electrons) we find that

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega)=\frac{n\mathbf{q}^2}{m}.} \tag{11.138}$$

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

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega)=\frac{i}{\hbar\mathcal{V}}\left\langle\left[\frac{\partial n_{\mathbf{q}}(t)}{\partial t},n_{-\mathbf{q}}(t)\right]\right\rangle \tag{11.139}$$

$$=-\frac{1}{\hbar^2\mathcal{V}}\left\langle\left[\left[H,n_{\mathbf{q}}(t)\right],n_{-\mathbf{q}}(t)\right]\right\rangle \tag{11.140}$$

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

$$\int d\left(\mathbf{r}-\mathbf{r}'\right)e^{-i\mathbf{q}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}f(\mathbf{r}-\mathbf{r}')=\frac{1}{\mathcal{V}}\int d\mathbf{r}e^{-i\mathbf{q}\cdot r}\int d\mathbf{r}'e^{-i\mathbf{q}\cdot r'}f(\mathbf{r}-\mathbf{r}') \tag{11.141}$$

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

$$n_{\mathbf{q}}=\int d\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\sum_{\alpha}\delta(\mathbf{r}-\mathbf{r}_{\alpha})=\sum_{\alpha}e^{-i\mathbf{q}\cdot\mathbf{r}_{\alpha}} \tag{11.142}$$

$$\left[p_{\beta}^{x},n_{\mathbf{q}}\right]=\frac{\hbar}{i}\left[\frac{\partial}{\partial x_{\beta}},\sum_{\alpha}e^{-i\mathbf{q}\cdot\mathbf{r}_{\alpha}}\right]=-\hbar q^{x}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}. \tag{11.143}$$

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

$$\left[H,n_{\mathbf{q}}(t)\right]=\sum_{\beta}\left[\frac{p_{\beta}^{2}}{2m},n_{\mathbf{q}}\right]=\frac{1}{2m}\sum_{\beta}\left(\mathbf{p}_{\beta}\cdot\left(-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}\right)+\left(-\hbar\mathbf{q}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}\right)\cdot\mathbf{p}_{\beta}\right) \tag{11.144}$$

$$\left[\left[H,n_{\mathbf{q}}(t)\right],n_{-\mathbf{q}}(t)\right]=-\frac{1}{m}\sum_{\beta=1}^{N}\hbar^{2}\mathbf{q}^{2}e^{-i\mathbf{q}\cdot\mathbf{r}_{\beta}}e^{i\mathbf{q}\cdot\mathbf{r}_{\beta}}=-\frac{\hbar^{2}\mathbf{q}^{2}N}{m} \tag{11.145}$$

which proves the result (C.9) when substituted in the expression in terms of commutator (11.140) 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.)

11.11 Exercice

11.11.1 Fonction de relaxation de Kubo.

Dans la limite classique, le théorème de fluctuation-dissipation devient:

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

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

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

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

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

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

11.11.2 Constante diélectrique et Kramers-Kronig.

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

$$\epsilon_1(\omega)-\epsilon_1(\infty)=\frac{2}{\pi}\mathcal{P}\int_0^\infty d\xi\frac{\xi\epsilon_2(\xi)}{\xi^2-\omega^2}\tag{11.146}$$

$$\epsilon_2(\omega)=-\frac{2}{\pi}\omega\mathcal{P}\int_0^\infty d\xi\frac{\epsilon_1(\xi)-\epsilon_1(\infty)}{\xi^2-\omega^2}\tag{11.147}$$

11.11.3 Lien entre fonctions de réponses, constante de diffusion et dérivées thermodynamiques. Rôle des règles de somme.

Soit un système uniforme de spins 1/2, comme par exemple l'helium ^3He. Les interactions dans le système de spin ne dépendent pas du spin. Donc, l'aimantation totale dans la direction z, que nous noterons M, est conservée, c'est-à-dire que

$$\partial_t M(\mathbf{r},t)+\nabla\cdot\mathbf{j}^M(\mathbf{r},t)=0\tag{11.148}$$

où $\mathbf{j}^M$ est le courant d'aimantation. Sur une base purement phénoménologique, ce courant dépend du gradient d'aimantation. En d'autres mots, comme M est conservée, il obéit à une dynamique diffusive. Dans un processus hors d'équilibre, (mais pas trop loin de l'équilibre!) et sur des échelles hydrodynamiques, (grand temps et grandes longueurs d'ondes) nous aurons donc

$$\left\langle\mathbf{j}^M(\mathbf{r},t)\right\rangle_{he}=-D\nabla\left\langle M(\mathbf{r},t)\right\rangle_{he}\tag{11.149}$$

où la moyenne fait référence à une moyenne hors d'équilibre.

Soit la fonction de corrélation aimantation-aimantation

$$S_{MM}(\mathbf{r},t)=\left\langle M(\mathbf{r},t)M(\mathbf{0},0)\right\rangle\tag{11.150}$$

Cette fonction de corrélation est accessible par exemple par diffusion neutronique.

a) Phénoménologie: En utilisant le fait que le couplage entre aimantation et champ magnétique est donné par

$$H_{int} = -\int d^3\mathbf{r} M(\mathbf{r})\, h(\mathbf{r})$$

et que l'Hamiltonien commute avec l'aimantation totale, montrez que

$$\lim_{\mathbf{k}\to 0} S_{MM}(\mathbf{k},t{=}0) = \frac{1}{\beta}\left(\frac{\partial M}{\partial h}\right) \equiv \frac{1}{\beta}\chi_{MM} \tag{11.151}$$

En supposant ensuite que la dynamique pour $\langle M(\mathbf{r},t)\, M(0,0)\rangle$ avec $t > 0$ est la même que celle obtenue phénoménologiquement pour une perturbation hors d'équilibre et en utilisant la réversibilité, soit

$$\langle M(\mathbf{r},t)\, M(\mathbf{0},0)\rangle = \langle M(\mathbf{0},0)\, M(\mathbf{r},-t)\rangle \tag{11.152}$$

pour déduire le résultat lorsque $t < 0$, montrez qu'aux grandes longueurs d'onde (c'est-à-dire dans la limite hydrodynamique)

$$S_{MM}(\mathbf{k},\omega) = \frac{2Dk^2}{\omega^2 + (Dk^2)^2} S_{MM}(\mathbf{k},t=0) \approx \frac{2Dk^2}{\omega^2 + (Dk^2)^2}\frac{1}{\beta}\chi_{MM} \tag{11.153}$$

- Vous pouvez utiliser l'invariance sous la transformation de parité $\mathbf{r} \to -\mathbf{r}$.
- L'hypothèses menant à ce résultat est connue sous le nom d'hypothèse de régression d'Onsager: "Les fluctuations spontanées à l'équilibre régressent vers l'équilibre de la même façon que les perturbations provoquées de l'extérieur, en autant que ces perturbations ne soient pas trop fortes (réponse linéaire)."

b) Lien entre calcul phénoménologique et microscopique. En utilisant le théorème de fluctuation-dissipation, obtenez une prédiction phénoménologique pour $\chi''_{MM}(\mathbf{k},\omega)$ à partir de $S_{MM}(\mathbf{k},\omega)$. Montrez ensuite que si un calcul microscopique nous donne $\chi''_{MM}(\mathbf{k},\omega)$ alors la constante de diffusion peut être obtenue de ce calcul microscopique en de la façon suivante:

$$D\chi = \lim_{\omega\to 0}\left[\lim_{\mathbf{k}\to\mathbf{0}} \frac{\omega}{k^2}\chi''_{MM}(\mathbf{k},\omega)\right] \tag{11.154}$$

tandis que la susceptibilité magnétique uniforme elle, s'obtient de

$$\chi_{MM} = \lim_{\mathbf{k}\to\mathbf{0}} \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{k},\omega)}{\omega} \tag{11.155}$$

c) Règles de somme: La dernière équation ci-dessus est la règle de somme thermodynamique pour la susceptibilité $\chi''_{MM}(\mathbf{k},\omega)$. Notre expression phénoménologique pour $\chi''_{MM}(\mathbf{k},\omega)$ satisfait cette règle de somme. Considérons maintenant la règle de somme f. L'expression microsopique pour l'aimantation est

$$M(\mathbf{r}) = \sum_{\alpha=1}^{N} 2\mu s_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) \tag{11.156}$$

où, dans ce système paramagnétique, $s_\alpha = \pm\frac{1}{2}$ et μ est le moment magnétique, alors que l'expression correspondante pour le courant d'aimantation est

$$\mathbf{j}^M(\mathbf{r}) = \frac{\mu}{m}\sum_{\alpha=1}^{N} s_\alpha \left[\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta(\mathbf{r} - \mathbf{r}_\alpha) + \delta(\mathbf{r} - \mathbf{r}_\alpha)\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\right] \tag{11.157}$$

avec m la masse. Utilisant ces expressions, démontrez la règle de somme f pour ce système de spins, soit

$$\int \frac{d\omega}{\pi} \omega \chi^{''}_{MM}(\mathbf{k},\omega) = \frac{n}{m}\mu^2 k^2 \tag{11.158}$$

où n est la densité. Vérifiez ensuite que l'expression phénoménologique trouvée ci-dessus pour $\chi^{''}_{MM}(\mathbf{k},\omega)$ à partir de considérations hydrodynamiques, ne satisfait *pas* la règle de somme f. Laquelle de nos hypothèses phénoménologiques devrait être raffinée pour arriver à satisfaire cette règle de somme?

12. 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.

12.1 Coupling between electromagnetic fields and matter, and gauge invariance

Electric and magnetic fields are related to vector and scalar potential by

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\nabla}\phi \tag{12.1}$$

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}. \tag{12.2}$$

The gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A} + \boldsymbol{\nabla}\Lambda \tag{12.3}$$

$$\phi \rightarrow \phi - \frac{\partial \Lambda}{\partial t} \tag{12.4}$$

leaves the electric and magnetic fields invariant. We say that the theory is gauge invariant. In other words, there are many equivalent ways of representing the same physics. It is not a symmetry in the usual sense.[9] We will give a more detailed derivation in the next subsection, but you only need to know the so-called minimal-coupling prescription to couple matter and electromagnetic field,[5] one of the most elegant results in physics

$$\mathbf{p}_\alpha = \frac{\hbar}{i}\nabla_\alpha \rightarrow \frac{\hbar}{i}\nabla_\alpha - e\mathbf{A}(\mathbf{r}_\alpha, t) \tag{12.5}$$

$$i\hbar\frac{\partial}{\partial t} \rightarrow i\hbar\frac{\partial}{\partial t} - e\phi(\mathbf{r}_\alpha, t). \tag{12.6}$$

In this expression e is the charge of the particle, not the elementary charge. The derivatives to the right are called covariant.

Given this, Schrödinger's equation in the presence of an electromagnetic field should read

$$\left(i\hbar\frac{\partial}{\partial t}-e\phi(\mathbf{r}_\alpha,t)\right)\psi=\frac{1}{2m}\left(\frac{\hbar}{i}\nabla_\alpha-e\mathbf{A}(\mathbf{r}_\alpha,t)\right)^2\psi+V\psi \tag{12.7}$$

where V is some potential energy. Suppose we write the equation in a different gauge

$$\left(i\hbar\frac{\partial}{\partial t}-e\phi(\mathbf{r}_\alpha,t)+e\frac{\partial\Lambda}{\partial t}\right)\psi'=\frac{1}{2m}\left(\frac{\hbar}{i}\nabla_\alpha-e\mathbf{A}(\mathbf{r}_\alpha,t)-e\boldsymbol{\nabla}\Lambda\right)^2\psi'+V\psi'. \tag{12.8}$$

The solution is different since it is not the same equation. Assume however that ψ and ψ' correspond to an eigenstate with the same value of the eigenenergy. The latter should be gauge invariant. Then, the solution ψ' that we find is related to ψ with the same eigenvalue in the following way

$$\psi'=e^{ie\Lambda/\hbar}\psi. \tag{12.9}$$

That is easy to check since if we substitute in the equation for ψ', then we recover the previous equation for ψ.

Observables should be gauge invariant. That is clearly the case for the potential,

$$\int d^3\mathbf{r}\psi^*V\psi=\int d^3\mathbf{r}\psi'^*V\psi' \tag{12.10}$$

since the phases cancel. The conjugate momentum operator however is not gauge invariant

$$\int d^3\mathbf{r}\psi^*\frac{\hbar}{i}\boldsymbol{\nabla}\psi\neq\int d^3\mathbf{r}\psi'^*\frac{\hbar}{i}\boldsymbol{\nabla}\psi' \tag{12.11}$$

since $\boldsymbol{\nabla}\Lambda\neq 0$. On the other hand, the following quantity $\left(\frac{\hbar}{i}\boldsymbol{\nabla}-e\mathbf{A}(\mathbf{r}_\alpha,t)\right)$ is gauge invariant since

$$\int d^3\mathbf{r}\psi^*\left(\frac{\hbar}{i}\boldsymbol{\nabla}-e\mathbf{A}(\mathbf{r}_\alpha,t)\right)\psi=\int d^3\mathbf{r}\psi'^*\left(\frac{\hbar}{i}\boldsymbol{\nabla}-e\mathbf{A}(\mathbf{r}_\alpha,t)-e\boldsymbol{\nabla}\Lambda\right)\psi'. \tag{12.12}$$

That quantity is the expectation of the mass times the velocity and is thus an observable. It is necessary to establish the correct expression for the current.

12.1.1 Invariant action, Lagrangian and coupling of matter and electromagnetic field[10]

This section is not necessary to understand any other section. It is just useful to recall the fundamental ideas about coupling electromagnetic fields and matter.

Take a single particle of charge e in classical mechanics. The action that couples that particle, or piece of charged matter, to the electromagnetic field should be invariant under a Lorentz transformation and a gauge transformation. The simplest candidate that satisfies this requirement is

$$S_{e-m}=e\int A_\mu dr^\mu \tag{12.13}$$

where we used the summation convention as usual and the four-vectors with r^μ the contravariant four-vector for position

$$A_\mu = (-\phi/c, A_a) \; ; \; r^\mu = \begin{pmatrix} ct \\ r_a \end{pmatrix} . \tag{12.14}$$

The action is clearly Lorentz invariant. It is also gauge invariant since, with $\partial_\mu = \left(\frac{1}{c\partial t}, \boldsymbol{\nabla}\right)$, the gauge transformation

$$S_{e-m} \to e \int \left(A_\mu + \partial_\mu \Lambda\right) dr^\mu = e \int A_\mu dr^\mu \tag{12.15}$$

only adds a total time derivative to the Lagrangian

$$e \int \left(\partial_\mu \Lambda\right) dr^\mu = e \int \left(\partial_\mu \Lambda\right) \frac{dr^\mu}{dt} dt = e \int \frac{d\Lambda}{dt} dt \tag{12.16}$$

and in the variational principle the Lagrangian does not vary at the limits of time integration.

Speaking of the Lagrangian, it can be deduced from

$$S_{e-m} = e \int A_\mu \frac{dr^\mu}{dt} dt = \int \left(-e\phi + e\mathbf{A}\cdot\frac{d\mathbf{r}}{dt}\right) dt = \int L_{e-m} dt \tag{12.17}$$

The coupling of light to matter appears at two places in the equations of motion obtained from the Euler-Lagrange equations. It appears in the Euler-Lagrange equations for matter that involve particle coordinates, and in the Euler-Lagrange equations for the electromagnetic field that involve electromagnetic potentials playing the role of coordinates. The former give Newton's equations with the Lorentz force and the latter Maxwell's equations.

The part of the Lagrangian that involve particle coordinates, neglecting potential energy terms that do not play any role in this derivation, is given by $L = m\mathbf{v}^2/2 + L_{e-m}$, namely

$$\begin{aligned} L &= \frac{1}{2} m\mathbf{v}^2 - e\left(\phi - \mathbf{A}\cdot\frac{d\mathbf{r}}{dt}\right) && (12.18) \\ &= \frac{1}{2} m\mathbf{v}^2 - e\left(\phi - \mathbf{A}\cdot\mathbf{v}\right) && (12.19) \end{aligned}$$

It can be verified that the Euler-Lagrange equations give Newton's equation with the Lorentz force. The conjugate moment, is

$$p_a = \left(\frac{\partial L}{\partial v_a}\right)_{\mathbf{r},\mathbf{A}} = m v_a + e A_a \to \frac{\hbar}{i} \frac{\partial}{\partial r_a}. \tag{12.20}$$

It is the conjugate moment $\mathbf{p}$ that obeys commutation relations with position in quantum mechanics, in other words it is $\mathbf{p}$ that becomes $\frac{\hbar}{i}\boldsymbol{\nabla}$.

The action of the electromagnetic field is written in terms of the Faraday tensor. What is important for our discussion is that the current in Maxwell's equation is generated by the following term

$$j_a = e v_a = \left(\frac{\partial L_{e-m}}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} = \frac{e}{m}\left(p_a - e A_a\right) \tag{12.21}$$

where in the last equation we have used the equation that relates the conjugate moment to the velocity and vector potential Eq.(12.20). Physically this makes a lot of sense. The current is simply charge times velocity.

In condensed matter physics, we do not generally write down the part of the Hamiltonian that involves only the pure electromagnetic field. But we are interested in coupling matter to the electromagnetic field and we would like to have the expression for the current that follows from the Hamiltonian where the minimal-coupling prescription has been used. It is indeed possible to satisfy this wish and to obtain the current from the Hamiltonian. It proceeds as follows. Taking for L the full Lagrangian, except for the part that contains only the electromagnetic field, we obtain

$$\left(\frac{\partial L}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}}=\left(\frac{\partial\left(p_b v_b-H\right)}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}} \tag{12.22}$$

where $\mathbf{p}\left(\mathbf{r},\mathbf{v},\mathbf{A}\right)$ is written in terms of $\mathbf{r},\mathbf{v}$ and $\mathbf{A}$ using the equation for the conjugate moment Eq.(12.21). With the chain rule, we thus find (components of p that are not differentiated are also kept constant)

$$\left(\frac{\partial\left(p_b v_b-H\right)}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}}=\left(\frac{\partial p_b}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}}v_b-\left(\frac{\partial H}{\partial p_b}\right)_{\mathbf{r},\mathbf{A}}\left(\frac{\partial p_b}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}}-\left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{r}}. \tag{12.23}$$

Since Hamilton's equations give $\left(\frac{\partial H}{\partial p_b}\right)_{\mathbf{r},\mathbf{A}}=v_b$, we are left with

$$j_a=ev_a=\left(\frac{\partial L}{\partial A_a}\right)_{\mathbf{r},\mathbf{v}}=-\left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{A}}. \tag{12.24}$$

This result comes out because, as usual in a Legendre transform, the first derivative with respect to the conjugate variable $\mathbf{p}$ vanishes. The above expression for the current in terms of a derivative of the Hamiltonian is often used in practice. In this expression, H does not contain the part that involves only electromagnetic potentials.

Remark 27 *In the four-vector notation of the present section, the prescription for minimal coupling, is*

$$\partial_\mu\rightarrow\partial_\mu-ieA_\mu/\hbar. \tag{12.25}$$

12.2 Response of the current to external vector and scalar potentials

We need to find the terms $\delta\mathcal{H}(t)=\delta\mathcal{H}(t)_\phi+\delta\mathcal{H}(t)_{\mathbf{A}}$ added to the Hamiltonian by the presence of the electromagnetic field. Let us begin by the term $\delta\mathcal{H}(t)_{\mathbf{A}}$ coming from the vector potential. Under the minimal coupling prescription, we find (recall that the gradient will also act on the wave function that will multiply the operator)

$$-\frac{\hbar^2}{2m}\nabla_\alpha^2\rightarrow-\frac{\hbar^2}{2m}\nabla_\alpha^2-\frac{e\hbar}{2mi}\left(\mathbf{A}(\mathbf{r}_\alpha)\cdot\nabla_\alpha+\nabla_\alpha\cdot\mathbf{A}(\mathbf{r}_\alpha)\right)+\frac{e^2}{2m}\mathbf{A}^2(\mathbf{r}_\alpha). \tag{12.26}$$

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

$$\delta\mathcal{H}(t)_{\mathbf{A}}=-\sum_\alpha\frac{e\hbar}{2mi}\left(\mathbf{A}(\mathbf{r}_\alpha)\cdot\nabla_\alpha+\nabla_\alpha\cdot\mathbf{A}(\mathbf{r}_\alpha)\right)=-\int d\mathbf{r}\mathbf{A}(\mathbf{r},t)\cdot\mathbf{j}(\mathbf{r}). \tag{12.27}$$

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

$$\mathbf{j}(\mathbf{r}) = \frac{e}{2m}\sum_{\alpha}\left(\delta(\mathbf{r}-\mathbf{r}_{\alpha})\mathbf{p}_{\alpha}+\mathbf{p}_{\alpha}\delta(\mathbf{r}-\mathbf{r}_{\alpha})\right). \tag{12.28}$$

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.

The paramagnetic current that we found above is the same as that which is found from Schrödinger's equation in the absence of electromagnetic field by requiring that probability density $\psi^*\psi$ be conserved. Given the minimal coupling prescription, Eq.(12.5) and the considerations of Sec.12.1 on gauge invariance of observables, the observable current operator $\mathbf{j}^A(\mathbf{r})$ is obtained from the minimal coupling prescription in the paramagnetic current operator Eq.(12.28)

$$\mathbf{j}^A(\mathbf{r}) = \mathbf{j}(\mathbf{r}) - \frac{e^2}{m}\sum_{\alpha}\mathbf{A}(\mathbf{r}_{\alpha})\delta(\mathbf{r}-\mathbf{r}_{\alpha}) = \mathbf{j}(\mathbf{r}) - \frac{e}{m}\mathbf{A}(\mathbf{r})\rho(\mathbf{r}) \tag{12.29}$$

where we have defined the charge density as before

$$\rho(\mathbf{r}) = en(\mathbf{r}) = e\sum_{\alpha}\delta\left(\mathbf{r}-\mathbf{r}_{\alpha}\right). \tag{12.30}$$

The last term in the equation for the current is called the *diamagnetic current.*

Remark 28 *Our definition of the current-density operator Eq.(12.28) automatically takes care of the relative position of the vector potential and of the gradients in the above equation. The current can also be obtained from* $-\left(\frac{\partial H}{\partial A_a}\right)_{\mathbf{p},\mathbf{A}}$*, as explained in the previous section.*

It is easier to add an ordinary scalar potential. From Schrödinger's equation in the presence of an electromagnetic field Eq.(12.7), the presence of a scalar potential introduces a term

$$\delta\mathcal{H}(t)_{\phi} = \int d\mathbf{r}\phi(\mathbf{r},t)\rho(\mathbf{r}) \tag{12.31}$$

in the Hamiltonian.

Using the explicit expression for the current Eq.(12.29) and our linear-response formulae in Chapter 10, we finally come to the general expression for the response,

$$\boxed{\delta\left\langle j_a^A(\mathbf{q},\omega)\right\rangle = \left[\chi^R_{j_a j_b}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{ab}\right]A_b(\mathbf{q},\omega) - \chi^R_{j_a\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega).} \tag{12.32}$$

There is a sum over the repeated indices a as usual. The term proportional to $-\frac{ne^2}{m}\delta_{ab}$ in this expression, called the diamagnetic term, comes from the last term in the expression for the gauge invariant current Eq.(12.29). Since the density operator there is already multiplied by the vector potential, its average can be taken for the equilibrium ensemble where the average density is independent of position.

The above expression is not gauge invariant in an obvious way. The response is not given in terms of gauge invariant fields. We will show below that there is indeed gauge invariant. We begin with the case of the transverse response, which is easier.

12.3 Kubo formula for the transverse conductivity

The above relation between current and electromagnetic potential still does not give us the conductivity. The conductivity relates current to electric field, not to poetntial. Roughly, for the conductivity σ we have $j = \sigma E$. We thus need to go back to the fields. In addition, the first thing to realize is that the conductivity is a tensor since it relates current in one direction to field applied in any other direction. Moreover, the electromagnetic fields can be transverse or longitudinal, i.e. perpendicular or transverse to the direction of propagation. Let us begin by discussing this point.

When we study the response to applied fields whose direction is perpendicular to the direction of the wave vector $\mathbf{q}$, we say that we are studying the transverse (or selenoidal) response**.** In this case, $\mathbf{q}\cdot\mathbf{E}(\mathbf{q},\omega)$=0. The scalar potential contributes only to the longitudinal component of the field (along with the longitudinal contribution from the vector potential) since the gradient is always along $\mathbf{q}$. We can thus disregard for the moment the contribution from the scalar potential and leave it for our study of the longitudinal response, where we will study in detail the question of gauge invariance. The magnetic field is always transverse since $\nabla\cdot\mathbf{B} = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\times\mathbf{A} = 0$. Let us decompose the vector potential into a transverse and a longitudinal part. This is easily done by using the unit vector $\widehat{\mathbf{q}} = \mathbf{q}/\left|\mathbf{q}\right|$

$$\mathbf{A}^L \equiv \widehat{\mathbf{q}}\widehat{\mathbf{q}}\cdot\mathbf{A} \equiv \widehat{\mathbf{q}}\left(\widehat{\mathbf{q}}\cdot\mathbf{A}\right) \tag{12.33}$$

$$\mathbf{A}^T \equiv \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right)\cdot\mathbf{A}. \tag{12.34}$$

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

$$\left(\overleftrightarrow{\sigma}\cdot\mathbf{A}\right)_a = \sum_b \sigma_{ab}A_b. \tag{12.35}$$

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

$$\overleftrightarrow{\sigma}^T(\mathbf{q},\omega) = \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right)\cdot\overleftrightarrow{\sigma}(\mathbf{q},\omega)\cdot\left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \tag{12.36}$$

$$\overleftrightarrow{\sigma}^L(\mathbf{q},\omega) = \widehat{\mathbf{q}}\widehat{\mathbf{q}}\cdot\overleftrightarrow{\sigma}(\mathbf{q},\omega)\cdot\widehat{\mathbf{q}}\widehat{\mathbf{q}} \tag{12.37}$$

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.(12-1).

Then the conductivity defined by

$$\delta\left\langle j_y^A(q_x,\omega)\right\rangle \equiv \sigma_{yy}(q_x,\omega)E_y(q_x,\omega) \tag{12.38}$$

follows from the relation between current and vector potential Eq.(12.32) and from the relation between electric field and vector potential

$$E_y(q_x,\omega) = i(\omega + i\eta)A_y(q_x,\omega) \tag{12.39}$$

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. We find for the transverse conductivity

$$\boxed{\sigma_{yy}(q_x,\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_yj_y}(q_x,\omega) - \frac{ne^2}{m}\right]} \tag{12.40}$$

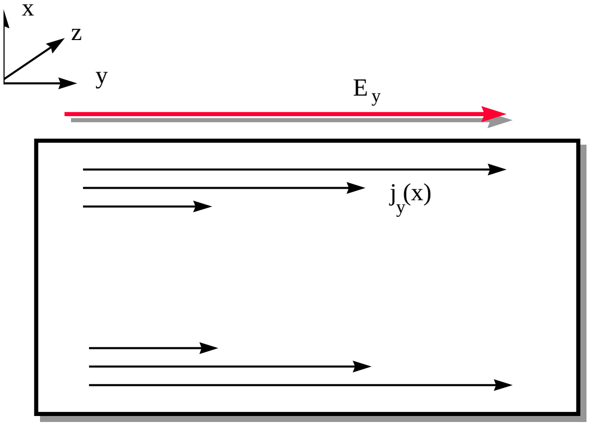

Figure 12-1 Application of a transverse electric field: skin effect.

12.4 Kubo formula for the longitudinal conductivity and *f*-sum rule

When $\mathbf{q}$ is in the direction of the electric field, we say that we are considering the longitudinal (or potential) response. Using the consequences of charge conservation on the response functions χ'', it is possible to rewrite the expression which involves both scalar and vector potential Eq.(12.32) in a way that makes the response look explicitly invariant under gauge transformations. This is the plan for this section.

As usual current conservation and gauge invariance are intimately related. More specifically, Noether's theorem states that to each continuous symmetry that leaves the action invariant, correponds a conserved quantity. Using this theorem, gauge invariance leads to current conservation, namely

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = -\nabla\cdot\mathbf{j}(\mathbf{r},t) \tag{12.41}$$

$$\frac{\partial \rho(\mathbf{q},t)}{\partial t} = -i\mathbf{q}\cdot\mathbf{j}(\mathbf{q},t). \tag{12.42}$$

We can use current conservation to replace the charge-density operator in the term describing the response of the scalar potential by a current density, which will make the response Eq.(12.32) look more gauge invariant. Take $\mathbf{q}$ in the x direction to be specific. Some gymnastics on the susceptibility in terms of commutator gives,

$$\frac{\partial \chi^R_{j_x\rho}(q_x,t)}{\partial t} = \delta(t)\frac{i}{\hbar\mathcal{V}}\left\langle [j_x(q_x,0),\rho(-q_x,0)]\right\rangle + \theta(t)\frac{i}{\hbar\mathcal{V}}(-iq_x)\left\langle [j_x(q_x,0),j_x(-q_x,-t)]\right\rangle . \tag{12.43}$$

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

$$\frac{i}{\hbar\mathcal{V}}\left\langle [j_x(q_x,0),\rho(-q_x,0)]\right\rangle = i\int \frac{d\omega}{\pi}\chi''_{j_x\rho}(q_x,\omega) \tag{12.44}$$

then current conservation

$$= i\int \frac{d\omega}{\pi}\frac{\omega}{q_x}\chi''_{\rho\rho}(q_x,\omega) \tag{12.45}$$

and finally the f sum rule Eq.(C.9) to rewrite the last expression as

$$= iq_x \frac{ne^2}{m} \tag{12.46}$$

Substituting back in the expression for the time derivative of the current-charge susceptibility Eq.(12.43) and Fourier transforming in frequency, we have

$$\boxed{-i(\omega + i\eta)\chi^R_{j_x\rho}(q_x, \omega) = iq_x \tfrac{ne^2}{m} - iq_x \chi^R_{j_x j_x}(q_x, \omega).} \tag{12.47}$$

Using this in the general formula for the response of the current Eq.(12.32) the longitudinal linear response function can be written in terms of the gauge invariant electric field in two different ways:

$$\delta \left\langle j^A_x(q_x,\omega)\right\rangle = \frac{1}{i(\omega + i\eta)} \left[\chi^R_{j_x j_x}(q_x, \omega) - \frac{ne^2}{m}\right] (i(\omega + i\eta)A_x(q_x, \omega) - iq_x\phi(q_x,\omega)) \tag{12.48}$$

$$= \left[\frac{1}{iq_x}\chi^R_{j_x\rho}(q_x, \omega)\right] (i(\omega + i\eta)A_x(q_x, \omega) - iq_x\phi(q_x,\omega))\,. \tag{12.49}$$

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

$$E_x(q_x, \omega) = i(\omega + i\eta)A_x(q_x, \omega) - iq_x\phi(q_x,\omega) \tag{12.50}$$

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

$$\boxed{\sigma_{xx}(q_x, \omega) = \tfrac{1}{i(\omega+i\eta)} \left[\chi^R_{j_x j_x}(q_x, \omega) - \tfrac{ne^2}{m}\right] = \left[\tfrac{1}{iq_x}\chi^R_{j_x\rho}(q_x, \omega)\right]}. \tag{12.51}$$

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.

12.4.1 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,

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda \tag{12.52}$$

$$\phi \rightarrow \phi - \frac{\partial \Lambda}{\partial t} \tag{12.53}$$

Let $\phi = 0$. Then

$$\delta \left\langle j^A_x(q_x,\omega)\right\rangle = \left[\chi^R_{j_x j_x}(q_x, \omega) - \frac{ne^2}{m}\right] A_x(q_x, \omega) \tag{12.54}$$

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

$$\boxed{\left[\chi^R_{j_x j_x}(q_x, 0) - \tfrac{ne^2}{m}\right] = 0}. \tag{12.55}$$

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

$$\chi^R_{j_x j_x}(q_x,0) = \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'} \tag{12.56}$$

as well as the conservation of charge,

$$= \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'} = \int \frac{d\omega'}{\pi} \frac{\omega'\chi''_{\rho\rho}(q_x,\omega')}{q_x^2} \tag{12.57}$$

and the f-sum rule (C.9)

$$= \frac{1}{q_x^2} \int \frac{d\omega'}{\pi} \omega'\chi''_{\rho\rho}(q_x,\omega') = \frac{ne^2}{m} = \chi^R_{j_x j_x}(q_x,0). \tag{12.58}$$

The form

$$\boxed{\int \frac{d\omega'}{\pi} \frac{\chi''_{j_x j_x}(q_x,\omega')}{\omega'} = \frac{ne^2}{m}} \tag{12.59}$$

of the above result, obtained by combining Eqs.(12.55) and (12.56) will be used quite often below.

Another possibility is to let A =0. Then, the general Kubo formula (12.32) gives

$$\delta \left\langle j_x\left(\mathbf{q},\omega\right)\right\rangle = -\chi^R_{j_x\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega). \tag{12.60}$$

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

$$\boxed{\chi^R_{j_x\rho}(0,\omega) = 0}. \tag{12.61}$$

That this is true, again follows from current conservation since

$$\chi^R_{j_x\rho}(0,\omega) = \int \frac{d\omega'}{\pi} \frac{\chi''_{j_x\rho}(0,\omega')}{\omega' - \omega - i\eta} \tag{12.62}$$

and

$$\chi''_{j_x\rho}(0,\omega') = \int dt e^{i\omega t} \frac{1}{2\hbar\mathcal{V}} \left\langle \left[\int d\mathbf{r} j_\mu(\mathbf{r},t), \int d\mathbf{r}'\rho(\mathbf{r}') \right] \right\rangle = 0 \tag{12.63}$$

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 29 *Both results Eq.(12.55) and Eq.(12.61) are consistent with the general relation found between both types of correlation functions Eq.(12.47). It suffices to take the* $\mathbf{q} \rightarrow 0$ *limit assuming that* $\chi^R_{j_x j_x}(q_x,\omega)$ *is finite or diverges less slowly than* $1/q_x$ *to prove Eq.(12.61) and to take* $\omega \rightarrow 0$ *assuming that* $\chi^R_{j_\mu\rho}(q_x,\omega)$ *is finite or diverges less slowly than* $1/\omega$ *to prove Eq.(12.55).*

12.4.2 Longitudinal conductivity sum-rule and a useful expression for the longitudinal conductivity.

The expression for the longitudinal conductivity

$$\sigma_{xx}(q_x,\omega)=\frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega)-\frac{ne^2}{m}\right] \tag{12.64}$$

can be written in an even more convenient manner by using our previous results Eq.(12.59) obtained from the $f-$sum rule and the spectral representation for the current-current correlation function

$$\begin{aligned}
\sigma_{xx}(q_x,\omega) &= \frac{1}{i(\omega+i\eta)}\left[\int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')}{\omega'-\omega-i\eta}-\int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')}{\omega'}\right] && (12.65)\\
&= \frac{1}{i(\omega+i\eta)}\left[\int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')(\omega+i\eta)}{\omega'\left(\omega'-\omega-i\eta\right)}\right] && (12.66)
\end{aligned}$$

$$\boxed{\sigma_{xx}(q_x,\omega)=\frac{1}{i}\left[\int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')}{\omega'(\omega'-\omega-i\eta)}\right]} \tag{12.67}$$

From this formula, we easily obtain with the usual identity for principal parts, Eq.(11.60)

$$\boxed{\mathrm{Re}\,\sigma_{xx}(q_x,\omega)=\frac{\chi''_{j_xj_x}(q_x,\omega)}{\omega}} \tag{12.68}$$

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

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathrm{Re}\left[\sigma_{xx}(q_x,\omega)\right]=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\chi''_{j_xj_x}(q_x,\omega)}{\omega}=\frac{ne^2}{2m}=\frac{\varepsilon_0\omega_p^2}{2}} \tag{12.69}$$

directly from the $f-$sum rule Eq.(12.59). In the above expression, ε_0 is the permittivity of the vacuum and ω_p^2 is the plasma frequency, which we will discuss later. Using the fact that the real part of the conductivity is an even function of ω, as follows from the fact that $\chi''_{j_xj_x}(q_x,\omega)$ 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 30 *Alternate expression: There is no principal part in the integrals appearing in the last expression. An equivalent but more cumbersome expression for the longitudinal conductivity, namely,*

$$\boxed{\sigma_{xx}(q_x,\omega)=\mathcal{P}\frac{1}{i\omega}\left[\chi^R_{j_xj_x}(q_x,\omega)-\frac{ne^2}{m}\right]-\pi\delta(\omega)\left[\chi^R_{j_xj_x}(q_x,\omega)-\frac{ne^2}{m}\right]} \tag{12.70}$$

is obtained from Eq.(12.64) by using the expression for principal parts. It is also possible to prove the optical-conductivity sum-rule from this starting point. Indeed, taking the real part and integrating both sides,

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

Note that since the conductivity sum rule is satisfied for abitrary q_x, it is also satisfied at $q_x=0$, a limit we will need when computing the conductivity in the next section.

Remark 31 *Practical use of sum rule: The* n *that appears in the conductivity sum rule is the full electronic density. In pratical calculations for experiment, one stops integrating at a finite frequency, which is smaller than the binding energy of core electrons. These electrons are then frozen, and the appropriate plasma frequency is calculated with the free electronic density in the conduction band.*

Remark 32 *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 33 *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.*

12.5 Exercices

12.5.1 Formule de Kubo pour la conductivité thermique

Dérivez les équations (1) à (19) de la section II de l'article "A Sum Rule for Thermal Conductivity and Dynamical Thermal Transport Coefficients in Condensed Matter -I" cond-mat/0508711 par Sriram Shastry (donnez les étapes manquantes et trouvez les fautes de typographie s'il y en a.). Notez que la représentation de Lehmann s'obtient facilement en utilisant un ensemble complet d'états intermédiaires et en utilisant l'évolution d'Heisenberg pour les opérateurs (il faut en un certain sens refaire à l'envers certaine des étapes qui nous ont permis de trouver la relation entre section efficace calculée par la règle d'or de Fermi et fonction de corrélation).

13. DRUDE WEIGHT, METALS, INSULATORS AND SUPERCONDUCTORS

All the above considerations about conductivity, correlation functions and sum rules may seem rather formal, and even useless. Let us put what we learned to work. In the present Chapter, we will find some powerful and unexpected results. For example, one can measure the penetration depth, i.e. the distance over which a static magnetic field is expelled by a superconductor, by doing instead a finite frequency conductivity measurement.

If we begin to talk about a superconductor, the first thing that comes to mind is the DC conductivity. Even if in the end we will see that zero resistance or infinite conductivity is not what characterizes a superconductor, this is a legitimate starting point. Suppose we are interested in the DC conductivity. We then need the response for a uniform, or very long wavelength field, i.e. the limit $q_x \to 0$ of our earlier formulae. It is important to notice that this is the proper way to compute the DC conductivity: Take the $\mathbf{q} \to 0$ limit, before the $\omega \to 0$ limit. In the opposite limit the response vanishes as we saw from gauge invariance (12.55). Physically, transport probes dynamical quantities. A DC measurement can be seen as the zero frequency limit of a microwave experiment for example. By taking the $\mathbf{q} \to \mathbf{0}$ limit first, we ensure that we are looking at an infinite volume, where energy levels can be arbitrarely close in energy. Then only can we take the zero frequency limit and still get absorption when the state is metallic. Otherwise the discrete nature of the energy states would not allow absorption in the zero frequency limit.

By asking questions about the DC conductivity, we are clearly beginning to ask what is the difference between a perfect metal, a superconductor, and an insulator. This is the question we will focus on in this chapter. The first step is to define the Drude weight.

13.1 The Drude weight

In the correct limit, the above formulae (12.68) and (12.70) for conductivity give us either the simple formula,

$$\operatorname{Re}\left[\sigma_{xx}(0,\omega)\right] = \frac{\chi''_{j_x j_x}(0,\omega)}{\omega} \tag{13.1}$$

or the more complicated-looking formula

$$\operatorname{Re}\left[\sigma_{xx}(0,\omega)\right] = \mathcal{P}\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} - \pi\delta(\omega)\left[\operatorname{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right] - \frac{ne^2}{m}\right] \tag{13.2}$$

The coefficient of the delta function at zero frequency $\delta(\omega)$ is called the Drude weight D:

$$\boxed{D = \pi \lim_{\omega\to 0}\left[\tfrac{ne^2}{m} - \operatorname{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right]\right]}. \tag{13.3}$$

Remark 34 *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.(12.64), that it can also be extracted from the imaginary part,*

$$D = \pi \lim_{\omega \to 0} \omega \, \mathrm{Im}\left[\sigma_{xx}(0,\omega)\right] \tag{13.4}$$

Remark 35 *Alternate derivation: To be reassured that the Drude weight would also come out from the first expression for the conductivity Eq.(13.1), it suffices to show that both expressions are equal, namely that*

$$\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} - \mathcal{P}\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} = -\pi\delta(\omega)\left[\mathrm{Re}\left[\chi^R_{j_x j_x}(0,\omega)\right] - \frac{ne^2}{m}\right] \tag{13.5}$$

To show this, one first notes that given the definition of principal part, the difference on the left-hand side can only be proportional to a delta function. To prove the equality of the coefficients of the delta functions on both sides, it then suffices to integrate over frequency. One obtains

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} - \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{j_x j_x}(0,\omega)}{\omega} \tag{13.6}$$

$$= \lim_{\omega\to 0}\lim_{q_x \to 0}\left[\frac{ne^2}{m} - \mathrm{Re}\left[\chi^R_{j_x j_x}(q_x,\omega)\right]\right] \tag{13.7}$$

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.(12.59).

Remark 36 *Contrary to what happened for conserved quantities in thermodynamic sum rules, principal parts here are very relevant.*

13.2 What is a metal

To understand what is a metal, let us first begin by asking what is the Drude weight for free electrons. The answer is that for free electrons, the $q_x \to 0$ conductivity is a delta function at zero-frequency whose Drude weight is $D = \pi ne^2/m$.

Proof: Let the current be $ne\mathbf{v}$. Then, using Newton's equation of motion in an electric field we find ,

$$\frac{\partial \mathbf{j}\left(\mathbf{q}=\mathbf{0},t\right)}{\partial t} = \frac{ne^2}{m}\mathbf{E}\left(\mathbf{q}=\mathbf{0},t\right) \tag{13.8}$$

or with a single applied frequency,

$$\mathbf{j}\left(\mathbf{q}=\mathbf{0},\omega\right) = -\frac{1}{i\left(\omega+i\eta\right)}\frac{ne^2}{m}\mathbf{E}\left(\mathbf{q}=\mathbf{0},\omega\right). \tag{13.9}$$

From this we see that the conductivity has only a Drude contribution (free acceleration).

$$\mathrm{Re}\,\frac{\mathbf{j}\left(\mathbf{q}=\mathbf{0},\omega\right)}{\mathbf{E}\left(\mathbf{q}=\mathbf{0},\omega\right)} = \mathrm{Re}\,\sigma\left(\mathbf{q}=\mathbf{0},\omega\right) = \pi\frac{ne^2}{m}\delta\left(\omega\right) \tag{13.10}$$

For interacting electrons, the current of a single particle is no longer a conserved quantity and there is a contribution from $\pi \lim_{\omega\to 0} Re\left[\chi^R_{j_xj_x}(0,\omega)\right]$. 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.(13.3) at zero temperature, in other words infinite conductivity or zero resistance even in the presence of interactions. At finite temperature or when there is inelastic scattering with some other system, like the phonons, the delta function is broadened. It can also be broadened at zero temperature by impurity scattering.

13.3 What is an insulator

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

$$\lim_{\omega\to 0} \mathrm{Re}\left[\chi^R_{j_xj_x}(0,\omega)\right] = \lim_{\omega\to 0} \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(0,\omega')}{\omega'-\omega} = \frac{ne^2}{m}. \tag{13.11}$$

Recalling the result obtained from the $f-$sum rule (or equivalently from gauge invariance), (12.59)

$$\chi^R_{j_xj_x}(q_x,0) = \int \frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}(q_x,\omega')}{\omega'} = \frac{ne^2}{m} \tag{13.12}$$

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

$$\lim_{\omega\to 0}\lim_{q_x\to 0} \mathrm{Re}\left[\chi^R_{j_xj_x}(q_x,\omega)\right] = \lim_{q_x\to 0}\lim_{\omega\to 0} \mathrm{Re}\left[\chi^R_{j_xj_x}(q_x,\omega)\right]. \tag{13.13}$$

This occurs in particular when there is a gap Δ. In this case, then $\chi^{''}_{j_xj_x}(q_x,\omega) = 0$ for all q_x as long as $\omega < \Delta$. In particular, there can be no contribution from zero frequency since $\chi^{''}_{j_xj_x}(q_x,0) = 0$ so that the principal part integral and the full integral are equal.

Remark 37 *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]*

13.4 What is a superconductor

Finally, *superconductors* are an interesting case. While gauge invariance (or $f-$sum rule) implies (12.55) that

$$\left[\chi^R_{j_xj_x}(q_x,0) - \frac{ne^2}{m}\right] = 0. \tag{13.14}$$

there is no such principle that forces the *transverse* response to vanish. Indeed, gauge transformations (12.3) are always longitudinal. Hence, it is possible to have,

$$\left[\chi^R_{j_yj_y}(q_x,0) - \frac{ne^2}{m}\right] = -\frac{n_s(q_x)\,e^2}{m} \tag{13.15}$$

where n_s is any density less than n. A superconductor will indeed have such a non-vanishing "transverse Drude weight". In general we will be interested in the long wave length limit and the q_x dependence can be neglected. We will show in Eq.(13.31) below that positivity of the dissipation implies that n_s cannot be larger than n.

Definition 7 *n_s is called the superfluid density.*

Remark 38 *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.*

To show why a non-vanishing value of n_s in Eq.(13.15) is related to superconductivity it suffices to show that in that case 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 (12.32)

$$\delta \left\langle j_a^A(\mathbf{q},\omega)^T \right\rangle = \left[\left(\chi^R_{j_a j_b}(\mathbf{q},\omega) \right)^T - \frac{ne^2}{m}\delta_{ab} \right] A_b^T(\mathbf{q},\omega).$$

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 $\mathbf{q}$),

$$\delta \left\langle j_a^A(\mathbf{q},0)^T \right\rangle = -\frac{n_s e^2}{m} A_a^T(\mathbf{q},0). \tag{13.16}$$

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. We take the curl on both sides of the Fourier transformed expression,

$$\nabla \times \delta \left\langle \mathbf{j}(\mathbf{r},\omega{=}0) \right\rangle = -\frac{n_s e^2}{m}\mathbf{B}(\mathbf{r},\omega{=}0) \tag{13.17}$$

and then multiply by μ_0, the permeability of the vacuum, and use Maxwell's equation $\nabla \times \mathbf{B}(\mathbf{r},\omega{=}0) = \mu_0 \mathbf{j}(\mathbf{r},\omega = 0)$ as well as $\nabla \times (\nabla \times \mathbf{B}) = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 (\mathbf{B})$ with $\nabla \cdot \mathbf{B} = 0$. The last equation takes the form,

$$\nabla^2 (\mathbf{B}) = \frac{n_s e^2}{m}\mu_0 \mathbf{B} \tag{13.18}$$

whose solution in the half-plane geometry shown in figure (13-1) is,

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

with the London penetration depth

$$\lambda_L^{-2} = \frac{n_s e^2}{m}\mu_0. \tag{13.19}$$

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

Remark 39 *In the case where $n_s = n$, which often occurs at zero temperature in BCS-like superconductors, we find*

$$\omega_p^2 \lambda_L^2 = \frac{ne^2}{\varepsilon_0 m}\frac{m}{ne^2\mu_0} = \frac{1}{\varepsilon_0\mu_0} = c^2. \tag{13.20}$$

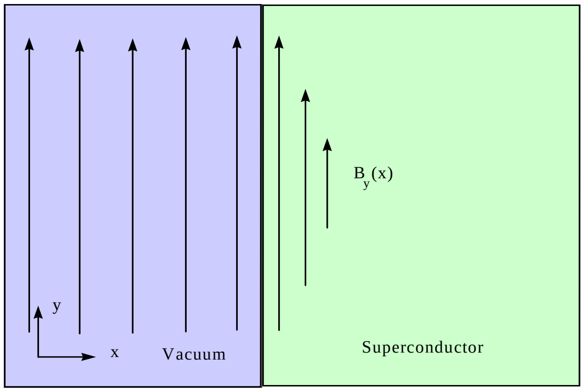

Figure 13-1 Penetration depth in a superconductor.

Why are the transverse and longitudinal zero-frequency responses different in a superconductor? By comparing the result of the f-sum rule Eq.(13.14) with the definition of the transverse Drude weight Eq.(13.15) this can happen only if

$$\lim_{q_x\to 0}\chi^R_{j_xj_x}(q_x,0,\omega=0)\neq\lim_{q_y\to 0}\chi^R_{j_xj_x}(0,q_y,\omega=0) \tag{13.21}$$

or in other words

$$\lim_{q_x\to 0}\int dt\int d\mathbf{r}e^{-iq_xx}\chi^R_{j_xj_x}(\mathbf{r},\omega=0)\neq\lim_{q_y\to 0}\int dt\int d\mathbf{r}e^{-iq_yy}\chi^R_{j_xj_x}(\mathbf{r},\omega=0). \tag{13.22}$$

That is the true definition of a superconductor. The above two limits cannot be inserted in a superconductor because long-range order leads to $\chi^R_{j_xj_x}(\mathbf{r},\omega=0)$ 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.

13.5 Metal, insulator and superconductor

In all cases, gauge invariance Eq.(12.55), or equivalently particle conservation, implies that

$$\left[\chi^R_{j_xj_x}(q_x,0)-\frac{ne^2}{m}\right]=0. \tag{13.23}$$

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 (13.3)

$$D=\pi\lim_{\omega\to 0}\lim_{q_x\to 0}\left[\frac{ne^2}{m}-\mathrm{Re}\left[\chi^R_{j_xj_x}(0,\omega)\right]\right] \tag{13.24}$$

and the transverse analog of the $f-$sum rule,

$$\boxed{D_S=\pi\lim_{q_x\to 0}\lim_{\omega\to 0}\left[\frac{ne^2}{m}-\chi^R_{j_yj_y}(q_x,\omega)\right]} \tag{13.25}$$

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

	D	D_S
Metal	D	0
Insulator	0	0
Superconductor	D	D_S

Table 13.1 Difference between metal, insulator and superconductor, as seen from the limiting value of correlation functions

in a superconductor. Since the London penetration depth is generally very long compared with the lattice spacing, the q_x dependense of D_S, or equivalently the superfluid density, can be neglected. The table summarizes the results.

A superconductor can unambiguously be defined by the non-vanishing of D_S. Indeed, a superconductor has a gap to single-particle excitations, like an insulator, and it has a delta response in the longitudinal direction at zero wave vector, like a metal. On the other hand, neither metal nor insulators have a non-zero D_S.

Remark 40 *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.*

13.6 Finding the London penetration depth from optical conductivity

Let us first establish the transverse conductivity sum rule for finite wave vector probes, such as microwaves, or electromagnetic radiation in general. In a metal, we already know that

$$\operatorname{Re}\sigma_{yy}(q_x,\omega)=\mathcal{P}\frac{1}{\omega}\left[\chi''_{j_yj_y}(q_x,\omega)\right]-\pi\delta\left(\omega\right)\left[\operatorname{Re}\chi^R_{j_yj_y}(q_x,\omega)-\frac{ne^2}{m}\right] \tag{13.26}$$

Let us imagine an experiment at finite temperature where the delta function is broadened. It is easier to also use the fact that the $q_x\to 0$ and $q_y\to 0$ limits can be interchanged and work with the equivalent formula Eq.(13.1)

$$\operatorname{Re}\left[\sigma_{yy}(0,\omega)\right]=\frac{\chi''_{j_yj_y}(0,\omega)}{\omega}. \tag{13.27}$$

When we integrate over frequency we find the same result as that predicted by the f-sum rule, namely

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\operatorname{Re}\left[\sigma_{yy}(0,\omega)\right]=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{\omega}\left[\chi''_{j_yj_y}(0,\omega)\right]=\frac{ne^2}{2m} \tag{13.28}$$

The experiment can be performed above the superconducting transition temperature for example and the integral over frequency done to find the value of the right-hand side.

Now, assume the system becomes a superconductor, then as we just saw a superconductor exhibits a true zero-frequency delta function response at finite wave-vector in the transverse response. This means that Eq.(13.26) for the transverse conductivity may be written

$$\operatorname{Re}\sigma_{yy}(q_x,\omega)=\mathcal{P}\frac{\chi''_{j_yj_y}(q_x,\omega)}{\omega}+D_S\left(q_x\right)\delta\left(\omega\right). \tag{13.29}$$

In that case, a conductivity experiment with electromagnetic radiation will not pick up the piece proportional to $\delta(\omega)$ in the transverse response Eq.(13.29), so doing the integral we will obtain

$$\begin{align}
\lim_{q_x\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{Re}\left[\sigma_{yy}(q_x,\omega)\right] &= \lim_{q_x\to 0}\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{\omega}\left[\chi''_{j_yj_y}(q_x,\omega)\right] \nonumber\\
&= \lim_{q_x\to 0}\frac{1}{2}\,\mathrm{Re}\,\chi^R_{j_yj_y}(q_x,0) \tag{13.30}\\
&= \frac{(n-n_s)\,e^2}{2m} \tag{13.31}
\end{align}$$

where we used the result Eq.(13.15) for $\mathrm{Re}\,\chi^R_{j_yj_y}(q_x,0)$. Note that there is no difference here between $\mathrm{Re}\,\chi^R_{j_yj_y}(q_x,0)$ and $\chi^R_{j_yj_y}(q_x,0)$ since this is a thermodynamic quantity at small q_x. The delta function in frequency in front of D_S this time forces us to take the $\omega=0$ limit first. The missing weight for the transverse response is in the delta function at the origin. The weight of that delta function is $D_S/(2\pi)=n_se^2/2m$. It is necessarily less than $ne^2/(2m)$ so that $n_s<n$ as we had promised to prove. This is called the Ferrell-Glover-Tinkham sum rule. It is quite remarkable that the penetration depth can be obtained from an optical conductivity experiment by looking at the missing weight in the f-sum rule.

As a recent example[11] of how this sum rule can be used is shown on Fig. (13-2). The nice aspect is that we do not need the frequency integral up to infinity. Indeed, at sufficiently high frequency, the absorption in the normal and in the superconducting state become identical, so the penetration depth is obtained from the missing area by using our previous result Eq.(13.19), namely $\lambda_L^{-2}=\mu_0n_se^2/2m$, to relate the two quantities. In a superconductor, many of the excitations are gapped, in other words they do not contribute to absorption. Let us call the typical gap energy Δ. For frequencies larger than a few times Δ, the results in the superconducting and in the normal state must become identical when $\hbar\omega$ becomes larger than the largest gap. For the example given here, this occurs around 6Δ.

In the cuprates, there is suggestion that there is missing weight when one tries to relate c axis conductivity to penetration depth in the underdoped regime.[12] The in-plane optical conductivity of $\mathrm{YBa_2Cu_3O_{7-x}}$ satisfies the sum-rule for the penetration depth but, in the underdoped case, the missing area extends over an unusually broad frequency range, suggesting that simple models based on Fermi liquids do not apply. [13]

Remark 41 *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 42 *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,*

$$\begin{align}
\mathrm{Im}\,\sigma_{yy}(q_x,\omega) &= \frac{1}{\omega}\left[\frac{ne^2}{m}-\mathrm{Re}\,\chi^R_{j_yj_y}(q_x,\omega)\right]-\pi\delta(\omega)\,\chi''_{j_yj_y}(q_x,\omega) \tag{13.32}\\
\lim_{\omega\to 0}\omega\,\mathrm{Im}\,\sigma_{yy}(q_x,\omega) &= \frac{D_S}{\pi} \tag{13.33}
\end{align}$$

since $\chi''_{j_yj_y}(q_x,0)=0$. That is another way to obtain the London penetration depth. In that case we do not need to know the conductivity at all frequencies, but only its high frequency tail.

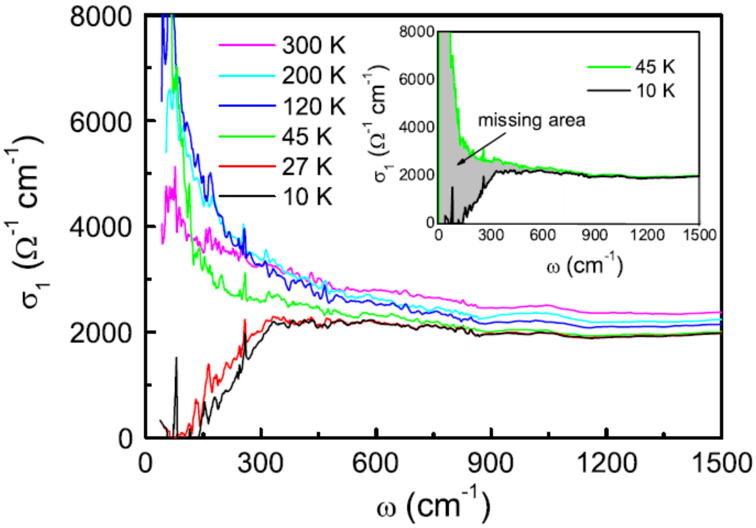

FIG. 3 (color online). T-dependent $\sigma_1(\omega)$ curves. The inset shows $\sigma_1(\omega)$ at 10 and 45 K. The shaded area represents the missing area due to the opening of superconducting energy gap.

Figure 13-2 A penetration depth of $2080\dot{A}$ was obtained from the missing aread in this infrared conductivity experiment on the pnictide Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ with a T_c of $37\ K$.

14. RELATION BETWEEN CONDUCTIVITY AND DIELECTRIC CONSTANT

The relation between dielectric constant and conductivity is a matter of macroscopic electromagnetism. Hence, since we already know the relation beween conductivity and correlation functions, we will be able to relate dielectric constant and correlation functions that we can compute later. The dielectric constant is basic to optical measurements. In infrared spectroscopy for example, one measures the reflectivity or the transmission coefficient, either of which is related to the complex index of refraction which follows from the dielectric constant.

We start from Maxwell's equations. We consider a translationally invariant system, so that it suffices to consider the Fourier-space version

$$i\mathbf{q}\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{14.1}$$

$$i\mathbf{q}\times\mathbf{E} = i\left(\omega+i\eta\right)\mathbf{B} \tag{14.2}$$

$$i\mathbf{q}\cdot\mathbf{B} = 0 \tag{14.3}$$

$$i\mathbf{q}\times\mathbf{B} = \mu_0\mathbf{j} - \frac{i\left(\omega+i\eta\right)}{c^2}\mathbf{E}. \tag{14.4}$$

where $\varepsilon_0 = 8.85\times10^{-12}$ farad/meter is the permittivity of vacuum and $\mu_0 = 4\pi\times10^{-7}$ henry/meter its permeability. The speed of light is related to these quantities by $\varepsilon_0\mu_0 = 1/c^2$.

14.1 Transverse dielectric constant.

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

$$i\mathbf{q}\times\mathbf{B} = \mu_0\overleftrightarrow{\sigma^T}\cdot\mathbf{E} - \frac{i\left(\omega+i\eta\right)}{c^2}\mathbf{E}. \tag{14.5}$$

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

$$q^2\mathbf{E} = \mu_0 i\left(\omega+i\eta\right)\overleftrightarrow{\sigma^T}\cdot\mathbf{E} + \frac{\left(\omega+i\eta\right)^2}{c^2}\mathbf{E} \equiv \frac{\left(\omega+i\eta\right)^2}{c^2}\frac{\overleftrightarrow{\epsilon^T}}{\varepsilon_0}\mathbf{E} \tag{14.6}$$

where the last equality is the definition of the dielectric tensor. If there was no coupling to matter, the electric field would have the usual pole for light $\omega = cq$. In general then,

$$\overleftrightarrow{\epsilon^T}\left(\mathbf{q},\omega\right) = \varepsilon_0 + \frac{ic^2\varepsilon_0\mu_0}{\left(\omega+i\eta\right)}\overleftrightarrow{\sigma^T} = \varepsilon_0 + \frac{i}{\left(\omega+i\eta\right)}\overleftrightarrow{\sigma^T} \tag{14.7}$$

In the simple case where the dielectric tensor is diagonal, it is related to the dielectric constant n and the attenuation constant κ through $\sqrt{\epsilon}=n+i\kappa$. Using the Kubo formula for the conductivity in terms of response function Eq.(12.40), we have that

$$\boxed{\overleftrightarrow{\epsilon^T}(\mathbf{q},\omega)=\varepsilon_0\left(1-\frac{\omega_p^2}{(\omega+i\eta)^2}\right)\overleftrightarrow{I}+\frac{1}{(\omega+i\eta)^2}\left(\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)\right)^T}. \tag{14.8}$$

Remark 43 *Bound charges: When one can separate the charges into bound and free in the calculation of* $\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)$*, the contribution of the bound charges to* $\frac{1}{(\omega+i\eta)^2}\overleftrightarrow{\chi^R_{\mathbf{jj}}}(\mathbf{q},\omega)$ *is usually included with the* 1 *and called,* $\overleftrightarrow{\epsilon^T}_{bound}$.

Remark 44 *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 45 *Electromagnetic field and plasmon: One can see from the equation for the electric field (14.6) that in general the electromagnetic field does see the plasmon (negative dielectric constant for* $\omega<\omega_p$ *in Eq.(14.8) means no propagation below the plasma frequency).*

14.2 Longitudinal dielectric constant.

Let the system be subjected to some external charge $\rho_e(\mathbf{q},\omega)$. The electric field depends on the total charge, including the induced one

$$i\mathbf{q}\cdot\mathbf{E}=\frac{(\rho_e+\delta\langle\rho\rangle)}{\varepsilon_0}. \tag{14.9}$$

The longitudinal dielectric constant is defined by

$$i\mathbf{q}\cdot\overleftrightarrow{\epsilon^L}\cdot\mathbf{E}=\rho_e. \tag{14.10}$$

$\overleftrightarrow{\epsilon^L}$ depends on $\mathbf{q}$ and ω, it is a retarded response function. With a longitudinal applied field, the previous two equations lead to

$$\left(\epsilon^L\right)^{-1}=\frac{\rho_e+\delta\langle\rho\rangle}{\varepsilon_0\rho_e}. \tag{14.11}$$

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

$$\phi_e(\mathbf{q},\omega)=\frac{1}{\varepsilon_0 q^2}\rho_e(\mathbf{q},\omega). \tag{14.12}$$

As above, linear response to

$$\delta\mathcal{H}(t)=\int d\mathbf{r}\rho(\mathbf{r})\,\phi_e(\mathbf{r},t) \tag{14.13}$$

is given by

$$\delta \left\langle \rho(\mathbf{q},\omega)\right\rangle = -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi_e(\mathbf{q},\omega) \tag{14.14}$$

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

$$\boxed{\tfrac{1}{\epsilon^L(\mathbf{q},\omega)} = \tfrac{1}{\varepsilon_0}\left(1-\tfrac{1}{q^2\varepsilon_0}\chi^R_{\rho\rho}(\mathbf{q},\omega)\right)}. \tag{14.15}$$

Remark 46 *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

$$S_{\rho\rho}(\mathbf{q},\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\,\mathrm{Im}\left[\chi^R_{\rho\rho}(\mathbf{q},\omega)\right] = -\frac{2\hbar}{1-e^{-\beta\hbar\omega}}q^2\,\mathrm{Im}\left[\frac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)}\right]. \tag{14.16}$$

The following properties of the dielectric constants are worthy of interest

Remark 47 *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 48 $\epsilon^L(\mathbf{q},\omega)\neq\epsilon^T(\mathbf{q},\omega)$ *in general*

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

Remark 49 *Collective transverse excitations: The poles of* ϵ^T *are at the collective transverse excitations. Indeed, let us look since* $\nabla\cdot\mathbf{D}=0$ *(no free charge) is garanteed by the fact the excitation is transverse, while* $\nabla\times\mathbf{E}=0$ *implies zero electric field in a transverse mode. Nevertheless,* $\mathbf{D}^T\neq 0$ *can occur even if the electric field is zero when* $\epsilon^T=\infty$*. The corresponding poles are those of the transverse part of* $\chi^R_{\mathbf{jj}}(\mathbf{q},\omega)$*.*

Remark 50 *Collective longitudinal excitations: The zeros of* ϵ^L *locate the longitudinal collective modes since* $\left(\epsilon^L\right)^{-1}=\frac{\rho_e+\delta\langle\rho\rangle}{\varepsilon_0\rho_e}=\infty$ *corresponds to internal charge oscillations. Alternatively,* $\mathbf{D}^L=0$ *as required by the no-free-charge constraint* $\nabla\cdot\mathbf{D}=0$ *but nevertheless* $\mathbf{E}^L\neq 0$ *is allowed if* $\epsilon^L=0$*. (*$\nabla\times\mathbf{E}=0$ *is automatic in a longitudinal mode). The corresponding collective modes are also the poles of* $\chi^R_{\rho\rho}(\mathbf{q},\omega)$*.*

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Part III

Introduction to Green's functions. One-body Schrödinger equation

We now know that correlation functions of charge, spin, current etc... allow us to predict the results of various experiments. In quantum mechanics, all these quantities, such as charge, spin, current, are bilinear in the Schrödinger field $\Psi(\mathbf{r},t)$, i.e $\rho\left(\mathbf{r},t\right)=\Psi^{*}(\mathbf{r},t)\Psi(\mathbf{r},t)$ for example. What about correlation functions of the field $\Psi(\mathbf{r},t)$ itself? They also are related to experiment, more specifically to photoemission and tunneling experiments for example. We will come back to this later. At this point, it suffices to say that if we do experiments where we actually inject or extract a single electron, then we need to know the correlation function for a single Ψ field. These correlation functions are called Green's functions, or propagators. They are absolutely necessary from a theoretical point of view to get a full description of the system. They turn out to be easier to compute than correlation functions for transport properties, such as charge-charge or current-current. So we will finally compute this type of correlation function, Green's functions, in this Part. 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. Finally, there is an alternate formulation of quantum mechanics, namely Feynman's path integral, that arises naturally when we think about the physical meaning of Green's functions.

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

15. DEFINITION OF THE PROPAGATOR, OR GREEN'S FUNCTION

Previously, we needed to know how an operator, such as charge for example, was correlated with another one at another time. The generalization of this idea for a one-body wave function is to know how it correlates with itself at different times. That is also useful because the main idea of perturbation theory is to prepare a state $\Psi_0(\mathbf{r}', t')$ and to let it evolve adiabatically in the presence of the perturbation into the new eigenstate $\Psi(\mathbf{r}, t)$. 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

$$\Psi(\mathbf{r}, t) = \langle \mathbf{r}| e^{-iHt} |\Psi_H\rangle . \tag{15.1}$$

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

$$|\Psi_0(t')\rangle = e^{-iHt'} |\Psi_H\rangle \tag{15.2}$$

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

$$\Psi(\mathbf{r}, t) = \langle \mathbf{r}| e^{-iH\left(t-t'\right)} |\Psi_0(t')\rangle . \tag{15.3}$$

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

$$\Psi_0(\mathbf{r}', t') = \langle \mathbf{r}'|\ \Psi_0\left(t'\right)\rangle \tag{15.4}$$

it suffices to use a complete set of states

$$\Psi(\mathbf{r}, t)\theta\left(t-t'\right) = \int d\mathbf{r}' \langle \mathbf{r}| e^{-iH\left(t-t'\right)} |\mathbf{r}'\rangle \langle \mathbf{r}'|\ \Psi_0\left(t'\right)\rangle \theta\left(t-t'\right) \tag{15.5}$$

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

$$\Psi(\mathbf{r}, t)\theta\left(t-t'\right) = i\int d\mathbf{r}' G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)\Psi_0(\mathbf{r}', t') \tag{15.6}$$

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

$$\boxed{G^R\left(\mathbf{r},t;\mathbf{r}',t'\right) = -i\langle \mathbf{r}| e^{-iH\left(t-t'\right)} |\mathbf{r}'\rangle \theta\left(t-t'\right)}. \tag{15.7}$$

This may look like a useless exercise in definitions, but in fact there are many reasons to work with the retarded Green's function $G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)$. Suppose we want to know the expectation value of two one-body operators at different times

- $G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)$ does not depend on the initial condition $\Psi_0(\mathbf{r}', t')$.
- $G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)$ 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 du to Feynman that we discuss in the last chapter of this part.

- $G^R(\mathbf{r},t;\mathbf{r}',t')$ 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 8 $G^R(\mathbf{r},t;\mathbf{r}',t')$ *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.*

16. 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

$$G^R(\mathbf{r},\mathbf{r}';\omega) = -i\int_0^\infty d(t-t')\, e^{i\omega(t-t')}\langle\mathbf{r}|\, e^{-iH(t-t')}\,|\mathbf{r}'\rangle\, e^{-\eta(t-t')}. \tag{16.1}$$

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

$$H|n\rangle = E_n|n\rangle \tag{16.2}$$

$$\langle n|\, e^{-iH(t-t')}\,|m\rangle = e^{-iE_n(t-t')}\delta_{n,m} \tag{16.3}$$

to obtain for the Green's function

$$G^R(\mathbf{r},\mathbf{r}';\omega) = -i\sum_n \langle\mathbf{r}|\, n\rangle\int_0^\infty dt e^{i(\omega+i\eta-E_n)t}\langle n\,|\mathbf{r}'\rangle \tag{16.4}$$

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

$$\boxed{G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \frac{\langle\mathbf{r}|\, n\rangle\langle n\,|\mathbf{r}'\rangle}{\omega+i\eta-E_n} = \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')}{\omega+i\eta-E_n}} \tag{16.5}$$

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

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 a Lehmann representation.

16.1 Operator representation

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

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega+i\eta-H}} \tag{16.6}$$

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

$$\boxed{\widehat{G}^R(t) = -ie^{-iHt}\theta(t)} \tag{16.7}$$

The advanced propagator is

$$\boxed{\widehat{G}^A(t) = ie^{-iHt}\theta(-t)} \tag{16.8}$$

$$\boxed{\widehat{G}^A(\omega) = \frac{1}{\omega - i\eta - H}} \tag{16.9}$$

Let us evaluate explicitly the Green's function for a simple case. Let us take a free particle. The eigenstates are momentum eigenstates, $H|\mathbf{k}\rangle = \varepsilon_{\mathbf{k}}|\mathbf{k}\rangle$ .Then,

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}'\rangle = \langle\mathbf{k}|\,\frac{1}{\omega + i\eta - H}\,|\mathbf{k}'\rangle = \frac{\langle\mathbf{k}|\,\mathbf{k}'\rangle}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \tag{16.10}$$

16.2 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

$$\boxed{\rho(E) = \sum_n \delta(E - E_n)} = \sum_n \int d\mathbf{r}\,\langle n\,|\mathbf{r}\rangle\,\langle\mathbf{r}|\,n\rangle\,\delta(E - E_n) \tag{16.11}$$

$$\boxed{= -\frac{1}{\pi}\int d\mathbf{r}\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r};E)} \tag{16.12}$$

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

$$\boxed{\rho(E) = -\frac{1}{\pi}Tr\left[\mathrm{Im}\,\widehat{G}^R(E)\right]}. \tag{16.13}$$

The quantity

$$\rho(\mathbf{r},E) = -\frac{1}{\pi}\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r};E) \tag{16.14}$$

is called the local density of states, a quantity relevant in particular when there is no translational invariance. This is what is measured by scanning tunnelin microscopes.

16.3 Spectral representation, sum rules and high frequency expansion

Green's functions are response functions for the wave function, hence they have many formal properties that are analogous to those of response functions that we saw earlier. We discuss some of them here.

16.3.1 Spectral representation and Kramers-Kronig relations.

Returning to the explicit representation in energy eigenstates, (16.5), it can be written in a manner which reminds us of the spectral representation

$$\boxed{G^R(\mathbf{r},\mathbf{r}';\omega)} = \sum_n \frac{\Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} = \int \frac{d\omega'}{2\pi}\frac{\sum_n \Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')\,2\pi\delta(\omega' - E_n)}{\omega + i\eta - \omega'} \tag{16.15}$$

$$\boxed{= \int \frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'} = \int \frac{d\omega'}{2\pi}\frac{-2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'} = \int d\omega'\frac{\rho(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'}} \tag{16.16}$$

which defines the spectral weight

$$A(\mathbf{r},\mathbf{r}';\omega') = \sum_n \Psi_n(\mathbf{r})\,\Psi_n^*(\mathbf{r}')\,2\pi\delta(\omega' - E_n) \tag{16.17}$$

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

$$\boxed{G^R(\mathbf{k};\omega) = \int \frac{d\omega'}{2\pi}\frac{A(\mathbf{k};\omega')}{\omega+i\eta-\omega'}} \tag{16.18}$$

with

$$\boxed{A(\mathbf{k};\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{k};\omega')} \tag{16.19}$$

$$\begin{aligned} A(\mathbf{k};\omega') &= \sum_n \Psi_n(\mathbf{k})\,\Psi_n^*(\mathbf{k})\,2\pi\delta(\omega' - E_n) && (16.20)\\ &= \sum_n \langle\mathbf{k}|\,n\rangle\,\langle n\,|\mathbf{k}\rangle\,2\pi\delta(\omega' - E_n)\,. && (16.21)\end{aligned}$$

In the case of free particles, there is only a single eigenstate $|n\rangle = |\mathbf{k}\rangle$ that contributes to the sum and we have a single delta function for the spectral weight. That occurs whenever we are in an eigenbasis.

Remark 51 *Assumptions in relating A to $\mathrm{Im}\,G^R$: It is only in the presence of a time-reversal invariant system that the Schrödinger wave functions $\Psi_n(\mathbf{r})$ can always be chosen real. In such a case, it is clear that we are allowed to write $A(\mathbf{r},\mathbf{r}';\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r}';\omega')$ as we did in Eq.(16.16).*

Remark 52 *Analogies with ordinary correlation functions. Contrary to the spectral representation for correlation functions introduced earlier, there is $\frac{d\omega'}{2\pi}$ instead of $\frac{d\omega'}{\pi}$. That is why there is a factor of two in relating the imaginary part of the Green's function to the spectral weight. Furthermore, the denominator involves $\omega + i\eta - \omega'$ instead of $\omega' - \omega - i\eta$, which explains the minus sign in $A(\mathbf{k};\omega') = -2\,\mathrm{Im}\,G^R(\mathbf{k};\omega')$, Eq.(16.19). Apart from these differences, it is clear that $A(\mathbf{k};\omega')$ here is analogous to $\chi''(\mathbf{k};\omega')$ for correlation functions.*

Analyticity in the upper half-plane implies Kramers-Kronig relations as before. In fact, the spectral representation itself leads immediately to

$$\mathrm{Re}\left[G^R(\mathbf{r},\mathbf{r}';\omega)\right] = \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Im}\left[G^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega' - \omega}. \tag{16.22}$$

The other reciprocal Kramers-Kronig relation follows as before.

$$\mathrm{Im}\left[G^R(\mathbf{r},\mathbf{r}';\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Re}\left[G^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega' - \omega} \tag{16.23}$$

16.3.2 Sum rules

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

$$\int \frac{d\omega'}{2\pi} \left(-2\,\mathrm{Im}\,G^R\left(\mathbf{r},\mathbf{r}';\omega'\right)\right) = \int \frac{d\omega'}{2\pi} \sum_n \Psi_n\left(\mathbf{r}\right)\Psi_n^*\left(\mathbf{r}'\right) 2\pi\delta\left(\omega' - E_n\right) \tag{16.24}$$

$$= \sum_n \Psi_n\left(\mathbf{r}\right)\Psi_n^*\left(\mathbf{r}'\right) = \delta\left(\mathbf{r}-\mathbf{r}'\right) \tag{16.25}$$

so that

$$\int d\left(\mathbf{r}-\mathbf{r}'\right) \int \frac{d\omega'}{2\pi} \left(-2\,\mathrm{Im}\,G^R\left(\mathbf{r},\mathbf{r}';\omega'\right)\right) = 1. \tag{16.26}$$

More sum rules are trivially derived. For example,

$$\boxed{\int d\mathbf{r} \int \tfrac{d\omega'}{2\pi}\omega'\left(-2\,\mathrm{Im}\,G^R\left(\mathbf{r},\mathbf{r};\omega'\right)\right)} = \int d\mathbf{r} \int d\omega'\omega'\rho(\mathbf{r},\omega') = \int d\mathbf{r} \sum_n E_n \Psi_n\left(\mathbf{r}\right)\Psi_n^*\left(\mathbf{r}\right) \tag{16.27}$$

$$\boxed{= \int d\mathbf{r} \left\langle \mathbf{r}\right| H \left|\mathbf{r}\right\rangle}. \tag{16.28}$$

In operator form, all of the above results are trivial

$$\boxed{\int \tfrac{d\omega}{2\pi}\omega^n \mathrm{Tr}\left[-2\,\mathrm{Im}\left(\widehat{G}^R\right)\right]} = \int \frac{d\omega}{2\pi}\omega^n \mathrm{Tr}\left[-2\,\mathrm{Im}\left(\frac{1}{\omega + i\eta - H}\right)\right] \tag{16.29}$$

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

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

$$\int d\mathbf{r} \int \frac{d\omega'}{2\pi} \left(\omega'\right)^n \left(-2\,\mathrm{Im}\,G^R\left(\mathbf{r},\mathbf{r};\omega'\right)\right) = \int d\mathbf{r} \left\langle \mathbf{r}\right| H^n \left|\mathbf{r}\right\rangle \tag{16.30}$$

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

You may be uneasy with the formal manipulations of operators we did in this section. If so, you should to back to the derivations at the beginning of this section which clearly explain what is meant by the formal manipulations.

Remark 53 *Recall that in the case of sum rules for χ'', there was also an implicit trace since we were computing equilibrium expectation values.*

16.3.3 High frequency expansion.

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

$$G^R\left(\mathbf{k},\mathbf{k};\omega\right) = \int \frac{d\omega'}{2\pi} \frac{-2\,\mathrm{Im}\,G^R\left(\mathbf{k},\mathbf{k};\omega'\right)}{\omega + i\eta - \omega'}. \tag{16.31}$$

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,

$$G^R(\mathbf{k},\mathbf{k};\omega) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\omega'}{2\pi} (\omega')^n \left(-2\operatorname{Im} G^R(\mathbf{k},\mathbf{k};\omega')\right) \tag{16.32}$$

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

$$\int \frac{d\mathbf{k}}{(2\pi)^3} G^R(\mathbf{k},\mathbf{k};\omega) \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\mathbf{k}}{(2\pi)^3} \langle \mathbf{k}| H^n |\mathbf{k}\rangle \tag{16.33}$$

or in more general terms,

$$\operatorname{Tr}\left[\widehat{G}^R(\omega)\right] \approx \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \operatorname{Tr}(H^n) \tag{16.34}$$

which is an obvious consequence of the high-frequency expansion of (16.6)

$$\widehat{G}^R(\omega) = \frac{1}{\omega + i\eta - H} \tag{16.35}$$

Remark 54 $\operatorname{Im} G^R(\mathbf{k},\mathbf{k};\omega) = 0$ *at high frequency. Indeed consider the relation of this quantity to the spectral weight Eq.(16.19) and the explicit representation of the spectral weight Eq.(16.21). 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 55 *The leading high-frequency behavior is in* $1/\omega$*, contrary to that of correlation functions which was in* $1/\omega^2$*.*

16.4 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.

$$S_{\rho\rho}(\mathbf{k},\omega) = \frac{1}{\mathcal{V}} \int dt e^{i\omega t} \langle \rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}\rangle = \frac{1}{\mathcal{V}} \int dt e^{i\omega t} \left\langle e^{iHt}\rho_{\mathbf{k}} e^{-iHt}\rho_{-\mathbf{k}}\right\rangle. \tag{16.36}$$

The real-time retarded propagator was

$$\widehat{G}^R(t) = -ie^{-iHt}\theta(t) \tag{16.37}$$

while the advanced propagator was

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

The charge structure factor is then expressed in terms of the propagators

$$S_{\rho\rho}(\mathbf{k},\omega) = \frac{-1}{\mathcal{V}} \int dt e^{i\omega t} \left\langle \left(\widehat{G}^R(-t) - \widehat{G}^A(-t)\right)\rho_{\mathbf{k}} \left(\widehat{G}^R(t) - \widehat{G}^A(t)\right)\rho_{-\mathbf{k}}\right\rangle. \tag{16.38}$$

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

Remark 56 *Alternate proof: We can also see this in the Fourier transform version*

$$S_{\rho\rho}(\mathbf{k},\omega)=\frac{-1}{\mathcal{V}}\int\frac{d\omega'}{2\pi}\left\langle\left(\widehat{G}^R(\omega')-\widehat{G}^A(\omega')\right)\rho_{\mathbf{k}}\left(\widehat{G}^R(\omega'+\omega)-\widehat{G}^A(\omega'+\omega)\right)\rho_{-\mathbf{k}}\right\rangle. \tag{16.39}$$

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

$$\boxed{S_{\rho\rho}(\mathbf{k},\omega)=\frac{1}{\mathcal{V}}\int\frac{d\omega'}{2\pi}\left\langle\widehat{G}^R(\omega')\rho_{\mathbf{k}}\widehat{G}^A(\omega'+\omega)\rho_{-\mathbf{k}}+\widehat{G}^A(\omega')\rho_{\mathbf{k}}\widehat{G}^R(\omega'+\omega)\rho_{-\mathbf{k}}\right\rangle} \tag{16.40}$$

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

$$G^R(n,n';E)=\langle n|\frac{1}{E-H+i\eta}|n'\rangle=\delta_{nn'}\frac{1}{E-E_n+i\eta} \tag{16.41}$$

$$G^A(n,n';E)=\langle n|\frac{1}{E-H-i\eta}|n'\rangle \tag{16.42}$$

16.5 Green's functions for differential equations

The expression for the propagator (15.6)

$$\Psi(\mathbf{r},t)\theta(t-t')=i\int d\mathbf{r}'G^R(\mathbf{r},t;\mathbf{r}',t')\Psi_0(\mathbf{r}',t') \tag{16.43}$$

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

$$i\frac{\partial}{\partial t}\left[\Psi(\mathbf{r},t)\theta(t-t')\right]=i\delta(t-t')\Psi(\mathbf{r},t)+i\theta(t-t')\frac{\partial}{\partial t}\Psi(\mathbf{r},t) \tag{16.44}$$

$$=i\delta(t-t')\Psi(\mathbf{r},t)+H(\mathbf{r})\theta(t-t')\Psi(\mathbf{r},t). \tag{16.45}$$

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

$$i\frac{\partial}{\partial t}\left[i\int d\mathbf{r}'G^R(\mathbf{r},t;\mathbf{r}',t')\Psi_0(\mathbf{r}',t')\right]= \tag{16.46}$$

$$\delta(t-t')i\int d\mathbf{r}'\delta^3(\mathbf{r}-\mathbf{r}')\Psi_0(\mathbf{r}',t')+H(\mathbf{r})\left[i\int d\mathbf{r}'G^R(\mathbf{r},t;\mathbf{r}',t')\Psi_0(\mathbf{r}',t')\right] \tag{16.47}$$

and since the equation is valid for arbitrary initial condition $\Psi_0(\mathbf{r}',t')$, then either by inspection or by taking $\Psi_0(\mathbf{r}',t')=\delta(\mathbf{r}'-\mathbf{r}'')$ we find,

$$\boxed{\left[i\frac{\partial}{\partial t}-H(\mathbf{r})\right]G^R(\mathbf{r},t;\mathbf{r}'',t')=\delta(t-t')\delta^3(\mathbf{r}-\mathbf{r}'')}. \tag{16.48}$$

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

Remark 57 *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

$$\widehat{G}^R(t) = -ie^{-iHt}\theta(t) \tag{16.49}$$

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

$$\left[i\frac{\partial}{\partial t} - H\right]\widehat{G}^R(t) = \delta(t) \tag{16.50}$$

which takes exactly the form above, (16.48) 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,

$$\boxed{\widehat{G}^R(t) = \left[i\tfrac{\partial}{\partial t} - H\right]^{-1}\delta(t)} \tag{16.51}$$

which is meaningless unless we specify that the boundary condition is that $G^R(-\infty) = 0$. This should be compared with Eq.(16.6).

Remark 58 *Boundary condition in time vs pole location in frequency space: From the equation for the propagator (16.48) 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* $i\eta$*) and is equal to* $-i$ *at* $t=0$ *makes the solution unique. For a first-order differential equation, one boundary condition at* $t-t'=0^+$ *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.(16.8).*

16.6 Exercices

16.6.1 Fonctions de Green retardées, avancées et causales.

Soit la fonction de Green pour des particules libres:

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2m}\nabla^2\right]G\left(\mathbf{r}-\mathbf{r}';t\right)=\delta^3\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t\right)$$

a) Calculez $G\left(\mathbf{k},\omega\right)$ en prenant la transformée de Fourier de cette équation d'abord dans l'espace, puis dans le temps. Pour la transformée de Foureir spatiale, on peut supposer que $G\left(\mathbf{r}-\mathbf{r}';t\right)=0$ à $\mathbf{r}-\mathbf{r}'=\pm\infty$. Dans le cas de la transformée de Fourier dans le temps, intégrez par parties et montrez que le choix $\pm i\eta$ est déterminé par l'endroit où G s'annulle, soit à $t=\infty$ ou à $t=-\infty$.. Une de ces fonctions de Green est la fonction dite avancée.

b) Rajoutez à la fonction retardée une solution de la version homogène de l'équation différentielle pour obtenir une fonction de Green qui ne s'annule ni à $t=\infty$ ni à $t=-\infty$ et qui est le plus symétrique possible sous le changement $(t\rightarrow -t)$, plus spécifiquement $G_c^*\left(\mathbf{k},t\right)=G_c\left(\mathbf{k},-t\right)$. C'est la fonction de Green "Causale" (Time-ordered).

c) Calculez la fonction de Green retardée $G^R\left(\mathbf{r}-\mathbf{r}';t\right)$ pour une particule libre en trois dimensions en prenant la transformée de Fourier de $G^R\left(\mathbf{k},\omega\right)$.

17. A FIRST PHENOMENOLOGICAL ENCOUNTER WITH SELF-ENERGY

In this short Chapter, we want to devlop an intuition for the concept of self-energy. The concept is simplest to understand if we start from a non-interacting system and assume to add interactions with a potentail or whatever that change the situation a little. We will be guided by simple ideas about the harmonic oscillator.

Let us start then from the Green function for a non-interacting particle in Eq.(16.10)

$$\langle \mathbf{k}| \widehat{G}_0^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) = \langle \mathbf{k}| \frac{1}{\omega + i\eta - H} |\mathbf{k}'\rangle = \frac{\langle \mathbf{k}|\, \mathbf{k}'\rangle}{\omega + i\eta - \varepsilon_{\mathbf{k}}}. \tag{17.1}$$

Since the momentum states are orthogonal, it is convenient to define $G_0^R(\mathbf{k},\omega)$ by

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

The corresponding spectral weight is particularly simple,

$$A_0(\mathbf{k},\omega) = -2\,\mathrm{Im}\, G_0^R(\mathbf{k},\omega) = 2\pi\delta(\omega - \varepsilon_{\mathbf{k}}). \tag{17.2}$$

We should think of the frequency as the energy. It is only for a non-interacting particle that specifying the energy specifies the wave vector, since it is only in that case that $\omega = \varepsilon_{\mathbf{k}}$.

In general, if momentum is not conserved, the spectral representation Eq.(16.18)

$$G^R(\mathbf{k};\omega) = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k};\omega')}{\omega + i\eta - \omega'} \tag{17.3}$$

and the explicit expression for the spectral weight Eq.(16.21)

$$A(\mathbf{k};\omega') = \sum_n \langle \mathbf{k}|\, n\rangle \langle n\, |\mathbf{k}\rangle\, 2\pi\delta(\omega' - E_n) \tag{17.4}$$

tells us that a momentum eigenstate has non-zero projection on several true eigenstates and hence $A(\mathbf{k};\omega')$ is not a delta function.

Intuitively, for weak perturbations, we simply expect that $A(\mathbf{k};\omega')$ will broaden in frequency around $\omega = \widetilde{\varepsilon}_{\mathbf{k}}$ where $\widetilde{\varepsilon}_{\mathbf{k}}$ is close to $\varepsilon_{\mathbf{k}}$.We take this intuition from the damped harmonic oscillator where the resonance is broadened and shifted by damping. If we take a Lorentzian as a phenomenological form for the spectral weight

$$A(\mathbf{k};\omega') = \frac{2\Gamma}{(\omega - \widetilde{\varepsilon}_{\mathbf{k}})^2 + \Gamma^2} \tag{17.5}$$

then the Green's function can be computed from the spectral representation Eq.(17.3) by using Cauch's residue theorem. The result is

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega - \widetilde{\varepsilon}_{\mathbf{k}} + i\Gamma}. \tag{17.6}$$

We have neglected $i\eta$ in front of $i\Gamma$.It is easy to verify that $-2\operatorname{Im} G^R(\mathbf{k},\omega)$ gives the spectral weight we started from.

With a jargon that we shall explain momentarily, we define the one-particle irreducible self-energy by

$$G^R(\mathbf{k},\omega)=\frac{1}{\omega+i\eta-\varepsilon_{\mathbf{k}}-\Sigma^R(\mathbf{k},\omega)}=\frac{1}{G_0^R(\mathbf{k},\omega)^{-1}-\Sigma^R(\mathbf{k},\omega)}. \tag{17.7}$$

Its physical meaning is clear. The imaginary part $\operatorname{Im}\Sigma^R(\mathbf{k},\omega)=\Gamma$ corresponds to the scattering rate, or inverse lifetime, whereas the real part, $\operatorname{Re}\Sigma^R(\mathbf{k},\omega)=\widetilde{\varepsilon}_{\mathbf{k}}-\varepsilon_{\mathbf{k}}$ leads to the shift in the position of the resonance in the spectral weight. In other words, $\Sigma^R(\mathbf{k},\omega)$ contains all the information about the interactions.

With the simple approximation that we did for the self-energy,

$$\Sigma^R(\mathbf{k},\omega)=\widetilde{\varepsilon}_{\mathbf{k}}-\varepsilon_{\mathbf{k}}-i\Gamma, \tag{17.8}$$

one notices that the second moment $n=2$ in Eq.(16.30) diverges because the second moment of a Lorentzian does. Hence, the high-frequency expansion becomes incorrect already at order $1/\omega^3$. We need to improve the approximation to recover higher frequency moments. Nevertheless, in the form

$$G^R(\mathbf{k},\omega)^{-1}=G_0^R(\mathbf{k},\omega)^{-1}-\Sigma^R(\mathbf{k},\omega) \tag{17.9}$$

equivalent to that given above, there is no loss in generality. The true self-energy is defined as the difference between the inverse of the non-interacting propagator and the inverse of the true propagator. Lifetimes and shifts must in general be momentum and frequency dependent.

18. PERTURBATION THEORY FOR ONE-BODY PROPAGATOR

Feynman diagrams in their most elementary form appear naturally in perturbation theory for a one-body potential. We will also be able to introduce more precisely the notion of self-energy and point out that the definition given above for the self-energy, $G^R(\mathbf{k},\omega)^{-1} = G_0^R(\mathbf{k},\omega)^{-1} - \Sigma^R(\mathbf{k},\omega)$ is nothing but Dyson's equation. As an example, we will treat in more details the propagation of an electron in a random potential.

18.1 General starting point for perturbation theory.

If we can diagonalize H, then we know the propagator

$$\boxed{\widehat{G}^R(\omega) = \frac{1}{\omega - H + i\eta}} \tag{18.1}$$

from the identities we developed above,

$$G^R(n,n';E) = \langle n|\frac{1}{E-H+i\eta}|n'\rangle = \delta_{nn'}\frac{1}{E-E_n+i\eta} \tag{18.2}$$

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} \tag{18.3}$$

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

$$(\omega + i\eta - H_0 - V)\,\widehat{G}^R(\omega) = 1. \tag{18.4}$$

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

$$\widehat{G}_0^R(\omega) = \frac{1}{\omega + i\eta - H_0} \tag{18.5}$$

we have

$$\left(\widehat{G}_0^R(\omega)\right)^{-1}\widehat{G}^R(\omega) = 1 + V\widehat{G}^R(\omega). \tag{18.6}$$

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

$$\boxed{\widehat{G}^R(\omega) = \widehat{G}_0^R(\omega) + \widehat{G}_0^R(\omega)\,V\widehat{G}^R(\omega)}. \tag{18.7}$$

In scattering theory, this is the propagator version of the Lippmann-Schwinger equation. Perturbation theory is obtained by iterating the above equation.

$$\widehat{G}^R(\omega) = \widehat{G}_0^R(\omega) + \widehat{G}_0^R(\omega)\,V\widehat{G}_0^R(\omega) + \widehat{G}_0^R(\omega)\,V\widehat{G}_0^R(\omega)\,V\widehat{G}_0^R(\omega) + \dots \tag{18.8}$$

At first sight we have done much progress. We cannot invert the large matrix H to compute $\widehat{G}^R(\omega)$ but we have expressed it in terms of quantities we know, namely $\widehat{G}_0^R(\omega)$ and V.We know $\widehat{G}_0^R(\omega)$ because by hypothesis H_0 can be diagonalized. At first sight, if we want to know the propagator to a given order, we just stop the above expansion at some order. Stopping the iteration at an arbitrary point may however lead to misleading results, as we shall discuss after discussing a simple representation of the above series in terms of pictures, Feynmann diagrams.

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

$$\boxed{\tfrac{1}{X+Y}=\tfrac{1}{X}-\tfrac{1}{X}Y\tfrac{1}{X+Y}} \tag{18.9}$$

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

$$\frac{1}{X+Y}(X+Y)=\frac{1}{X}X+\frac{1}{X}Y-\frac{1}{X}Y\frac{1}{X+Y}(X+Y)=1 \tag{18.10}$$

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

The Lippmann Schwinger equation Eq.(18.7) may be represented by diagrams. The thick line stands for $\widehat{G}^R(\omega)$ while the thin line stands for $\widehat{G}_0^R(\omega)$ and the dotted line with a cross represents the action of V.

Iterating the basic equation (18.7), one obtains the series

$$\widehat{G}^R(\omega)=\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)V\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)V\widehat{G}_0^R(\omega)V\widehat{G}_0^R(\omega)+\ldots \tag{18.11}$$

which we represent diagrammatically by Fig.(18-1). Physically, one sees that the full propagator is obtained by free propagation between scatterings off the potential.

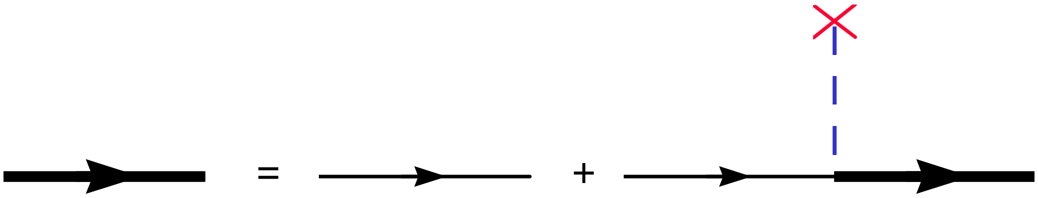

Figure 18-1 Diagrammatic representation of the Lippmann-Schwinger equation for scattering.

18.2.1 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

$$\langle \mathbf{r} | \widehat{G}^R(\omega) | \mathbf{r}' \rangle = \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | V | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \ldots \tag{18.12}$$

$$= \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \int d\mathbf{r}_1 \langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | V | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle + \ldots \tag{18.13}$$

Remark 59 *Physical interpretation and path integral: Given that* $\langle \mathbf{r} | \widehat{G}^R(\omega) | \mathbf{r}' \rangle$ *is the amplitude to propagate from* $\langle \mathbf{r}|$ *to* $|\mathbf{r}'\rangle$*, the last result may be interpreted as saying that the full propagator is obtained by adding up the amplitudes to go with free propagation between* $\langle \mathbf{r}|$ *and* $|\mathbf{r}'\rangle$*, then with two free propagations and one scattering at all possible intermediate points, then with three free propagations and two scatterings at all possible intermediate points etc... The Physics is the same as that seen in Feynman's path integral formulation of quantum mechanics that we discuss below.*

One can read off the terms of the perturbation series from the diagrams above by using the following simple diagrammatic rules which go with the following figure (18-2).

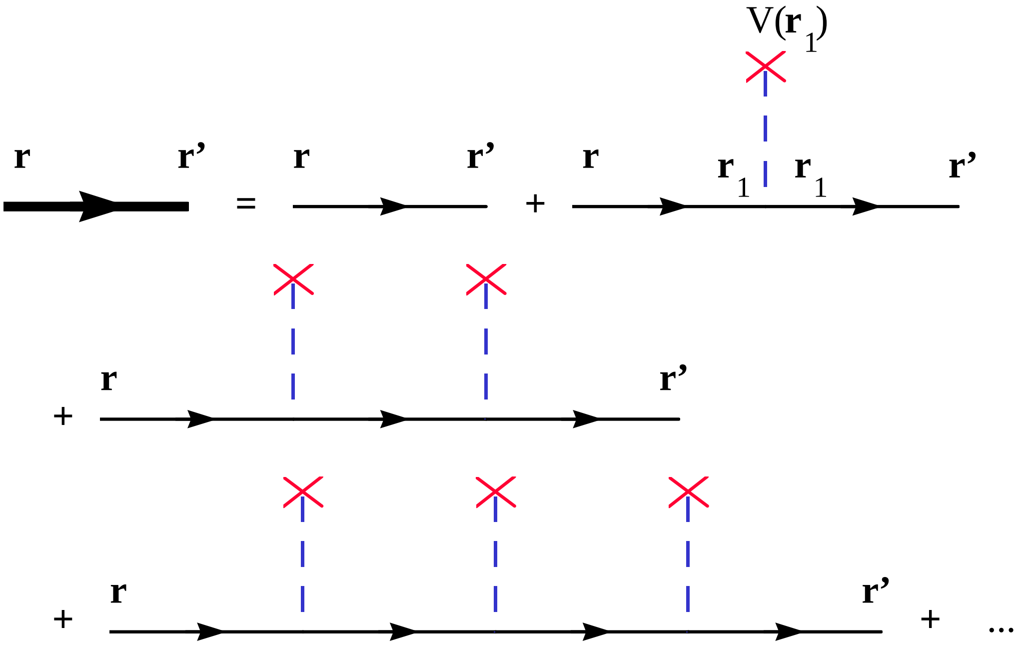

Figure 18-2 Iteration of the progagator for scattering off impurities.

- Let each thin line with an arrow stand for $\langle \mathbf{r} | \widehat{G}_0^R(\omega) | \mathbf{r}' \rangle$. One end of the arrow represents the original position $\mathbf{r}$ while the other represents the final position $\mathbf{r}'$ so that the line propagates from $\mathbf{r}$ to $\mathbf{r}'$. Strictly speaking, from the way we have defined the retarded propagator in terms of propagation of wave functions, this should be the other way around. But the convention we are using now is more common.
- The X at the end of a dotted line stands for a potential $\langle \mathbf{r}_1 | V | \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_1)$.

- Diagrams are built by attaching each potential represented by an X to the end of a propagator line and the beginning of another propagator line by a dotted line.
- The intersection of a dotted line with the two propagator lines is called a vertex.
- There is one dummy integration variable $\int d\mathbf{r}_1$ over coordinates for each vertex inside the diagram.
- The beginning point of each continuous line is $\langle \mathbf{r}|$ and the last point is $|\mathbf{r}'\rangle$. These coordinates are not integrated over.
- The propagator is obtained by summing all diagrams formed with free propagators scattering off one or more potentials. All topologically distinct possibilities must be considered in the sum. One scattering is distinct from two etc...

18.2.2 Diagrams in momentum space

Since the propagator for a free particle is diagonal in the momentum space representation, this is often a convenient basis to write the perturbation expansion in (18.11). Using complete sets of states again, as well as the definition $\langle \mathbf{k}| \widehat{G}_0^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) \langle \mathbf{k}|\, \mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) (2\pi)^3 \delta(\mathbf{k}-\mathbf{k}')$ we have that for a particle with a quadratic dispersion law, or a Hamiltonian $H_0 = p^2/2m$

$$G_0^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \frac{k^2}{2m}}. \tag{18.14}$$

In this basis, the perturbation series becomes

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) \langle \mathbf{k}|\, \mathbf{k}'\rangle + \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| V |\mathbf{k}_1\rangle \langle \mathbf{k}_1| \widehat{G}^R(\omega) |\mathbf{k}'\rangle. \tag{18.15}$$

Solving by iteration to second order, we obtain,

$$\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}'\rangle = G_0^R(\mathbf{k},\omega) \langle \mathbf{k}|\, \mathbf{k}'\rangle + G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| V |\mathbf{k}'\rangle G_0^R(\mathbf{k}',\omega) \tag{18.16}$$

$$+ \int \frac{d\mathbf{k}_1}{(2\pi)^3} G_0^R(\mathbf{k},\omega) \langle \mathbf{k}| V |\mathbf{k}_1\rangle G_0^R(\mathbf{k}_1,\omega) \langle \mathbf{k}_1| V |\mathbf{k}'\rangle G_0^R(\mathbf{k}',\omega) + ... \tag{18.17}$$

The diagrams shown in the following figure Fig.(18-3) are now labeled differently. The drawing is exactly the same as well as the rule of summing over all topologically distinct diagrams.

However,

- Each free propagator has a label $\mathbf{k}$,ω. One can think of momentum $\mathbf{k}$ flowing along the arrow.
- 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.

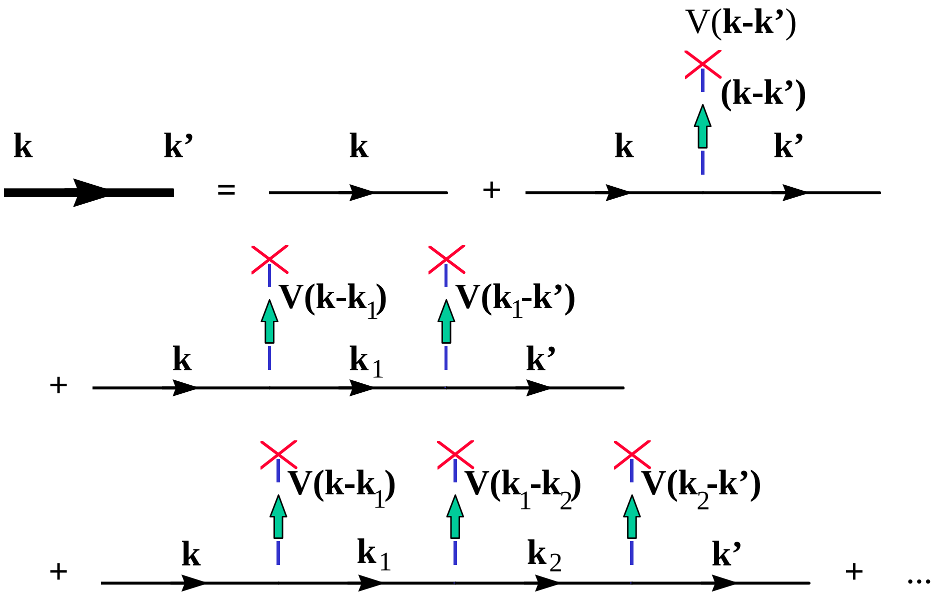

Figure 18-3 Feynman diagrams for scattering off impurities in momentum space (before impurity averaging).

18.3 Dyson's equation, irreducible self-energy

How do we rescue the power series idea. We need to rearrange the power series so that it becomes a power series not for the Green's function, but for the self-energy that we introduced earlier. This idea will come back over and over again. We discuss it here in the simple context of scattering off impurities. Even in this simple context we would need in principle to introduce the impurity averaging technique, but we can avoid this.

The Green's function describes how a wave propagates through a medium. We know from experience that even in a random potential, such as that which light encounters when going through glass, the wave can be scattered forward, i.e. if it comes in an eigenstate of momentum, a plane wave, it can come out in the same eigenstate of momentum. So let us compute the amplitude for propagating from $\langle\mathbf{k}|$ to $|\mathbf{k}\rangle$ using perturbation theory. Suppose we truncate the perturbation expansion to some finite order. For example, consider the truncated series for the diagonal element $\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle$

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle \tag{18.18}$$

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.(16.19) and (16.21) 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

$$\operatorname{Im}\frac{1}{\left(\omega+i\eta-\frac{k^2}{2m}\right)^2} = -\frac{\partial}{\partial\omega}\operatorname{Im}\frac{1}{\omega+i\eta-\frac{k^2}{2m}} \tag{18.19}$$

$$= \pi\frac{\partial}{\partial\omega}\delta\left(\omega-\frac{k^2}{2m}\right) \tag{18.20}$$

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

$$\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,G_0^R(\mathbf{k},\omega)=\frac{\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle}{\omega+i\eta-\frac{k^2}{2m}} \tag{18.21}$$

a quantity which is not smal 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

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle \tag{18.22}$$

$$+\,G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle+... \tag{18.23}$$

which may be generated by

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle\,\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle \tag{18.24}$$

then things start to make more sense since the solution

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = \frac{\langle\mathbf{k}|\,\mathbf{k}\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1}-\langle\mathbf{k}|\,V\,|\mathbf{k}\rangle} \tag{18.25}$$

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 $\int\frac{d\omega}{2\pi}Tr\left[-2\operatorname{Im}\left(\widehat{G}^R(\omega)\right)\right]=Tr\left[H^0\right]=1$ as well as the second $\int\frac{d\omega}{2\pi}\omega Tr\left[-2\operatorname{Im}\left(\widehat{G}^R\right)\right]=Tr\left[H\right]$.

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* $\sum(\mathbf{k},\omega)$ by the equation

$$\boxed{\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = G_0^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\mathbf{k}\rangle + G_0^R(\mathbf{k},\omega)\,\Sigma^R(\mathbf{k},\omega)\,\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle}. \tag{18.26}$$

This is the so-called *Dyson equation* whose diagrammatic representation is given in Fig.(18-4) and whose solution can be found algebraically

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}\rangle = \frac{\langle\mathbf{k}|\,\mathbf{k}\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1}-\Sigma^R(\mathbf{k},\omega)}. \tag{18.27}$$

The definition of the self-energy is found in principle by comparing with the exact result Eq.(18.15) obtained from the Lippmann-Schwinger equation. The

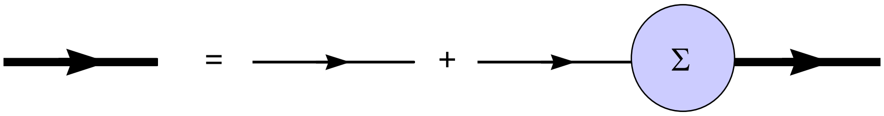

Figure 18-4 Dyson's equation and irreducible self-energy.

algebraic derivation is discussed in the following section, but diagrammatically one can see what to do. The self-energy $\sum(\mathbf{k},\omega)$ should contain all possible diagrams that start with an interaction vertex with entering momentum $\mathbf{k}$, and end with an interaction vertex with outgoing momentum $\mathbf{k}$ and never have in the intermediate states $G_0^R(\mathbf{k}',\omega)$ with $\mathbf{k}'$ equal to the value of $\mathbf{k}$ we 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 (18.26) will give back all missing $G_0^R(\mathbf{k},\omega)$ in intermediate states.

$\sum(\mathbf{k},\omega)$ is called *irreducible* because a diagram in the self-energy cannot be cut in two separate pieces by cutting one $G_0^R(\mathbf{k},\omega)$ with the same $\mathbf{k}$. In the context of self-energy, one usually drops the term *irreducible* since the *reducible* self-energy $\widetilde{\Sigma}^R(\omega)$, defined by $\widehat{G}^R(\omega)=\widehat{G}_0^R(\omega)+\widehat{G}_0^R(\omega)\widetilde{\Sigma}^R(\omega)\widehat{G}_0^R(\omega)$, does not have much interest from the point of view of calculations. The last factor in that last equation is $\widehat{G}_0^R(\omega)$ instead of the full $\widehat{G}^R(\omega)$ .Hence $\widetilde{\Sigma}^R$ contains diagrams that can be cut in two pieces by cutting one $G_0^R(\mathbf{k},\omega)$.

To first order then, $\sum(\mathbf{k},\omega)$ is given by the diagram in Fig.(18-5) whose algebraic expression can be read off

$$\Sigma^{R(1)}(\mathbf{k},\omega)=\langle\mathbf{k}|V|\mathbf{k}\rangle. \tag{18.28}$$

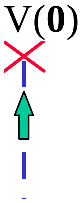

Figure 18-5 First-order irreducible self-energy.

This is the first-order shift to the energies we had found above. To second order, the diagram is given in Fig.(18-6) and its algebraic expression is

$$\Sigma^{R(2)}(\mathbf{k},\omega)=\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}\langle\mathbf{k}|V|\mathbf{k}_1\rangle G_0^R(\mathbf{k}_1,\omega)\langle\mathbf{k}_1|V|\mathbf{k}\rangle. \tag{18.29}$$

The result is now frequency dependent and less trivial than the previous one. There will be a non-zero imaginary part, corresponding to the finite lifetime we described previously in our introduction to the self-energy in Chap.17

What have we achieved? We have rearranged the series in such a way that simple expansion in powers of V is possible, but for the irreducible self-energy.

Remark 60 *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".*

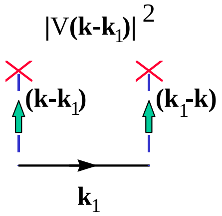

Figure 18-6 Second order irreducible self-energy (before impurity averaging).

Remark 61 *Strictly speaking the irreducible self-energy starting at order three will contain double poles, but at locations different from* $\varepsilon_{\mathbf{k}}$ *and in addition these will have negligible weight in integrals so they will not damage analyticity properties.*

18.4 Exercices

18.4.1 Règles de somme dans les systèmes désordonnés.

La seconde quantification est prérequise à cet exercice. Soit l'Hamiltonien de liaisons fortes pour une chaîne unidimensionnelle:

$$H = \sum_i \epsilon_i a_i^+ a_i + t \sum_i \left(a_i^+ a_{i+1} + a_{i+1}^+ a_i \right)$$

où a_i est un opérateur de destruction sur le site i. Les énergies ϵ_i des sites ont une valeur ϵ_0 avec une probabilité x et une valeur ϵ_1 avec une probabilité $1-x$. Il n'y a qu'une particule.

a) Utilisez les règles de somme pour calculer la valeur moyenne sur le désordre du moment d'ordre 0 et du moment d'ordre 1 de la densité d'états totale $\rho(\omega)$, i.e. calculez la valeur moyenne sur le désordre de $\int d\omega \omega^n \rho(\omega)$ pour $n = 0, 1$.

b) Calculez aussi $\rho(\omega)$ lorsque la chaîne est ordonnée, i.e. $x = 1$.

18.4.2 Développement du locateur dans les systèmes désordonnés.

Soit une particule sur un réseau où l'énergie potentielle sur chaque site i est aléatoire (L'espace des positions est maintenant discret et les intégrales peuvent être remplacées par des sommes).

a) Décrivez dans l'espace des positions les diagrammes pour la théorie des perturbations permettant de calculer G_{ii} lorsque le potentiel joue le rôle de H_0 —diagonal dans l'espace des positions i— et les éléments de matrice H_{ij} de la perturbation sont non-nuls seulement lorsque deux sites i et j sont premiers voisins. Il n'est pas nécessaire de faire la moyenne sur le désordre.

b) Comment définirait-on la self-énergie de Dyson pour G_{ii}, toujours sans faire la moyenne sur le désordre?

18.4.3 Une impureté dans un réseau: état lié, résonnance, matrice T.

Considérons des électrons qui n'interagissent pas l'un avec l'autre mais qui sautent d'un site à l'autre sur un réseau. Les intégrales sur la position deviennent des sommes discrètes. On suppose ce réseau invariant sous translation et on note les éléments de matrice de l'Hamiltonien $\langle i|\, H \,|j\rangle = t_{ij}$ sauf pour une impureté, située à l'origine, caractérisée par un potentiel V local. À partir de l'équation de Lippmann-Schwinger, on voit que l'équation du mouvement pour la fonction de Green retardée dans ce cas est

$$\sum_{\ell} \left(\delta_{i,\ell}\left(\omega+i\eta\right)-t_{i\ell}\right) G^{R}\left(\ell,j;\omega\right)=\delta_{i,j}+\delta_{i,0} V G^{R}\left(0,j;\omega\right) \tag{18.30}$$

On suppose qu'on connaît la solution du problème lorsque l'impureté est absente, *i.e.* qu'on connaît

$$\sum_{\ell} \left(\delta_{i,\ell}\left(\omega+i\eta\right)-t_{i\ell}\right) G_{0}^{R}\left(\ell,j;\omega\right)=\delta_{i,j} \tag{18.31}$$

a) Utilisant ce dernier résultat, montrez que

$$G^{R}\left(i,j;\omega\right)=G_{0}^{R}\left(i,j;\omega\right)+G_{0}^{R}\left(i,0;\omega\right) V G^{R}\left(0,j;\omega\right) \tag{18.32}$$

b) Résolvez l'équation précédente pour $G^{R}\left(0,j;\omega\right)$ en posant $i=0$ puis démontrez que dans le cas général

$$G^{R}\left(i,j;\omega\right)=G_{0}^{R}\left(i,j;\omega\right)+G_{0}^{R}\left(i,0;\omega\right) T^{R}\left(0,0;\omega\right) G_{0}^{R}\left(0,j;\omega\right) \tag{18.33}$$

où la matrice T est définie par

$$T^{R}\left(0,0;\omega\right)=\frac{V}{1-V G_{0}^{R}\left(0,0;\omega\right)} \tag{18.34}$$

La matrice T tient compte exactement de la diffusion provoquée par l'impureté. Dans le cas de l'approximation de Born, il n'y aurait eu que le numérateur pour la matrice T.

Nous allons calculer maintenant la densité d'états locale sur l'impureté.

c) Démontrez d'abord que les pôles $G_{0}^{R}\left(0,0;\omega\right)$ du problème sans impureté n'apparaissent plus directement dans ceux du nouveau propagateur $G^{R}\left(0,0;\omega\right)$ et que les pôles de ce dernier sont plutôt situés là où

$$1-V G_{0}^{R}\left(0,0;\omega\right)=0 \tag{18.35}$$

d) Posons ($\hbar=1$)

$$G_{0}^{R}\left(0,0;\omega\right)=\frac{1}{N}\sum_{\mathbf{k}=\mathbf{1}}^{N}\frac{1}{\omega+i\eta-\varepsilon_{\mathbf{k}}} \tag{18.36}$$

où les $\varepsilon_{\mathbf{k}}$ sont les énergies propres du système sans impureté. En ne dessinant qu'un petit nombre des valeurs de $\varepsilon_{\mathbf{k}}$ possibles et en notant que celles-ci sont très près l'une de l'autres (distantes de $O\left(1/N\right)$), montrez graphiquement que les nouveaux pôles donnés par la solution de $1-V\operatorname{Re}G_{0}^{R}\left(0,0;\omega\right)=0$ ne sont que légèrement déplacés par rapport à la position des anciens pôles, sauf pour un nouvel état lié (ou anti-lié) qui peut se situer loin de l'un ou de l'autre des bords de l'ancienne bande à condition que $V\geq V_{0}$ ou $V\leq V_{0}^{\prime}$. Pour ce dernier calcul, on utilise la limite $N=\infty$,

$$\frac{1}{N}\sum_{\mathbf{k}=\mathbf{1}}^{N}\rightarrow\int N\left(\varepsilon\right) d\varepsilon \tag{18.37}$$

et les définitions

$$\frac{1}{V_0} \equiv \int \frac{N(\varepsilon)\, d\varepsilon}{\omega_B - \varepsilon} \quad ; \quad \frac{1}{V_0'} \equiv \int \frac{N(\varepsilon)\, d\varepsilon}{\omega_{B'} - \varepsilon} \tag{18.38}$$

ω_B et $\omega_{B'}$ étant respectivement définies comme les fréquences supérieures et inférieures des bords de la bande .

e) Montrez que la densité d'états locale sur l'impureté est donnée par

$$\frac{N(\omega)}{\left[1 - V\mathcal{P}\int \frac{N(\varepsilon)d\varepsilon}{\omega-\varepsilon}\right]^2 + V^2\pi^2 N(\omega)^2} \tag{18.39}$$

Par rapport à la densité d'états $N(\omega)$ de la bande originale, cette densité d'états est donc augmentée ou réduite, selon que le dénominateur est plus petit ou plus grand que l'unité. En particulier, même lorsqu'il n'y a pas d'état lié ou anti-lié, il est quand même possible qu'il y ait une forte augmentation de la densité d'états pour une énergie située à l'intérieur de la bande. La position de la résonnance ω_r est donnée par

$$1 - V\mathcal{P}\int \frac{N(\varepsilon)\, d\varepsilon}{\omega_r - \varepsilon} = 0 \tag{18.40}$$

et sa largeur est approximativement donnée par $V\pi N(\omega_r)$.

f) À partir du résultat précédent, montrez qu'en dehors de l'ancienne bande, c'est-à-dire là où $N(\omega) \to 0$, une fonction delta apparaît dans la densité d'états lorsqu'il y a un état lié ou anti-lié et calculez le poids de cette fonction delta. Laissez les résultats sous forme d'intégrale sans les évaluer explicitement.

19. FORMAL PROPERTIES OF THE SELF-ENERGY

We will come back in the next chapter on the properties of the self-energy and of the Green function but we give a preview. Given the place where the self-energy occurs in the denominator of the full Green function Eq.(18.27), we see that its imaginary part has to be negative if we want the poles of $\widehat{G}^R(\omega)$ to be in the lower half-plane. Also, from the Dyson equation (18.26), the self-energy is analytic in the upper half-plane since $\langle \mathbf{k}| \widehat{G}^R(\omega) |\mathbf{k}\rangle$ itself is. Analyticity in the upper half-plane means that $\Sigma^R(\mathbf{k},\omega)$ obeys Kramers-Kronig equations analogous to those found before for response functions,

$$\mathrm{Re}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega) - \Sigma^R(\mathbf{r},\mathbf{r}';\infty)\right] = \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Im}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega')\right]}{\omega'-\omega}. \tag{19.1}$$

$$\mathrm{Im}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Re}\left[\Sigma^R(\mathbf{r},\mathbf{r}';\omega') - \Sigma^R(\mathbf{r},\mathbf{r}';\infty)\right]}{\omega'-\omega} \tag{19.2}$$

One motivation for the definition of the self-energy is that to compute the shift in the energy associated with $\mathbf{k}$, we have to treat exactly the free propagation with $G_0^R(\mathbf{k},\omega)$.

The self-energy itself has a spectral representation, and obeys sum rules. To find its formal expression, let us first define projection operators:

$$\mathcal{P} = |\mathbf{k}\rangle\langle\mathbf{k}| \quad ; \quad \mathcal{Q} = 1-\mathcal{P} = \int \frac{d\mathbf{k}'}{(2\pi)^3}|\mathbf{k}'\rangle\langle\mathbf{k}'| - |\mathbf{k}\rangle\langle\mathbf{k}| \tag{19.3}$$

with the usual properties for projection operators

$$\mathcal{P}^2 = \mathcal{P} \quad ; \quad \mathcal{Q}^2 = \mathcal{Q} \quad ; \quad \mathcal{P}+\mathcal{Q} = 1 \tag{19.4}$$

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

Since H_0 is diagonal in this representation, we have that

$$\mathcal{P}G_0^R(\mathbf{k},\omega)\,\mathcal{Q} = \mathcal{Q}G_0^R(\mathbf{k},\omega)\,\mathcal{P} = 0 \tag{19.5}$$

We will use the above two equations freely in the following calculations.

We want to evaluate the full propagator in the subspace $|\mathbf{k}\rangle$. Let us thus project the Lippmann-Schwinger equation

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R V\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R V\mathcal{P}\widehat{G}^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R V\mathcal{Q}\widehat{G}^R\mathcal{P}. \tag{19.6}$$

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

$$\mathcal{Q}\widehat{G}^R\mathcal{P} = \mathcal{Q}\widehat{G}_0^R V\widehat{G}^R\mathcal{P} = \mathcal{Q}\widehat{G}_0^R V\mathcal{P}\widehat{G}^R\mathcal{P} + \mathcal{Q}\widehat{G}_0^R V\mathcal{Q}\widehat{G}^R\mathcal{P} \tag{19.7}$$

$$\mathcal{Q}\widehat{G}^R\mathcal{P} = \frac{1}{1-\mathcal{Q}\widehat{G}_0^R V\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R V\mathcal{P}\widehat{G}^R\mathcal{P}. \tag{19.8}$$

Substituting in the previous result, we find

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R V\left[1+\frac{1}{1-\mathcal{Q}\widehat{G}_0^R V\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R V\right]\mathcal{P}\widehat{G}^R\mathcal{P} \tag{19.9}$$

$$\mathcal{P}\widehat{G}^R\mathcal{P} = \mathcal{P}\widehat{G}_0^R\mathcal{P} + \mathcal{P}\widehat{G}_0^R\mathcal{P}V\left[1 + \frac{1}{1 - \mathcal{Q}\widehat{G}_0^R V \mathcal{Q}}\mathcal{Q}\widehat{G}_0^R V\mathcal{P}\right]\mathcal{P}\widehat{G}^R\mathcal{P} \tag{19.10}$$

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

$$\boxed{\widehat{\Sigma}^R = \mathcal{P}V\mathcal{P} + \mathcal{P}V\mathcal{Q}\tfrac{1}{1-\mathcal{Q}\widehat{G}_0^R\mathcal{Q}V\mathcal{Q}}\mathcal{Q}\widehat{G}_0^R\mathcal{Q}V\mathcal{P}}. \tag{19.11}$$

This is precisely the algebraic version of the diagrammatic definition which we gave before. The state $\mathbf{k}$ corresponding to the projection $\mathcal{P}$ never occurs in intermediate states, but the initial and final states are in $\mathcal{P}$.

Remark 62 *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 63 *High-frequency behavior of self-energy and sum rules: Given the* $1/\omega$ *high-frequency behavior of* $\widehat{G}_0^R$, *one can see that the infinite frequency limit of the self-energy is a constant given by* $\mathcal{P}V\mathcal{P} = |\mathbf{k}\rangle\langle\mathbf{k}|V|\mathbf{k}\rangle\langle\mathbf{k}|$ *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* $\widehat{G}_0^R$. *We will see in the interacting electrons case that the Hartree-Fock result is the infinite-frequency limit of the self-energy.*

Remark 64 *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.*

20. ELECTRONS IN A RANDOM POTENTIAL: IMPURITY AVERAGING TECHNIQUE.

We treat in detail the important special case of an electron being scattered by a random distribution of impurities. This serves as a model of the residual resistivity of metals. It is the Green's function version of the Drude model for elastic impurity scattering. One must however add the presence of the Fermi sea. When this is done in the many-body context, very little changes compared with the derivation that follows. The many-body calculation will also allow us to take into account inelastic scattering. We start by discussing how to average over impurities, and then we apply these results to the averaging of the perturbation series for the Green's function.

20.1 Impurity averaging

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

$$V_C(\mathbf{r}) = \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) \tag{20.1}$$

where each of the N_i impurities produces the same potential v but centered at a different position $\mathbf{R}_i$. We have added the index C to emphasize the fact that at this point the potential depends on the actual configuration of impurities. We want to work in momentum space since after averaging over impurities translational invariance will be recovered. This means that the momentum representation will be the most convenient one for the Green's functions.

$$V_C(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{i=1}^{N_i} v(\mathbf{r} - \mathbf{R}_i) = \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \int d\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_i)} v(\mathbf{r} - \mathbf{R}_i) \tag{20.2}$$

$$= v(\mathbf{q}) \sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \tag{20.3}$$

We assume that the impurities are distributed in a uniform and statistically independent manner (The joint probability distribution is a product of a factor $1/\mathcal{V}$ for each impurity). Denoting the average over impurity positions by an overbar, we have for this distribution of impurities,

$$\overline{V_C(\mathbf{q})} = v(\mathbf{q}) \sum_{i=1}^{N_i} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}}\right) = v(\mathbf{q}) \sum_{i=1}^{N_i} \frac{1}{\mathcal{V}} \int d\mathbf{R}_i e^{-i\mathbf{q}\cdot\mathbf{R}_i} = v(\mathbf{q}) \frac{N_i}{\mathcal{V}} (2\pi)^3 \delta(\mathbf{q}) \tag{20.4}$$

$$= n_i v(\mathbf{0}) (2\pi)^3 \delta(\mathbf{q}) \tag{20.5}$$

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

$$\overline{V_C\left(\mathbf{q}\right)V_C\left(\mathbf{q}'\right)} = v\left(\mathbf{q}\right)v\left(\mathbf{q}'\right)\overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i}\sum_{j=1}^{N_i} e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}. \tag{20.6}$$

To compute the average, we need to know the joint probability distribution for having an impurity at site i and an impurity at site j. The most simple-minded model takes no correlations, in other words, the probability is the product of probabilities for a single impurity, which in the present case were uniform probability distributions. (This is not such a bad approximation in the dilute-impurity case). So for $i \neq j$, we write

$$\overline{\sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{-i\mathbf{q}'\cdot\mathbf{R}_j}} = \sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i}\left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}}\quad\overline{e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}\right) = \frac{\left(N_i^2-N_i\right)}{\mathcal{V}^2}\left(2\pi\right)^3\delta\left(\mathbf{q}\right)\left(2\pi\right)^3\delta\left(\mathbf{q}'\right). \tag{20.7}$$

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

$$\overline{\sum_{i=1}^{N_i} e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{-i\mathbf{q}'\cdot\mathbf{R}_i}} = n_i\left(2\pi\right)^3\delta\left(\mathbf{q}+\mathbf{q}'\right). \tag{20.8}$$

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

$$\overline{V_C\left(\mathbf{q}\right)V_C\left(\mathbf{q}'\right)} = \frac{\left(N_i^2-N_i\right)}{\mathcal{V}^2}\left(v\left(\mathbf{0}\right)\left(2\pi\right)^3\delta\left(\mathbf{q}\right)\right)\left(v\left(\mathbf{0}\right)\left(2\pi\right)^3\delta\left(\mathbf{q}'\right)\right)+n_i\left|v\left(\mathbf{q}\right)\right|^2\left(2\pi\right)^3\delta\left(\mathbf{q}+\mathbf{q}'\right). \tag{20.9}$$

20.2 Averaging of the perturbation expansion for the propagator

Let us return to the perturbation expansion in momentum space to second order Eq.(18.17).Using

$$\left\langle\mathbf{k}\right|V_C\left|\mathbf{k}'\right\rangle = \int d\mathbf{r}\left\langle\mathbf{k}\right|\left.\mathbf{r}\right\rangle V_C\left(\mathbf{r}\right)\left\langle\mathbf{r}\right|\left.\mathbf{k}'\right\rangle = V_C\left(\mathbf{k}-\mathbf{k}'\right) \tag{20.10}$$

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

$$\overline{\left\langle\mathbf{k}\right|\widehat{G}^R\left(\omega\right)\left|\mathbf{k}'\right\rangle} = G_0^R\left(\mathbf{k},\omega\right)\left(2\pi\right)^3\delta\left(\mathbf{k}-\mathbf{k}'\right)+G_0^R\left(\mathbf{k},\omega\right)\overline{V_C\left(\mathbf{k}-\mathbf{k}'\right)}G_0^R\left(\mathbf{k}',\omega\right) \tag{20.11}$$

$$+\int\frac{d\mathbf{k}_1}{\left(2\pi\right)^3}G_0^R\left(\mathbf{k},\omega\right)\overline{V_C\left(\mathbf{k}-\mathbf{k}_1\right)G_0^R\left(\mathbf{k}_1,\omega\right)V_C\left(\mathbf{k}_1-\mathbf{k}'\right)}G_0^R\left(\mathbf{k}',\omega\right)+\ldots \tag{20.12}$$

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

$$\begin{aligned}\left\langle\mathbf{k}\right|\widehat{G}^R\left(\omega\right)\left|\mathbf{k}'\right\rangle = \quad & \left\{G_0^R\left(\mathbf{k},\omega\right)+G_0^R\left(\mathbf{k},\omega\right)\left[n_iv\left(\mathbf{0}\right)\right]G_0^R\left(\mathbf{k},\omega\right)\right.\\ & +G_0^R\left(\mathbf{k},\omega\right)\left[n_iv\left(\mathbf{0}\right)\right]G_0^R\left(\mathbf{k},\omega\right)\left[n_iv\left(\mathbf{0}\right)\right]G_0^R\left(\mathbf{k},\omega\right)\end{aligned}$$

$$-G_0^R(\mathbf{k},\omega)\left[n_i\left|v(\mathbf{0})\right|^2\frac{1}{\mathcal{V}}\right]G_0^R(\mathbf{k},\omega)\,G_0^R(\mathbf{k},\omega)$$

$$+\,G_0^R(\mathbf{k},\omega)\int\frac{d\mathbf{k}_1}{(2\pi)^3}G_0^R(\mathbf{k}_1,\omega)\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]G_0^R(\mathbf{k},\omega)+...\}\,(2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right)\tag{20.13}$$

Recalling the relation between discrete sums and integrals,

$$\int\frac{d\mathbf{k}_1}{(2\pi)^3}=\frac{1}{\mathcal{V}}\sum_{\mathbf{k}_1}\tag{20.14}$$

we see that the term with a negative sign above removes the $\mathbf{k}=\mathbf{k}_1$ term from the integral. We are thus left with the series

$$\begin{aligned}\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}'\rangle = \quad &\left\{G_0^R(\mathbf{k},\omega)+G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)\right.\\ &+G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)\left[n_i v(\mathbf{0})\right]G_0^R(\mathbf{k},\omega)\\ +G_0^R(\mathbf{k},\omega)&\left(\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}G_0^R(\mathbf{k}_1,\omega)\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\right)G_0^R(\mathbf{k},\omega)+...\}\,(2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right)\end{aligned}\tag{20.15}$$

The diagrams corresponding to this expansion are illustrated in Fig.(20-1)

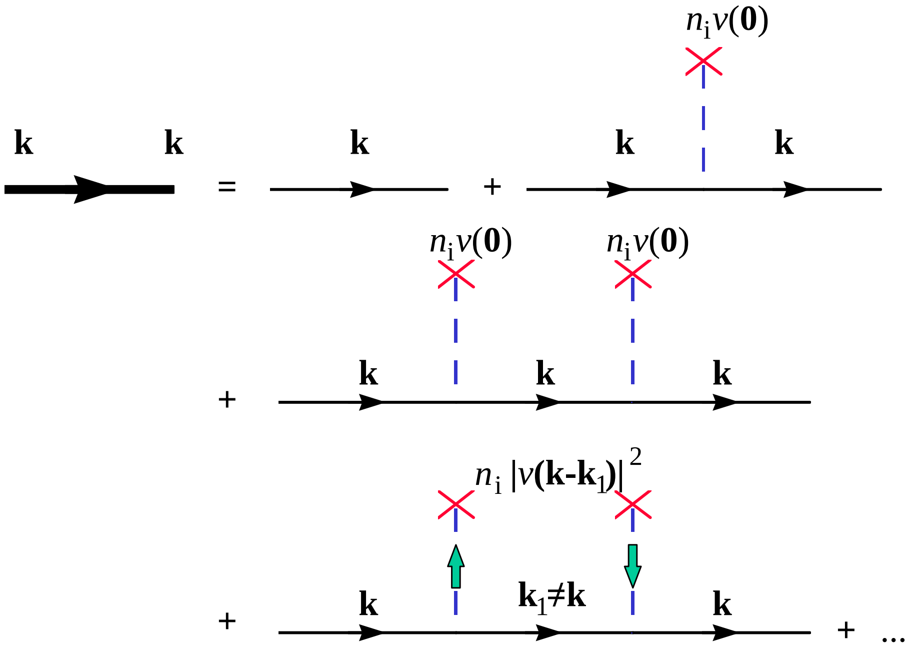

Figure 20-1 Direct iterated solution to the Lippmann-Schwinger equation after impurity averaging.

The diagrammatic rules have changed a little bit. Momentum is still conserved at every vertex, but this time,

- No momentum can flow through an isolated X (in other words, at the vertex the momentum continues only along the line.)
- A factor $[n_i v(\mathbf{0})]$ is associated with every isolated X.

- Various X can be joined together, accounting for the fact that in different X the impurity can be the same.

- When various X are joined together, some momentum can flow along the dotted lines. Each dotted line has a factor $v(\mathbf{k}-\mathbf{k}_1)$ associated with it, with the momentum determined by the momentum conservation rule (which comes from the fact that if in $\int d\mathbf{r} f_1(\mathbf{r}) f_2(\mathbf{r}) f_3(\mathbf{r})$ we replace each function by its Fourier representation, the integral $\int d\mathbf{r}$ will lead to a delta function of the Fourier variables, i.e. $\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0$.)

- The overall impurity concentration factor associated with a single X linking many dotted lines, is n_i, however many dotted lines are associated with it.

- There is an integral over all momentum variables that are not purely determined by the momentum conservation.

Once again, one cannot truncate the series to any finite order since this leads to double poles, triple poles and the other pathologies discussed above. One must resum infinite subsets of diagrams. Clearly, one possibility is to write a self-energy so that

$$\langle\mathbf{k}|\,\widehat{G}^R(\omega)\,|\mathbf{k}'\rangle = \frac{\langle\mathbf{k}|\,\mathbf{k}'\rangle}{\left(G_0^R(\mathbf{k},\omega)\right)^{-1}-\Sigma^R(\mathbf{k},\omega)}. \tag{20.16}$$

If we take the diagrams in Fig.(20-2) for the self-energy, expansion of the last equation for the Green's function, or iteration of Dyson's equation in diagrammatic Fig.(18-4), regive the terms discussed above in the straightforward expansion since the algebraic expression for the self-energy we just defined is

$$\boxed{\Sigma^R(\mathbf{k},\omega) = [n_i v(\mathbf{0})] + \int_{\mathbf{k}_1\neq\mathbf{k}} \frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right] G_0^R(\mathbf{k}_1,\omega)}. \tag{20.17}$$

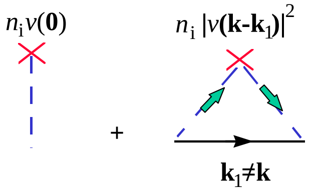

Figure 20-2 Second-order irreducible self-energy in the impurity averaging technique.

Remark 65 *Energy shift: This self-energy gives us the displacements of the poles to linear order in the impurity concentration and to second order in the impurity potential. The displacement of the poles is found by solving the equation*

$$E = \frac{k^2}{2m} + \mathrm{Re}\left[\Sigma^R(\mathbf{k},E)\right]. \tag{20.18}$$

Remark 66 *Lifetime: Taking the Fourier transform to return to real time, it is easy to see that a constant imaginary self-energy corresponds to a life-time, in other words to the fact that the amplitude for being in state* $\mathbf{k}$ *"leaks out" as other states become populated. Indeed, take* $\Sigma^R(\mathbf{k},\omega) = a - i/\tau$ *for example, as an approximation for the self-energy. The corresponding spectral weight is a Lorenzian and the corresponding propagator in time is* $G^R(\mathbf{k},\omega) = -ie^{-i\left(k^2/2m-a\right)t}e^{-t/\tau}$. *We see that the probability of being in state* $\mathbf{k}$ *decreases exponentially. One can* *also check explicitly that the formula found for the lifetime by taking the imaginary part of the self-energy corresponds to what would be obtained from Fermi's Golden rule. For example, the second order contribution from the self-energy expression Eq.(20.17) is*

$$\begin{aligned}\operatorname{Im}\Sigma^R(\mathbf{k},\omega) &= -\pi\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\delta\left(\omega-\frac{k_1^2}{2m}\right) &(20.19)\\ &= -\pi\int d\varepsilon N(\varepsilon)\frac{d\Omega}{4\pi}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]\delta(\omega-\varepsilon) &(20.20)\end{aligned}$$

where in the last expression, $N(\varepsilon)$ is the density of states, and Ω the solid angle. One recognizes the density of states at the frequency of interest ω that will come in and the square of the matrix element. We have an overall factor of π instead of 2π because $-\operatorname{Im}\Sigma^R(\mathbf{k},\omega)$ is the scattering rate for the amplitude instead of the probability. In the continuum, we do not need to worry about $\mathbf{k}_1\neq\mathbf{k}$ for this calculation.

Remark 67 *Self-energy and sum rules: One can check that this self-energy is explicitly analytic in the upper half-plane and that the corresponding Green's function satisfies the first sum rule $\int\frac{d\omega}{2\pi}Tr\left[-2\operatorname{Im}\left(\widehat{G}^R(\omega)\right)\right]=Tr\left[H^0\right]=1$ as well as the second $\int\frac{d\omega}{2\pi}\omega Tr\left[-2\operatorname{Im}\left(\widehat{G}^R\right)\right]=Tr\left[H\right]$. However, at this level of approximation, none of the other sum rules are satisfied because the second and higher moments of a Lorentzian are not defined.*

Remark 68 *Average self-energy and self-averaging: We could have obtained precisely the same result by directly averaging the self-energies (18.28)(18.29) defined in the previous subsection (18.26). Indeed, since the rule there was that $G_0^R(\mathbf{k},\omega)$ could not occur in the intermediate states, impurity averaging of the second-order diagram (18.29) would have given only the correlated contribution $\int_{\mathbf{k}_1\neq\mathbf{k}}\frac{d\mathbf{k}_1}{(2\pi)^3}\left[n_i\left|v(\mathbf{k}-\mathbf{k}_1)\right|^2\right]G_0^R(\mathbf{k}_1,\omega)$. A $G_0^R(\mathbf{k},\omega)$ in the intermediate state would be necessary to obtain a contribution $\left[n_iv(\mathbf{0})\right]^2$. It is possible to average directly the self-energy in the Dyson equation Eq.(18.26) 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 69 *Correlations in the impurity distribution: If we had taken into account impurity-impurity correlations in the joint average (20.7),*

$$\overline{\sum_{i=1}^{N_i}\sum_{j\neq i}^{N_i}e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{-i\mathbf{q}'\cdot\mathbf{R}_j}}, \qquad (20.21)$$

then we would have found that instead of two delta functions leading eventually to forward scattering only, $(2\pi)^3\delta\left(\mathbf{k}-\mathbf{k}'\right)$, 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 70 *Strong impurity potential: It is easy to take into account the scattering by a single impurity more carefully in the self-energy. The set of diagrams* *in Fig.(20-3) are all first-order in impurity concentration. Their summation corresponds to summing the full Born series. In other words, the summation would correspond to replacing the Born cross section entering the expression for the imaginary part of the Green's function by the full T-matrix expression. The cross section for the impurity is then evaluated beyond the Born approximation. This is important when the phase shifts associated with scattering from the impurity are important.*

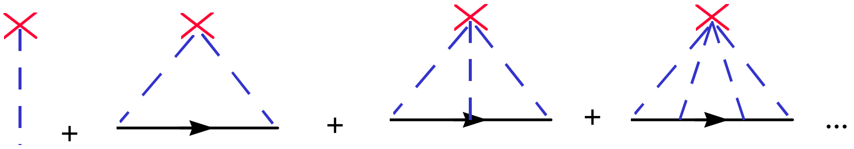

Figure 20-3 Taking into account multiple scattering from a single impurity.

Remark 71 *Irreversibility and infinite volume limit: We have proven that the poles of the Green's function are infinitesimally close to the real axis. In particular, suppose that $|n\rangle$ labels the true eigenstates of our one-body Schrödinger equation in the presence of the impurity potential. Then, our momentum space Green's function will be given by Eq.(16.5)*

$$G^R(\mathbf{k},\mathbf{k};\omega)=\sum_n\frac{\langle\mathbf{k}|\,n\rangle\,\langle n\,|\mathbf{k}\rangle}{\omega+i\eta-E_n}\tag{20.22}$$

$$-\frac{1}{\pi}\operatorname{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right]=\sum_n\langle\mathbf{k}|\,n\rangle\,\langle n\,|\mathbf{k}\rangle\,\delta(\omega-E_n)\,.\tag{20.23}$$

In the case we are considering here, **k** *is no longer a good quantum number. Hence, instead of a single delta function, the spectral weight* $-\frac{1}{\pi}\operatorname{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right]$ *contains a sum of delta functions whose weight is determined by the projection of the true eigenstate on* **k** *states. However, if we go to the infinite volume limit, or equivalently assume that the level separation is smaller than* η*, the discrete sum over* n *can be replaced by an integral, and we obtain a continuous function for the spectral weight. As long as the Green's function has discrete poles, the Fourier transform in time of* G^R *is an oscillatory function and we have reversibility (apart from the damping* η*). Going to the infinite volume limit, (level spacing goes to zero before* η*), we obtained instead a continuous function of frequency instead of a sum over discrete poles. The Fourier transform of this continuous function will in general decay in time. In other words, we have obtained irreversibility by taking the infinite volume limit before the* $\eta\to 0$ *limit.*

Remark 72 *Origin of poles far from the real axis: We come back to the phenomenological considerations on the self-energy in Chap.17. In the case of a continuous spectral weight, when we start to do approximations there may appear poles that are not infinitesimally close to the real axis. Indeed, return to our calculation of the imaginary part of the self-energy above. If we write*

$$-\frac{1}{\pi}\operatorname{Im}\left[G^R(\mathbf{k},\mathbf{k};\omega)\right]=\frac{1}{\pi}\frac{-\operatorname{Im}\left[\Sigma^R(\mathbf{k},\omega)\right]}{\left(\omega-\frac{k^2}{2m}-\operatorname{Re}\left[\Sigma^R(\mathbf{k},\omega)\right]\right)^2+\left(\operatorname{Im}\left[\Sigma^R(\mathbf{k},\omega)\right]\right)^2}\tag{20.24}$$

then there are many cases, such as the one of degenerate electrons scattering off impurities, where for small ω *we can approximate* $\operatorname{Im}\left(\Sigma^R(\mathbf{k},\omega)\right)$ *by a constant and* $\operatorname{Re}\left[\Sigma^R(\mathbf{k},\omega)\right]$ *by a constant plus a linear function of frequency. Then* $G^R(\mathbf{k},\mathbf{k};\omega)$

has a single pole, far from the real axis. In reality, we see from the spectral representation Eq.(16.18) that this single pole is the result of the contribution of a series of poles near the real axis, each of which gives a different residue contribution to the spectral weight. (In the impurity problem, $\mathbf{k}$ *is not a good quantum number anymore so that several of the true eigenstates* E_n *entering the spectral weight Eq.(16.21) 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* $\eta \rightarrow 0$*.*

20.3 Exercices

20.3.1 Diffusion sur des impuretés. Résistance résiduelle des métaux.

Continuons le problème de la diffusion d'une particule sur des impuretés abordé précédemment. Supposez qu'on s'intéresse à des quantités de mouvement et des énergies près de la surface de Fermi d'un métal. $(d = 3)$ Mesurant l'énergie par rapport à la surface de Fermi, on a alors comme propagateur non-perturbé

$$G_0^R(\mathbf{k}, \omega) = \frac{1}{\omega + i\eta - \xi(\mathbf{k})}$$

où $\xi(\mathbf{k}) \equiv (\epsilon(\mathbf{k}) - \mu)$ avec $\epsilon(\mathbf{k}) = k^2/2m$ et μ le potentiel chimique.

Dans tous les calculs qui suivent vous pouvez faire l'approximation que les contributions principales viennent des énergies près du niveau de Fermi. Cela veut dire que vous pouvez partout faire la substitution

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \approx N(0) \int_{-\infty}^{\infty} d\xi$$

où $N(0)$ est la densité d'états au niveau de Fermi, que l'on prend constante. Dans le cas où l'intégrale sur ξ ne converge pas, on régularise de la façon suivante

$$N(0) \int_{-E_0}^{E_0} d\xi$$

où E_0 est une coupure de l'ordre de l'énergie de Fermi.

a) Calculez explicitement la valeur de la règle de somme $Tr[H]$ pour ce problème de diffusion sur un potentiel aléatoire.

b) Calculez les parties réelle et imaginaire de $\sum^R(\mathbf{k}, \omega)$ dans l'approximation illustrée sur la figure 20-4

en prenant une fonction delta ($v(\mathbf{r}) = u\boldsymbol{\delta}(\mathbf{r})$) pour le potentiel diffuseur. Exprimez le résultat en fonction de la densité d'états.

c) En négligeant toute dépendance en $\mathbf{k}$ et ω de $\sum(\mathbf{k}, \omega)$, vérifiez que dans cette approximation, les deux règles de somme sur $G^R(\mathbf{k},\omega)$ correspondant à $Tr\left[H^0\right] = Tr[1]$ et à $Tr[H]$ sont satisfaites, mais qu'aucune autre ne l'est.

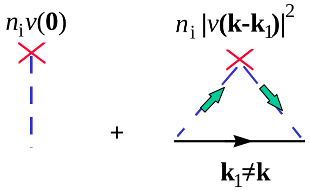

Figure 20-4 Second-order irreducible self-energy in the impurity averaging technique.

d) En approximant encore la self-énergie par une constante indépendante de $\mathbf{k}$ et ω, prenez la transformée de Fourier du résultat que vous avez trouvé pour $G^R(\mathbf{k},\omega)$ et calculez $G^R(\mathbf{k},t)$. (N.B. Il est utile de définir un temps de relaxation pour votre résultat en vous basant sur des considérations dimensionnelles.) Donnez une interprétation physique de votre résultat pour $G^R(\mathbf{k},t)$.

e) Supposons que dans le diagramme de ci-haut qui contient une fonction de Green, on fait une approximation auto-cohérente, i.e. on utilise la fonction de Green "habillée" plutôt que la fonction de Green des particules libres. Montrez que, moyennant des hypothèse raisonnables, les résultats précédents ne sont pas vraiment modifiés.

f) Dessinez quelques-uns des diagrammes de la série de perturbation originale pour la self-énergie que l'approximation auto-cohérente décrite ci-dessus resomme automatiquement.

21. OTHER PERTURBATION RESUMMATION TECHNIQUES: A PREVIEW

The ground state energy may be obtained by the first sum rule. But in the more general case, one can develop a perturbation expansion for it. The corresponding diagrams are a sum of connected diagrams. The so-called "linked cluster theorem" is a key theorem that will come back over and over again.

Given the expression we found above for the density-density correlation, the reader will not be surprised to learn that the diagrams to be considered are, before impurity averaging, of the type illustrated in Fig.(21-1). The density operators act at the far left and far right of these diagrams.

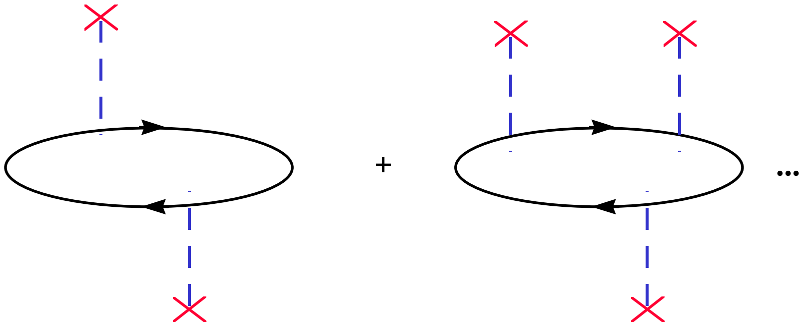

Figure 21-1 Some diagrams contributing to the density-density correlation function before impurity averaging.

After impurity averaging, we obtain for example diagrams of the form illustrated in Fig.(21-2)

Subset of diagrams corresponding to dressing internal lines with the self-energy can be easily resummed. The corresponding diagrams are so-called skeleton diagrams. The first two diagrams in Fig.(21-2) could be generated simply by using lines that contain the full self-energy. The diagrams that do not correspond to self-energy insertions, such as the last on in Fig.(21-2), are so-called vertex corrections.

Subsets of vertex corrections that can be resummed correspond to ladders or bubbles. Ladder diagrams, illustrated in Fig.(21-3) correspond to the so-called Bethe-Salpeter equation, or T-matrix equation. They occur in the problem of superconductivity and of localization.

The bubbles illustrated in Fig.(21-4) are useful especially for long-range forces. They account for dielectric screening, and either renormalize particle-hole excitations or give new collective modes: excitons, plasmons, spin wave, zero sound and the like.

Finally, self-consistent Hartree-Fock theory can be formulated using skeleton diagrams, as illustrated in Fig.(21-5). The self-consistency contained in Hartree-Fock diagrams is crucial for any mean-field type of approximation, such as the BCS theory for superconductivity and Stoner theory for magnetism.

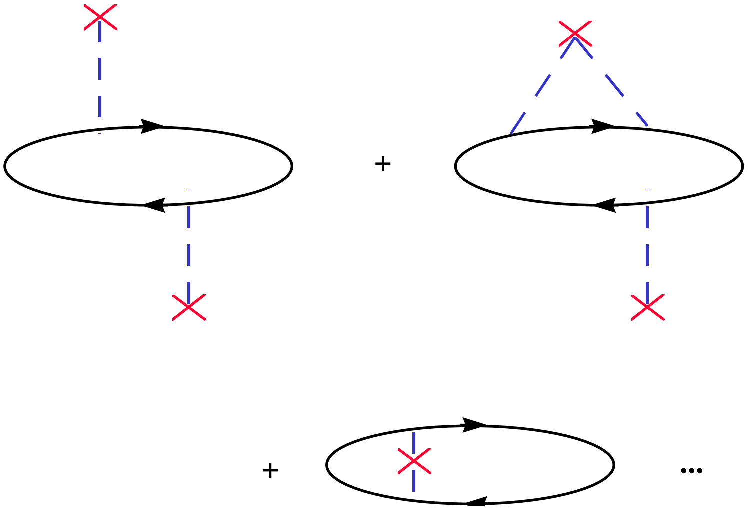

Figure 21-2   Some of the density-density diagrams after impurity averaging.

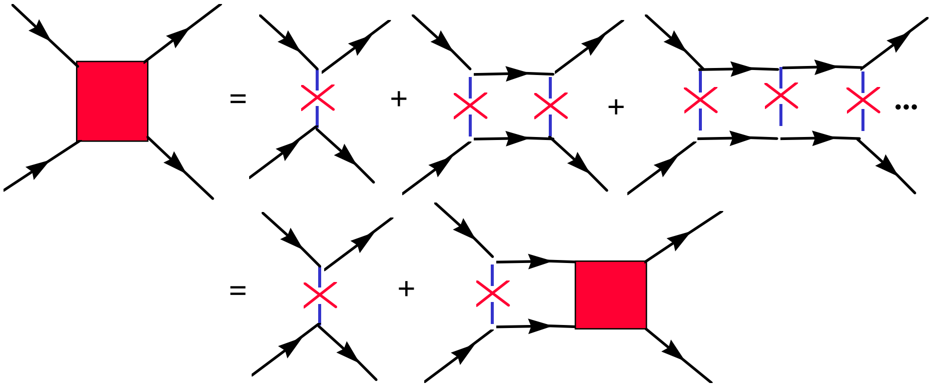

Figure 21-3   Ladder diagrams for T-matrix or Bethe-Salpeter equation.

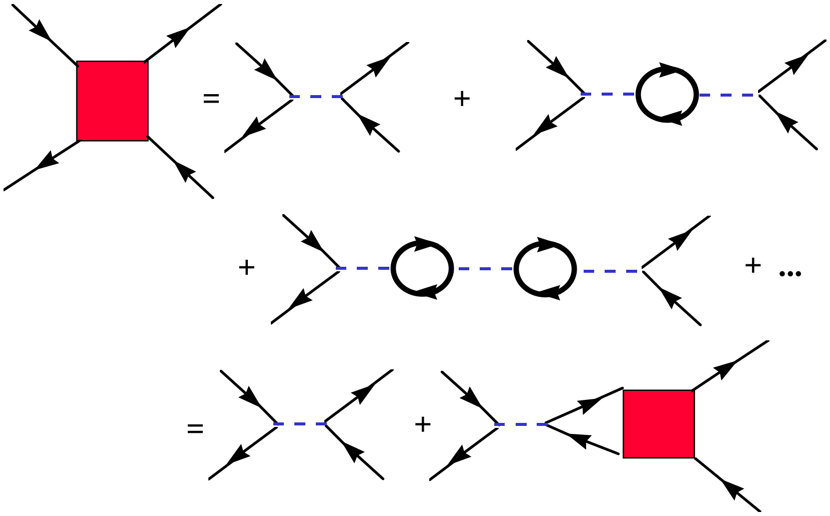

Figure 21-4   Bubble diagrams for particle-hole exitations.

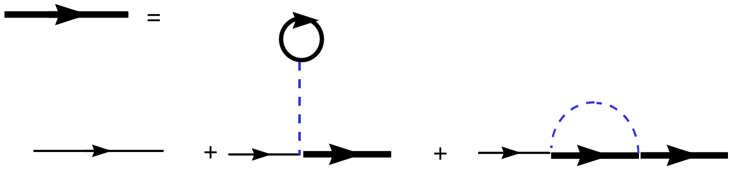

Figure 21-5 Diagrammatic representation of the Hartree-Fock approximation.

Parquet diagrams sum bubble and ladder simultaneously. They are essential if one wants to formulate a theory at the two-particle level which satisfies fully the antisymmetry of the many-body wave-function. In diagrammatic language, this is known as crossing symmetry.

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

22. FEYNMAN PATH INTEGRAL FOR THE PROPAGATOR, AND ALTERNATE FORMULATION OF QUANTUM MECHANICS

We have seen that all the information is in the one-particle propagator. It is thus possible to postulate how the propagator is calculated in quantum mechanics and obtain a new formulation that is different from Schrödinger's, but that can be proven equivalent. This formulation is Feynman's path integral, that was stimulated by ideas of Dirac. The final outcome will be that the amplitude to go from one point to another is equal to the sum over all possible ways of going between the points, each path being weighted by a term proportional to $e^{iS(\dot{x},x)}$ where S is the action. To understand that all intermediate paths are explored, it suffices to think of Young's interference through two slits. If we add more and more slits, we see that the wave must go everywhere. In quantum mechanics there is no trajectory, one of the most surprising results of that theory. However, if the action is large, as in the classical limit, the most likely path will be that which minimizes the action, just as we know from the least action principle in classical mechanics. Instead of postulating it, here we derive the path integral formulation from Schrödinger's quantum mechanics. In practice, this method is now used mostly for numerical calculations and for deriving semi-classical approximations.

We take a single particle in one dimension to simplify the discussion. The relevant object is the amplitude for a particle to go from position x_i to position x_f in a time t.Feynman calls that the probability amplitude or the kernel $K\left(x_f,t;x_i,0\right)$. We will use the notation $G^{>}\left(x_f,t;x_i,0\right)$ for reasons that will be come clear when we discuss propagators in second quantized notation. Mathematically then,

$$G^{>}\left(x_f,t;x_i,0\right) \equiv \left\langle x_f\right| e^{-iHt/\hbar}\left|x_i\right\rangle . \tag{22.1}$$

It is the basic object of this section.

22.1 Physical interpretation

There are several ways to physically understand the quantity defined above. From the basic postulates of quantum mechanics, squaring $G^{>}\left(x_f,t;x_i,0\right)$ gives the probability $\left|\left\langle x_f\right| e^{-iHt/\hbar}\left|x_i\right\rangle\right|^{2.}$ that we are in eigenstate of position x_f at time t if the starting state is a position eigenstate x_i. Also, if we know $G^{>}\left(x_f,t;x_i,0\right)$ we know the amplitude to go from any state to any other one. Indeed, inserting complete sets of position eigenstates we find that

$$\left\langle \psi_f\right| e^{-iHt/\hbar}\left|\psi_i\right\rangle = \int dx_i dx_f \psi_f^*\left(x_f\right)\psi_i\left(x_i\right)\left\langle x_f\right| e^{-iHt}\left|x_i\right\rangle \tag{22.2}$$

Another way to see how to use $G^{>}(x_f,t;x_i,0)$ is to relate it to the retarded propagator,

$$G^{R}(x_f,t;x_i,0) \equiv -i\langle x_f|\,e^{-iHt}\,|x_i\rangle\,\theta(t) = -iG^{>}(x_f,t;x_i,0)\,\theta(t) \tag{22.3}$$

where $\theta(t)$ is the heaviside step function. Inserting a complete set of energy eigenstates, we find

$$\begin{aligned} G^{R}(x_f,t;x_i,0) &\equiv -i\sum_n \langle x_f|\,n\rangle\,e^{-iE_nt}\,\langle n\,|x_i\rangle\,\theta(t) \\ &= -i\sum_n \psi_n(x_f)\,\psi_n^*(x_i)\,e^{-iE_nt}\theta(t) \end{aligned} \tag{22.4}$$

As we saw before, the Fourier transform of this quantity with η a positive real number is

$$\int_{-\infty}^{\infty} dte^{i(z+i\eta)t}G^{R}(x_f,t;x_i,0) = \sum_n \frac{\psi_n(x_f)\,\psi_n^*(x_i)}{z+i\eta-E_n}. \tag{22.5}$$

The poles of this function, as we already know, give the eigenenergies and the residues are related to the wave functions. In the many-body context, a generalization of the propagator occurs very naturally in perturbation theory.

Remark 73 *In statistical physics,* $\langle x_f|\,\rho\,|x_i\rangle$ *is a quantity of interest. Using the known form of the density matrix, we have* $\langle x_f|\,\rho\,|x_i\rangle = \langle x_f|\,e^{-\beta H}\,|x_i\rangle/Z$*. Hence, computing these matrix elements is like computing the propagator in imaginary time* τ *with the substitution* $t \rightarrow -i\tau$*. This analogy holds also in the many-body context. The density matrix is much better behaved in numerical evaluations of the path integral than the equivalent in real time because it does not have unpleasant oscillations as a function of time.*

22.2 Computing the propagator with the path integral

In general, H contains non-commuting pieces. The potential energy V is diagonal in position space, but the kinetic energy K is diagonal in momentum space. Hence, computing the action of e^{-iHt} on $|x_i\rangle$ is non-trivial since we need to diagonalize the Hamiltonian to compute the value of the exponential of an operator and that Hamiltonian contains two non-commuting pieces that are diagonal in different basis. The key observation is that if the time interval t is very small, say ε, then the error that we do in writing the exponential as a product of exponentials is of order ε^2 since it depends on the commutator of $K\varepsilon$ with $V\varepsilon$

$$e^{-iH\varepsilon} \sim e^{-iK\varepsilon}e^{-iV\varepsilon} + O\left(\varepsilon^2\right). \tag{22.6}$$

In fact the error of order ε^2 is in the argument of the exponential, as one can see from the Baker-Campbell-Hausdorff formula $e^Ae^B = e^M$ with

$$M = A + B + \frac{1}{2}[A,B] + a_2[A,[A,B]] + \ldots \tag{22.7}$$

In numerical calculations it is important to keep the exponential form since this garantees unitarity.

Other factorizations give errors of even higher order. For example,

$$e^{-iH\varepsilon} \sim e^{-iV\varepsilon/2}e^{-iK\varepsilon}e^{-iV\varepsilon/2} \tag{22.8}$$

gives an error of order ε^3. In practice, for numerical simulations it is quite useful to use factorizations that lead to higher order errors. To continue analytically however, the simplest factorization suffices.

In the factorized form, we can take advantage of the fact that we can introduce complete sets of states where the various pieces of the Hamiltonian are diagonal to compute the propagator for an infinitesimal time

$$\begin{aligned} \langle x_f| e^{-iK\varepsilon}e^{-iV\varepsilon} |x_i\rangle &= \int \frac{dp}{2\pi} \langle x_f| e^{-iK\varepsilon} |p\rangle \langle p| e^{-iV\varepsilon} |x_i\rangle & (22.9) \\ &= \int \frac{dp}{2\pi} e^{i\left[-\varepsilon\frac{p^2}{2m}+p(x_f-x_i)-\varepsilon V(x_i)\right]} & (22.10) \end{aligned}$$

where we used $\langle x| p\rangle = e^{ipx}$. The last formula can be rewritten

$$\int \frac{dp}{2\pi} e^{i(p\dot{x}-H)\varepsilon} \tag{22.11}$$

where

$$\dot{x} \equiv \frac{x_f - x_i}{\varepsilon}. \tag{22.12}$$

The argument of the exponential is the Lagrangian times the time interval. It thus has the units of action and is made dimensionless by dividing by the quantum of action $\hbar$ that we have set to unity.

For a finite time interval, we simply split the time evolution operator into evolution pieces that involve over an infinitesimal time interval

$$e^{-iHt} = \prod_{i=1}^{N} e^{-iH\varepsilon} \tag{22.13}$$

where $\varepsilon = t/N$. There is no approximation here. Inserting $N-1$ complete sets of states, we have

$$\begin{aligned} \langle x_f| e^{-iHt} |x_i\rangle &= \int \prod_{j=1}^{N-1} dx_j \, \langle x_f| e^{-iH\varepsilon} |x_{N-1}\rangle \langle x_{N-1}| e^{-iH\varepsilon} |x_{N-2}\rangle \langle x_2| \ldots \\ & \quad |x_1\rangle \langle x_1| e^{-iH\varepsilon} |x_i\rangle . & (22.14) \end{aligned}$$

Each of the N matrix elements can be evaluated now using the previous trick so that the propagator is given by the formally exact expression

$$\begin{aligned} \langle x_f| e^{-iHt} |x_i\rangle &= \lim_{N\to\infty} \int \prod_{j=1}^{N-1} dx_j \int \prod_{j=1}^{N} dp_j \exp\left[i\left(p_N \frac{x_f - x_{N-1}}{\varepsilon} - \frac{p_N^2}{2m} - V\left(x_{N-1}\right)\right)\varepsilon \right. \\ & +i\left(p_{N-1}\frac{x_{N-1}-x_{N-2}}{\varepsilon} - \frac{p_{N-1}^2}{2m} - V\left(x_{N-2}\right)\right)\varepsilon \\ & +\ldots \\ & \left. + \, i\left(p_1 \frac{x_1 - x_i}{\varepsilon} - \frac{p_1^2}{2m} - V\left(x_i\right)\right)\varepsilon \right] & (22.15) \end{aligned}$$

To do the calculation, this is what one has to do. Formally however, the final expression is quite nice. It can be written as a path integral in phase space

$$\begin{aligned} \langle x_f| e^{-iHt} |x_i\rangle &= \int [DxDp] \exp\left\{ i\int dt \left[p\dot{x} - H\left(p,x\right)\right]\right\} & (22.16) \\ &= \int [DxDp] \exp iS\left(x,p\right) & (22.17) \end{aligned}$$

where the definition of the measure $[DxDp]$ is clear by comparison and where S is the action.

It is more natural to work in configuration space where the Lagrangian is normally defined. This comes out automatically by doing the integral over all the intermediate momenta. They can be done exactly since they are all Gaussian integrals that are easily obtained by completing the square

$$\begin{aligned}\int \frac{dp}{2\pi} \exp i \left(p_{N-1} \frac{x_{N-1} - x_{N-2}}{\varepsilon} - \frac{p_{N-1}^2}{2m} \right) \varepsilon &= \sqrt{\frac{m}{2\pi i \varepsilon}} \exp \left[\frac{im}{2} \left(\frac{x_{N-1} - x_{N-2}}{\varepsilon} \right)^2 \varepsilon \right] \\ &= \sqrt{\frac{m}{2\pi i \varepsilon}} \exp \left[\frac{im}{2} \dot{x}_{N-1}^2 \varepsilon \right]. \qquad (22.18)\end{aligned}$$

Remark 74 *The above is the propagator for a free particle. In that case, the time interval could be arbitrary and the result could also be obtained using our earlier decomposition on energy eigenstates since*

$$\sum_n \phi_n (x_f) \phi_n^* (x_i) e^{-iE_n t} = \int \frac{dp}{2\pi} e^{ip(x_f - x_i) - it\frac{p^2}{2m}}. \qquad (22.19)$$

Once the integrals over momenta have been done, we are left with

$$\begin{aligned}\langle x_f | e^{-iHt} | x_i \rangle &= \lim_{N\to\infty} \int \prod_{j=1}^{N-1} dx_j \left(\sqrt{\frac{mN}{2\pi i t}} \right)^N \exp \left[i\varepsilon \left(\frac{m}{2} \left(\frac{x_f - x_{N-1}}{\varepsilon} \right)^2 - V(x_{N-1}) \right) \right. \\ &\quad + i\varepsilon \left(\frac{m}{2} \left(\frac{x_{N-1} - x_{N-2}}{\varepsilon} \right)^2 - V(x_{N-2}) \right) \\ &\quad + \dots \\ &\quad \left. + \, i\varepsilon \left(\frac{m}{2} \left(\frac{x_1 - x_i}{\varepsilon} \right)^2 - V(x_i) \right) \right] \qquad (22.20) \\ &= \int_{x_i}^{x_f} Dx \exp \left(i \int_0^t dt' \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) \right) = \int_{x_i}^{x_f} Dx e^{iS(\dot{x}, x)} \qquad (22.21)\end{aligned}$$

where the formal expression makes clear only that it is the integral of the Lagrangian, hence the action, that comes in the argument of the exponential. The integration measure here is different from the one we had before. This form is particularly useful for statistical physics where all the integrals are clearly convergent, as opposed to the present case where they oscillate rapidly and do not always have a clear meaning.

The physical interpretation of this result is quite interesting. It says that the amplitude for going from one point to another in a given time is given by the sum amplitydes for all possible ways of going between these two points in the given time, each path, or trajectory, being weighted by an exponential whose phase is the classical action measured in units of the action quantum $\hbar$.

Remark 75 *Classical limit: The classical limit is obtained when the action is large compared with the quantum of action. Indeed, in that case the integral can be evaluated in the stationary phase approximation. In that approximation, one expands the action to quadratic order around the trajectory that minimizes the action. That trajectory, given by the Euler-Lagrange equation, is the classical trajectory according to the principle of least action. By including gaussian fluctuations around the classical trajectory, one includes a first set of quantum corrections.*

Remark 76 *The exponentials in the path integral are time-ordered, i.e. the ones corresponding to later times are always to the left of those with earlier times. This time-ordering feature will be very relevant later for Green functions.*

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Part IV

The one-particle Green's function at finite temperature

In the many-body context we need to find a generalization of the Green's function that will reduce to that found for the one-body Schrödinger equation in the appropriate limit. This object comes in naturally from two perspectives. From the experimental point a view, a photoemission experiment probes the Green's function in the same way that our scattering experiment at the very beginning probed the density-density correlation function. Just from an experimental point of view then, it is important to define that quantity. From the theoretical point of view, any quantum mechanical calculation of a correlation function involves the Green's function as an intermediate step. That is one more reason to want to know more about it.

We will begin with a brief recall of second quantization and then move on to show that to predict the results of a photoemission experiment, we need a Green's function. We will establish the correspondance with the Green's function we already know. When there are interactions, one needs perturbation theory to treat the problem. Time-ordered products will come in naturally in that context. Such time-ordered products motivate the definition of the Matsubara Green's function at finite temperature. The finite temperature formalism is more general and not more difficult than the zero-temperature one. We will once more spend some time on the interpretation of the spectral weight, develop some formulas for working with the Fourier series representation of the imaginary time functions (Matsubara frequencies). This should put us in a good position to start doing perturbation theory, which is all based on Wick's theorem. Hence, we will spend some time proving this theorem as well as the very general linked-cluster theorem that is very useful in practice.

23. MAIN RESULTS FROM SECOND QUANTIZATION

When there is more than one particle and they are identical, the wave function say $\psi(x_1, x_2, x_3)$ is not arbitrary. If we want particles to be indistinguishable, all coordinates should be equivalent. This means in particular that if x_1 takes any particular value, say a and x_2 takes another value, say b, then we expect that $\psi(a, b, x_3) = \psi(b, a, x_3)$. But that is not the only possibility since the only thing we know for sure is that if we exchange twice the coordinates of two particles then we should return to the same wave function. This means that under one permutation of two coordinates (exchange), the wave function can not only stay invariant, or have an eigenvalue of $+1$ as in the example we just gave, it can also have an eigenvalue of -1. These two cases are clearly the only possibilities and they correspond respectively to bosons and fermions. There are more possibilities in two dimensions, but that is beyond the scope of this chapter.

When dealing with many identical particles, a basis of single-particle states is most convenient. Given what we just said however, it is clear that a simple direct product such as $|\alpha_1\rangle \otimes |\alpha_2\rangle$ cannot be used without further care because many-particle states must be symmetrized or antisymmetrized depending on whether we deal with Bosons or Fermions. For example, for two fermions an acceptable wave function would have the form $\sqrt{2}^{-1} \langle \mathbf{r}_1| \otimes \langle \mathbf{r}_2| \left[|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle\right]$. Second quantization allows us to take into account these symmetry or antisymmetry properties in a straightforward fashion. To take matrix elements directly between wave functions would be very cumbersome.

The single-particle basis state is a complete basis that is used most often. Note however that a simple wave-function such as

$$\psi(x, y) = (x - y) N e^{-|x-y|/a} \tag{23.1}$$

for two electrons in one dimension, with N and a constants, is a perfectly acceptable antisymmetric wave function. To expand it in a single-particle basis state however requires a sum over many (in general an infinite number of) antisymmetrized one-particle states. There are cases, such as the quantum Hall effect, where working directly with wave functions is desirable, but for our purposes this is not so.

23.1 Fock space, creation and annihilation operators

As is often the case in mathematics, working in a space that is larger than the one we are interested in may simplify matters. Think of the use of functions of a complex variable to do integrals on the real axis. Here we are interested most of the time in Hamiltonians that conserve the number of particles. Nevertheless, it is easier to work in a space that contains an arbitrary number of particles. That is Fock space. Annihilation and creation operators allow us to change the number of particles while preservin indistinguishability and antisymmetry. In this representation, a three electron state comes out as three excitations of the same vacuum state $|0\rangle$, a rather satisfactory state of affairs.

It will be very helpful if you review creation-annihilation operators, also called ladder operators, in the context of the harmonic oscillator.

23.1.1 Creation-annihilation operators for fermion wave functions

For the time being our fermions are spinless, it will be easy to add spin later on. We assume that the one-particle states $|\alpha_i\rangle$ form an orthonormal basis for one particle, namely $\langle\alpha_i|\,\alpha_j\rangle = \delta_{i,j}$. The state $|\alpha_1\alpha_2\rangle$ has particle 1 in state α_1 and particle 2 in state α_2. If we write $|\alpha_2\alpha_1\rangle$ then particle 1 is in state α_2 and particle 2 in state α_1. Antisymmetry means that $|\alpha_1\alpha_2\rangle = -|\alpha_2\alpha_1\rangle$.

We define a vaccum $|0\rangle$ that contains no particle. Then, we define $a^\dagger_{\alpha_1}$ that creates a particle from the vacuum to put it in state $|\alpha_1\rangle$ and for fermions it antisymmetrizes that state will all others. In other words, $a^\dagger_{\alpha_1}|0\rangle = |\alpha_1\rangle$. Up to now, there is nothing to antisymmetrize with, but if we add another particle, $a^\dagger_{\alpha_2}|\alpha_1\rangle = |\alpha_2\alpha_1\rangle = a^\dagger_{\alpha_2}a^\dagger_{\alpha_1}|0\rangle$, then that state has to be antisymmetric. In other words, we need to have $|\alpha_2\alpha_1\rangle = -|\alpha_1\alpha_2\rangle$. Clearly this will automatically be the case if we impose that the creation operators anticommute, i.e. $a^\dagger_{\alpha_i}a^\dagger_{\alpha_j} = -a^\dagger_{\alpha_j}a^\dagger_{\alpha_i}$ or

$$\left\{a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \equiv a^\dagger_{\alpha_i}a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j}a^\dagger_{\alpha_i} = 0. \tag{23.2}$$

This property is a property of the operators, independently of the specific state they act on. The anticommutation property garantees the Pauli principle as we know it since if $i = j$ then the above leads to

$$a^\dagger_{\alpha_i}a^\dagger_{\alpha_i} = -a^\dagger_{\alpha_i}a^\dagger_{\alpha_i}. \tag{23.3}$$

The only operator that is equal to minus itself is zero. Hence we cannot create two particles in the same state.

That same anticommutation property will automatically be satisfied by the adjoint operators

$$\left\{a_{\alpha_i}, a_{\alpha_j}\right\} \equiv a_{\alpha_i}a_{\alpha_j} + a_{\alpha_j}a_{\alpha_i} = 0. \tag{23.4}$$

These adjoint operators are defined as follows

$$\langle\alpha_1| = \langle 0|\, a_{\alpha_1}. \tag{23.5}$$

The create and antisymmetrize in bras instead of kets. When the destruction operators act on kets instead of bras, they remove a particle instead of adding it. In particular,

$$a_{\alpha_1}|0\rangle = 0. \tag{23.6}$$

This is consistent with $\langle\alpha_1|\,0\rangle = 0 = \langle 0|\,a_{\alpha_1}|0\rangle$.

Since we also want states to be normalized, we need

$$\langle\alpha_i|\,\alpha_j\rangle = \langle 0|\,a_{\alpha_i}a^\dagger_{\alpha_j}|0\rangle = \delta_{i,j}. \tag{23.7}$$

Since we already know that $a_{\alpha_1}|0\rangle = 0$, that will automatically be satisfied if we write the following anticommutation realtion between creation and annihilation operators

$$\left\{a_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \equiv a_{\alpha_i}a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j}a_{\alpha_i} = \delta_{i,j} \tag{23.8}$$

because then $\langle 0| a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = -\langle 0| a^\dagger_{\alpha_j} a_{\alpha_i} |0\rangle + \langle 0| \delta_{i,j} |0\rangle = 0 + \delta_{i,j}$. The above thress sets of anticommutation relations are called canonical.

At this point one may ask why anticommutation instead of commutation. Well, two reasons. The first one is that given the previous anticommutation rules, this one seems elegant. The second one is that with this rule, we can define the very useful operator, the number operator

$$\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{23.9}$$

That operator just counts the number of particles in state α_i. To see that this is so and that anticommutation is needed for this to work, we look at a few simple cases. First note that if $\widehat{n}_{\alpha_i}$ acts on a state where α_i is not occupied, then

$$\widehat{n}_{\alpha_i} |\alpha_j\rangle = \widehat{n}_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_j} |0\rangle = -a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_i} |0\rangle = 0. \tag{23.10}$$

If I build an arbitrary many-particle state $|\alpha_j, \alpha_k, \ldots\rangle$, if the state α_i does not appear in the list, then when I compute $\widehat{n}_{\alpha_i} |\alpha_j, \alpha_k, \ldots\rangle$, I will be able to anticommute the destruction operator all the way to the vacuum and obtain zero. On the other hand, if α_i appears in the list then

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots \widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle . \tag{23.11}$$

I have been able to move the operator all the way to the indicated position without any additional minus sign because both the destruction and the annihilation operators anticommute with the creation operators that do not have the same labels. The minus signs from the creation and from the annihilation operators in $a^\dagger_{\alpha_i} a_{\alpha_i}$ cancel each other. Now, let us focus on $\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i}$ in the last equation. Using our anticommutation properties, one can check that

$$\widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i} \left(1 - a^\dagger_{\alpha_i} a_{\alpha_i} \right). \tag{23.12}$$

Since there are never two fermions in the same state, now the destruction operator in the above equation is free to move and annihilate the vacuum state, and

$$\widehat{n}_{\alpha_i} \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right) = \left(a^\dagger_{\alpha_j} a^\dagger_{\alpha_k} \ldots a^\dagger_{\alpha_i} \ldots a^\dagger_{\alpha_l} |0\rangle \right). \tag{23.13}$$

This means that $\widehat{n}_{\alpha_i}$ does simply count the number of particles. It gives one or zero depending on whether the state is occupied or not.

One last thing with fermions. If we want the whole formalism to make sense, we want to have a change sign to occur whenever we interchange two fermions, wherever they are in the list. In other words, we want $|\alpha_i \alpha_j \ldots \alpha_k \ldots \alpha_l \ldots \alpha_m\rangle = -|\alpha_i \alpha_j \ldots \alpha_l \ldots \alpha_k \ldots \alpha_m\rangle$. To see that our formalism works, you can write the state to the left in terms of creation operators on the vacuum and convince yourself by a series of pairwise interchange of operators that you will recover the state to the right with the proper sign, wherever α_k and α_l are in the list of operators. With fermions we need to determine an initial order of operators. That is totally arbitrary because of the phase arbitrariness of quantum mechanics. But then, during the calculations we need to keep track of the minus signs.

23.1.2 Creation-annihilation operators for boson wave functions

In the case of bosons, the state must be symmetric. Following Negele and Orland[1] we introduce the symmetrized many-body state

$$|\alpha_1 \alpha_2 ... \alpha_N\} . \tag{23.14}$$

The state is not normalized at this point, which explains the unusual notation. The state is symmetric means that $|\alpha_1\alpha_2\} = |\alpha_2\alpha_1\} = a^\dagger_{\alpha_2} a^\dagger_{\alpha_1} |0\rangle$. Hence in this case, the creation operators and their corresponding annihilation operators must commute:

$$\left[a^\dagger_{\alpha_i}, a^\dagger_{\alpha_j}\right] \equiv a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} - a^\dagger_{\alpha_j} a^\dagger_{\alpha_i} = 0 \tag{23.15}$$

$$\left[a_{\alpha_i}, a_{\alpha_j}\right] \equiv a_{\alpha_i} a_{\alpha_j} - a_{\alpha_j} a_{\alpha_i} = 0. \tag{23.16}$$

This time there is no Pauli principle. Several particles can occupy the same state. So what happens when we exchange creation and annihilation operators. By analogy with the fermions, it is natural to expect that they must commute, namely

$$\left[a_{\alpha_i}, a^\dagger_{\alpha_j}\right] \equiv a_{\alpha_i} a^\dagger_{\alpha_j} - a^\dagger_{\alpha_j} a_{\alpha_i} = \delta_{i,j} \tag{23.17}$$

The above set of commutation relations is called canonical. The same considerations as before tell us that annihilation operators destroy the vacuum.

And again the number operator is defined by

$$\widehat{n}_{\alpha_i} = a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{23.18}$$

Why is that true? If the state α_i is unoccupied or occupied only once, one can check the effect of the operator $\widehat{n}_{\alpha_i}$ the same way we did it for fermions. And note that when there are many other particles around, one must take commutation and not anticommutation between creation and annihilation operators to make sure that the many-particle state is an eigenstate of $\widehat{n}_{\alpha_i}$ with eigenvalue unity when a single state is occupied.

What happens if the same state is occupied multiple times? Then,

$$\begin{aligned} \widehat{n}_{\alpha_i} a^\dagger_{\alpha_i} &= a^\dagger_{\alpha_i} a_{\alpha_i} a^\dagger_{\alpha_i} = a^\dagger_{\alpha_i}\left(1 + a^\dagger_{\alpha_i} a_{\alpha_i}\right) & (23.19)\\ &= a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i}\widehat{n}_{\alpha_i}. & (23.20)\end{aligned}$$

The destruction operator in $\widehat{n}_{\alpha_i}$ will not be able to complete its jurney to the vacuum to annihilate it. Every time it encounters an operator $a^\dagger_{\alpha_i}$ it leaves it behind and adds a new term $a^\dagger_{\alpha_i}\widehat{n}_{\alpha_i}$ just like above. Once we have done that repeatedly, the desturction operator accomplishes its task and we are left with n_{α_i} times the original state, where n_{α_i} is the number of times the label α_i appeared in the list. So $\widehat{n}_{\alpha_i}$ really has the meaning of a number operator, i.e. an operator that counts the number of times a given label appears in a many-body state. All that we are left to do is normalize the symmetrized state.

23.1.3 Number operator and normalization

To fix the normalization in the case of bosons, it suffices to consider a single state that can be multiply occupied and then to generalize. Let us drop then all indices and ask how the state $\left(a^\dagger\right)^n |0\rangle$ can be normalized. First, notice that Eq.(23.12) above can be written as

$$\left[\widehat{n}, a^\dagger\right] = a^\dagger \tag{23.21}$$

By the way, using the fact that $\left(a^\dagger\right)^2 = 0$ on the right-hand side of Eq.(23.12) we see that the latter equation is true for fermions as well. Taking the adjoint of the above equation we find

$$\left[\widehat{n}, a\right] = -a \tag{23.22}$$

We can now use a very useful theorem that is trivial to prove. We will call it the theorem on commutators of ladder operators.

Theorem 9 *Let* $|n\rangle$ *be an eigenstate of* $\widehat{n}$ *with eigenvalue* n*. If* $\left[\widehat{n},a^\dagger\right]=Ba^\dagger$ *with* B *a real or complex number, then* $a^\dagger|n\rangle$ *is an eigenstate of* $\widehat{n}$ *with eigenvalue* $n+B$*.*

Proof: $\left[\widehat{n},a^\dagger\right]|n\rangle=\widehat{n}\left(a^\dagger|n\rangle\right)-a^\dagger n|n\rangle=Ba^\dagger|n\rangle$, so that $\widehat{n}\left(a^\dagger|n\rangle\right)=(n+B)\left(a^\dagger|n\rangle\right)$ Q.E.D.

Using this theorem with our result for the commutator of the number operator with the creation operator Eq.(23.21) we have that $\widehat{n}\left(a^\dagger|n\rangle\right)=(n+1)\left(a^\dagger|n\rangle\right)$ hence $a^\dagger|n\rangle=C|n+1\rangle$. Assuming that $|n\rangle$ and $|n+1\rangle$ are normalized we can find the normalization constant as follows

$$\begin{aligned}\langle n|aa^\dagger|n\rangle &= |C|^2\langle n+1\,|n+1\rangle=|C|^2\\ &= \langle n|1+a^\dagger a|n\rangle=(n+1)\langle n\,|n\rangle=(n+1)\,. \end{aligned}\tag{23.23}$$

We are free to choose the phase real so that $C=\sqrt{n+1}$.We thus have recursively

$$\begin{aligned}a^\dagger|0\rangle &= |1\rangle\\ \left(a^\dagger\right)^2|0\rangle &= \sqrt{2}\,|2\rangle\\ \left(a^\dagger\right)^3|0\rangle &= \sqrt{3}\sqrt{2}\,|3\rangle\end{aligned}\tag{23.24}$$

and

$$|n\rangle=\frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|0\rangle\,.\tag{23.25}$$

From this we conclude that for a general many-body state,

$$|\alpha_i\alpha_j...\alpha_m\rangle=\frac{1}{\sqrt{\prod_i n_{\alpha_i}!}}\,|\alpha_i\alpha_j...\alpha_m\}=\frac{1}{\sqrt{\prod_i n_{\alpha_i}!}}a^\dagger_{\alpha_i}a^\dagger_{\alpha_j}\dots a^\dagger_{\alpha_m}|0\rangle\tag{23.26}$$

where the product in the denominator is over the indices that label the occupied one-particle states and n_{α_i} counts the number of times a given one-particle state appears.

Remark 77 *Since with fermions a state is occupied only once, we did not need to worry about the* $n_{\alpha_i}!$*.*

Remark 78 *By recalling the theorem proven in this section, it is also easy to remember that* $\left[\widehat{n},a^\dagger\right]=a^\dagger$ *and* $[\widehat{n},a]=-a$*,*

23.1.4 Wave function

With N-particles, the wave function

$$\langle\mathbf{r}_1\mathbf{r}_2...\mathbf{r}_N|\,\alpha_1\alpha_2...\alpha_N\rangle\tag{23.27}$$

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

23.2 Change of basis

Creation-annihilation operators change basis in a way that is completely determined by the way one changes basis in single-particle states. Suppose one wants to change from the α basis to the μ basis, namely

$$\left|\mu_m\right\rangle = \sum_i \left|\alpha_i\right\rangle \left\langle\alpha_i\right| \left.\mu_m\right\rangle \tag{23.28}$$

which is found by inserting the completeness relation. Let creation operator $a^\dagger_{\alpha_i}$ create single particle state $\left|\alpha_i\right\rangle$ and antisymmetrize while creation operator $c^\dagger_{\mu_m}$ creates single particle state $\left|\mu_m\right\rangle$ and antisymmetrize. Then the correspondance between both sets of operators is clearly

$$c^\dagger_{\mu_m} = \sum_i a^\dagger_{\alpha_i} \left\langle\alpha_i\right| \left.\mu_m\right\rangle \tag{23.29}$$

with the adjoint

$$c_{\mu_m} = \sum_i \left\langle\mu_m\right| \left.\alpha_i\right\rangle a_{\alpha_i} \tag{23.30}$$

given as usual that $\left\langle\alpha_i\right| \left.\mu_m\right\rangle = \left\langle\mu_m\right| \left.\alpha_i\right\rangle^*$. Physically then, creating a particle in a state $\left|\mu_m\right\rangle$ is like creating it in a linear combination of states $\left|\alpha_i\right\rangle$. We can do the change of basis in the other direction as well.

Since we have defined new creation annihilation operators, it is quite natural to ask what are their commutation or anticommutation relations. It is easy to find using the change of basis formula and the completeness relation. Assuming that the cration-annihilation operators are for fermions, we find

$$\begin{aligned}
\left\{c_{\mu_m}, c^\dagger_{\mu_n}\right\} &= \sum_i \sum_j \left\langle\mu_m\right| \left.\alpha_i\right\rangle \left\{a_{\alpha_i}, a^\dagger_{\alpha_j}\right\} \left\langle\alpha_j\right| \left.\mu_n\right\rangle && (23.31)\\
&= \sum_i \sum_j \left\langle\mu_m\right| \left.\alpha_i\right\rangle \delta_{i,j} \left\langle\alpha_j\right| \left.\mu_n\right\rangle && (23.32)\\
&= \sum_i \left\langle\mu_m\right| \left.\alpha_i\right\rangle \left\langle\alpha_i\right| \left.\mu_n\right\rangle = \left\langle\mu_m\right| \left.\mu_n\right\rangle . && (23.33)
\end{aligned}$$

Hence, if the transformation between basis is unitary, the new operators, obey canonical anticommutation relations, namely

$$\left\{c_{\mu_m}, c^\dagger_{\mu_n}\right\} = \delta_{m,n}. \tag{23.34}$$

When the change of basis is unitary, we say that we have made a canonical transformation. The same steps show that a unitary basis change also preserves the canonical commutation relations for bosons.

23.2.1 The position and momentum space basis

We use this strange, but commonly used, basis where we take continuum notation for space and discrete notation for momentum. Then, we have the conventions

$$\sum_{\mathbf{k}} \left|\mathbf{k}\right\rangle \left\langle\mathbf{k}\right| = 1 = \int d\mathbf{r} \left|\mathbf{r}\right\rangle \left\langle\mathbf{r}\right|$$

$$\langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{23.35}$$

$$\langle \mathbf{k} | \mathbf{r} \rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{23.36}$$

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

$$\langle \mathbf{r} | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}') \tag{23.37}$$

$$\langle \mathbf{k} | \mathbf{k}' \rangle = \int d\mathbf{r} \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k}' \rangle = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')} = \delta_{\mathbf{k},\mathbf{k}'} \tag{23.38}$$

Creation operators in eigenstates of position are usually denoted, $\psi^\dagger(\mathbf{r})$, while creation operators in eigenstates of momentum are denoted $c^\dagger_{\mathbf{k}}$. The basis change between them leads to

$$\psi^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} \langle \mathbf{k} | \mathbf{r} \rangle = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{23.39}$$

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle c_{\mathbf{k}} = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}}. \tag{23.40}$$

Given our above convention, the momentum operators obey the algebra of a discrete set of creation operators. Taking fermions as an example, then we have

$$\boxed{\left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = \delta_{\mathbf{k},\mathbf{k}'} \quad ; \quad \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = \left\{c^\dagger_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} = 0} \tag{23.41}$$

while the position space creation-annihilation operators obey

$$\boxed{\left\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = \textstyle\sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle \mathbf{r} | \mathbf{k} \rangle \left\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\right\} \langle \mathbf{k}' | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r}-\mathbf{r}')} \tag{23.42}$$

$$\boxed{\{\psi(\mathbf{r}), \psi(\mathbf{r}')\} = \left\{\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right\} = 0} \tag{23.43a}$$

23.3 One-body operators

The matrix elements of an arbitrary one-body operator $\widehat{U}$ (in the $N-$particle case) may be computed in the many-body basis made of one-body states where $\widehat{U}$ is diagonal. As an example of one-body operator, the operator $\widehat{U}$ could be an external potential so that the diagonal basis is position space. In the diagonal basis,

$$\widehat{U} |\alpha_i\rangle = U_{\alpha_i} |\alpha_i\rangle = \langle \alpha_i | \widehat{U} | \alpha_i \rangle |\alpha_i\rangle \tag{23.44}$$

where U_{α_i} is the eigenvalue. In this basis, one sees that the effect of the one-body operator is to produce the same eigenvalue, whatever the particular order of the states on which the first-quantized operator acts. For example, suppose we have three particles in an external potential, then the potential energy operator is

$$V(\mathbf{R}_1) + V(\mathbf{R}_2) + V(\mathbf{R}_3) \tag{23.45}$$

where $\mathbf{R}_i$ acts on the i^{th} position of the many body state. If this state is not symmetrized or antisymmetrized, then for example

$$\left(V\left(\mathbf{R}_1\right)+V\left(\mathbf{R}_2\right)+V\left(\mathbf{R}_3\right)\right)\left|\mathbf{r}'\right\rangle\otimes\left|\mathbf{r}\right\rangle\otimes\left|\mathbf{r}''\right\rangle=\left(V\left(\mathbf{r}'\right)+V\left(\mathbf{r}\right)+V\left(\mathbf{r}''\right)\right)\left|\mathbf{r}'\right\rangle\otimes\left|\mathbf{r}\right\rangle\otimes\left|\mathbf{r}''\right\rangle . \tag{23.46}$$

If that operator $V\left(\mathbf{R}_1\right)+V\left(\mathbf{R}_2\right)+V\left(\mathbf{R}_3\right)$ had acted on onother ordering such as $\left|\mathbf{r}\right\rangle\otimes\left|\mathbf{r}''\right\rangle\otimes\left|\mathbf{r}'\right\rangle$, the eigenvalue would have been identical, $V\left(\mathbf{r}\right)+V\left(\mathbf{r}''\right)+V\left(\mathbf{r}'\right)$. This means that if we act on a symmetrized or antisymmetrized version of that state, then

$$\left(V\left(\mathbf{R}_1\right)+V\left(\mathbf{R}_2\right)+V\left(\mathbf{R}_3\right)\right)\left|\mathbf{r}',\mathbf{r},\mathbf{r}''\right\rangle=\left(V\left(\mathbf{r}'\right)+V\left(\mathbf{r}\right)+V\left(\mathbf{r}''\right)\right)\left|\mathbf{r}',\mathbf{r},\mathbf{r}''\right\rangle \tag{23.47}$$

In general then when we have N particles in a many-body state, the action of the one-body operator is

$$\sum_{\mu=1}^{N}\widehat{U}_{\mu}\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle=\left(U_{\alpha_i}+U_{\alpha_j}+U_{\alpha_k}+\ldots\right)\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle \tag{23.48}$$

Knowing the action of the number operator, we can write the same result differently

$$\sum_{\mu=1}^{N}\widehat{U}_{\mu}\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle=\sum_m U_{\alpha_m}\widehat{n}_{\alpha_m}\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle \tag{23.49}$$

in other words, there will be a contribution as long as α_i appears in the state. And if α_i occurs more than once, the corresponding eigenvalue U_{α_i} will appear more than once.

We hold a very elegant result. The one-body operator $\sum_m U_{\alpha_m}\widehat{n}_{\alpha_m}$ in second quantized notation makes no reference to the total number of particles nor to whether we are dealing with bosons of fermions. Note that in first quantization the sum extends over all particle coordinates whereas in second quantization the sum over m extends over all *states*.

Using the change of basis formula explained above, we have that

$$\sum_i\left\langle\alpha_i\right|U\left|\alpha_i\right\rangle a_{\alpha_i}^{\dagger}a_{\alpha_i}=\sum_i\sum_m\sum_n c_{\mu_m}^{\dagger}\left\langle\mu_m\right.\left|\alpha_i\right\rangle\left\langle\alpha_i\right|U\left|\alpha_i\right\rangle\left\langle\alpha_i\right.\left|\mu_n\right\rangle c_{\mu_n}. \tag{23.50}$$

Since U is diagonal, we can add a sum over α_j and use the closure relation to arrive at the final result

$$\boxed{\sum_i U_{\alpha_i}\widehat{n}_{\alpha_i}=\sum_m\sum_n c_{\mu_m}^{\dagger}\left\langle\mu_m\right|U\left|\mu_n\right\rangle c_{\mu_n}.} \tag{23.51}$$

Let us give examples in the position and momentum representation. A one-body scattering potential in the continuum would be represented by

$$\boxed{\widehat{U}=\int d\mathbf{r}U\left(\mathbf{r}\right)\psi^{\dagger}\left(\mathbf{r}\right)\psi\left(\mathbf{r}\right)} \tag{23.52}$$

which looks similar to the usual Schrödinger average. Similarly, the kinetic energy operator in the momentum representation becomes

$$\widehat{T}=\sum_{\mathbf{k}}\left\langle\mathbf{k}\right|\frac{k^2}{2m}\left|\mathbf{k}\right\rangle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}=\sum_{\mathbf{k}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)\left\langle\mathbf{r}\right.\left|\mathbf{k}\right\rangle\left\langle\mathbf{k}\right|\frac{k^2}{2m}\left|\mathbf{k}\right\rangle\left\langle\mathbf{k}\right.\left|\mathbf{r}'\right\rangle\psi\left(\mathbf{r}'\right) \tag{23.53}$$

$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)e^{i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\frac{k^2}{2m}\psi\left(\mathbf{r}'\right) \tag{23.54}$$

$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\int d\mathbf{r}\int d\mathbf{r}'\psi^{\dagger}\left(\mathbf{r}\right)\left(-\frac{1}{2m}\nabla^2\right)e^{i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\psi\left(\mathbf{r}'\right). \tag{23.55}$$

Performing the $\mathbf{k}$ summation and using partial integration assuming that everything vanishes at infinity or is periodic, we obtain,

$$\boxed{\widehat{T} = \left(-\frac{1}{2m}\right)\int d\mathbf{r}\psi^{\dagger}(\mathbf{r})\left(\nabla^{2}\psi(\mathbf{r})\right) = \frac{1}{2m}\int d\mathbf{r}\boldsymbol{\nabla}\psi^{\dagger}(\mathbf{r})\cdot\nabla\psi(\mathbf{r})}. \tag{23.56}$$

Again notice that second-quantized operators look like simple Schrödinger averages over wave functions.

23.4 Two-body operators.

A two-body operator involves the coordinates of two particles. An example is the Coulomb potential. If we let the indices in $\widehat{V}_{1,2}$ refer to the potential energy between the first and second particles in the direct product, and if we are in the diagonal basis, we have that

$$\widehat{V}_{1,2}\left|\alpha_i\right\rangle \otimes \left|\alpha_j\right\rangle = V_{\alpha_i\alpha_j}\left|\alpha_i\right\rangle \otimes \left|\alpha_j\right\rangle. \tag{23.57}$$

In this basis, one sees that again the eigenvalue does not depend on the order in which the states are when the first-quantized operator acts. This means that

$$\frac{1}{2}\sum_{\mu=1}^{N}\sum_{\substack{\nu=1\\ \nu\neq\mu}}^{N}\widehat{V}_{\mu,\nu}\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle = \frac{1}{2}\left(V_{\alpha_i\alpha_j}+V_{\alpha_i\alpha_k}+V_{\alpha_j\alpha_k}+\ldots\right)\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle \tag{23.58}$$

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,

$$\frac{1}{2}\sum_{\mu=1}^{N}\sum_{\substack{\nu=1\\ \nu\neq\mu}}^{N}\widehat{V}_{\mu,\nu}\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle = \frac{1}{2}\sum_{i}\sum_{j}V_{\alpha_i\alpha_j}\left(\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j}-\delta_{i,j}\widehat{n}_{\alpha_i}\right)\left|\alpha_i,\alpha_j,\alpha_k\ldots\right\rangle. \tag{23.59}$$

Again the expression to the right is independent of the state it acts on. It is valid in general.

We can simplify the expression further. Defining

$$\boxed{\zeta = -1 \quad \text{for} \quad \text{fermions}} \tag{23.60}$$

$$\boxed{\zeta = 1 \quad \text{for} \quad \text{bosons}} \tag{23.61}$$

we can rewrite $\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j}-\delta_{i,j}\widehat{n}_{\alpha_i}$ in terms of creation and annihilation operators in such a way that the form is valid for both fermions and bosons

$$\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j}-\delta_{i,j}\widehat{n}_{\alpha_i} = a^{\dagger}_{\alpha_i}a_{\alpha_i}a^{\dagger}_{\alpha_j}a_{\alpha_j}-\delta_{i,j}a^{\dagger}_{\alpha_i}a_{\alpha_i} = a^{\dagger}_{\alpha_i}\zeta a^{\dagger}_{\alpha_j}a_{\alpha_i}a_{\alpha_j} = a^{\dagger}_{\alpha_i}a^{\dagger}_{\alpha_j}a_{\alpha_j}a_{\alpha_i}. \tag{23.62}$$

Second quantized operators are thus written in the simple form

$$\boxed{\tfrac{1}{2}\sum_i\sum_j V_{\alpha_i\alpha_j}\left(\widehat{n}_{\alpha_i}\widehat{n}_{\alpha_j}-\delta_{i,j}\widehat{n}_{\alpha_i}\right) \equiv \tfrac{1}{2}\sum_i\sum_j \left(\alpha_i\alpha_j\right|V\left|\alpha_i\alpha_j\right) a^{\dagger}_{\alpha_i}a^{\dagger}_{\alpha_j}a_{\alpha_j}a_{\alpha_i}} \tag{23.63}$$

where

$$\left|\alpha_i\alpha_j\right) \equiv \left|\alpha_i\right\rangle \otimes \left|\alpha_j\right\rangle. \tag{23.64}$$

Under unitary transformation to an arbitrary basis we have

$$\boxed{\widehat{V}=\frac{1}{2}\sum_m\sum_n\sum_p\sum_q\left(\mu_m\mu_n\right|V\left|\mu_p\mu_q\right)c^\dagger_{\mu_m}c^\dagger_{\mu_n}c_{\mu_q}c_{\mu_p}}. \tag{23.65}$$

Definition 10 *When a series of creation and annihilation operators are placed in such an order where all destruction operators are to the right, one calls this "normal order".*

Remark 79 *Note the inversion in the order of μ_p and μ_q in the annihilation operators compared with the order in the matrix elements (This could have been for the creation operator instead).*

Remark 80 *The notation $\left(\mu_m\mu_n\right|V\left|\mu_p\mu_q\right)$ for the two-body matrix element means, in the coordinate representation for example,*

$$\int d\mathbf{r}_1 d\mathbf{r}_2\phi^*_{\mu_m}(\mathbf{r}_1)\,\phi^*_{\mu_n}(\mathbf{r}_2)\,V(\mathbf{r}_1-\mathbf{r}_2)\,\phi_{\mu_p}(\mathbf{r}_1)\,\phi_{\mu_q}(\mathbf{r}_2)\,. \tag{23.66}$$

Exemple 11 *In the case of a potential, such as the Coulomb potential, which acts on the densities, we have*

$$\boxed{\widehat{V}=\frac{1}{2}\int d\mathbf{x}\int d\mathbf{y}v\left(\mathbf{x}-\mathbf{y}\right)\psi^\dagger(\mathbf{x})\,\psi^\dagger(\mathbf{y})\,\psi(\mathbf{y})\,\psi(\mathbf{x})}. \tag{23.67}$$

23.5 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

$$\boxed{c_{\mathbf{k}}(t)=e^{i\widehat{H}t}c_{\mathbf{k}}e^{-i\widehat{H}t}\quad;\quad c^\dagger_{\mathbf{k}}(t)=e^{i\widehat{H}t}c^\dagger_{\mathbf{k}}e^{-i\widehat{H}t}} \tag{23.68}$$

It is easy to compute the time evolution in the case where the Hamiltonian is quadratic in creation and annihilation operators. Take for example

$$\widehat{H}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}}c_{\mathbf{k}} \tag{23.69}$$

The time evolution may be found from the Heisenberg equation of motion, which follows from differentiating the definition of the Heisenberg operators

$$i\frac{\partial c_{\mathbf{k}}(t)}{\partial t}=\left[c_{\mathbf{k}}(t)\,,\widehat{H}\right]. \tag{23.70}$$

To evaluate the commutator, we note that since $\widehat{H}$ commutes with itself is is time independent and

$$\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}}c_{\mathbf{k}}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}}(t)\,c_{\mathbf{k}}(t)\,.$$

To compute the commutator, we only need the equal-time commutator of the number operator $c_{\mathbf{k}}^{\dagger}(t)\, c_{\mathbf{k}}(t)$ with $c_{\mathbf{k}}(t)$, which is given by Eq.(23.22) and leads, for both fermions and bosons, to

$$i\frac{\partial c_{\mathbf{k}}(t)}{\partial t} = \left[c_{\mathbf{k}}(t), \widehat{H}\right] = \sum_{\mathbf{k}'} \epsilon_{\mathbf{k}'} \left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\, c_{\mathbf{k}'}(t)\right] = \epsilon_{\mathbf{k}} c_{\mathbf{k}}(t) \tag{23.71}$$

whose solution is

$$\boxed{c_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}}t} c_{\mathbf{k}}} \tag{23.72}$$

Taking the adjoint,

$$\boxed{c_{\mathbf{k}}^{\dagger}(t) = c_{\mathbf{k}}^{\dagger} e^{i\epsilon_{\mathbf{k}}t}}. \tag{23.73}$$

If we had been working in a basis where $\widehat{H}$ was not diagonal, then repeating the steps above,

$$i\frac{\partial a_{\alpha}(t)}{\partial t} = \left[a_{\alpha}(t), \widehat{H}\right] = \sum_{\beta,\gamma} \langle\beta|\, \widehat{H}\, |\gamma\rangle \left[a_{\alpha}(t), a_{\beta}^{\dagger}(t)\, a_{\gamma}(t)\right] = \sum_{\gamma} \langle\alpha|\, \widehat{H}\, |\gamma\rangle\, a_{\gamma}(t) \tag{23.74}$$

Commutator identities: The following are very useful identities to get equations of motions, and in general equal-time commutators.

$$[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA \tag{23.75}$$

$$\boxed{[A, BC] = [A, B]\, C + B\, [A, C]} \tag{23.76}$$

$$\boxed{[A, BC] = \{A, B\}\, C - B\, \{A, C\}} \tag{23.77}$$

The first commutator identity is familiar from elementary quantum mechanics. The last one can be memorized by noting that it behaves as if the B had anticommuted with the A.It is always easier to remember the commutator of the number operator with creation or annihilation operators, but if you need to prove it again for yourself, the above identities can be used to evaluate the needed commutator either for fermions

$$\left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\, c_{\mathbf{k}'}(t)\right] = \left\{c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\right\} c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}}(t) \tag{23.78}$$

or for bosons

$$\left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\, c_{\mathbf{k}'}(t)\right] = \left[c_{\mathbf{k}}(t), c_{\mathbf{k}'}^{\dagger}(t)\right] c_{\mathbf{k}'}(t) + 0 = \delta_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}}(t) \tag{23.79}$$

24. MOTIVATION FOR THE DEFINITION OF THE SECOND QUANTIZED GREEN'S FUNCTION G^R

Just as we showed that scattering and transport experiments measure correlation functions such as the density-density or current-current correlation function, we begin this chapter by showing that photoemission directly probes a one-particle correlation function. The last section will introduce and motivate further the definition of the second quantized Green's function.

24.1 Measuring a two-point correlation function (ARPES)

In a photoemission experiment, a photon ejects an electron from a solid. This is nothing but the old familiar photoelectric effect. In the angle resolved version of this experiment (ARPES), the energy and the direction of the outgoing electron are measured. This is illustrated in Fig.(24-1). The outgoing electron energy can be measured. Because it is a free electron, this measurement gives the value of the wave vector through $k^2/2m$. Using energy conservation, the energy of the outgoing electron is equal to the energy of the incident photon E_{ph}, minus the work function W plus the energy of the electron in the system, ω, measured relative to the Fermi level.

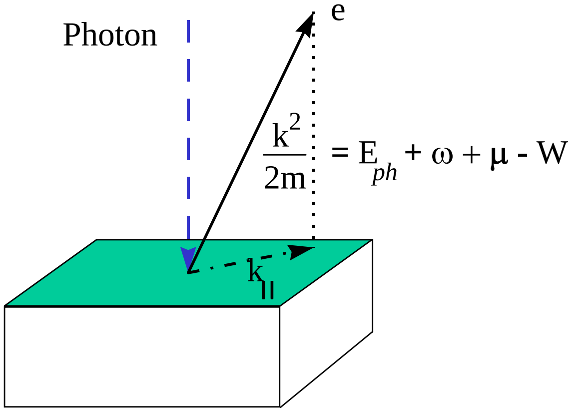

Figure 24-1 Schematic representation of an angle-resolved photoemission experiment. W is the work function.

The energy of the electron in the system ω will be mostly negative. The value of $\mathbf{k}_{||}$ may be extracted by simple geometric considerations from the value of k. Since in this experiment there is translational invariance only in the direction parallel to the plane, this means that in fact it is only the value of $\mathbf{k}_{||}$ that is conserved. Hence, it is only for layered systems that we really have access to both energy ω and total momentum $\mathbf{k}_{||}$ of the electron when it was in the system.

We can give a sketchy derivation of the calculation of the cross-section as follows. The cross-section the we will find below neglects. amongst other things, processes where energy is transferred from the outgoing electron to phonons or other excitations before it is detected (multiple scattering of outgoing electron). Such processes are referred to as "inelastic background". We start from Fermi's Golden rule. The initial state is a direct product $|m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em}$ of the state of the system $|m\rangle$, the state $|0\rangle$ with no electron far away from the detector and of the state of the elctromagnetic field that has one incoming photon $|1_{\mathbf{q}}\rangle_{em}$. The final state $|n\rangle \otimes |\mathbf{k}\rangle \otimes |0\rangle_{em}$ has the system in state $|n\rangle$ with one less electron, the detector with one electron in state $|\mathbf{k}\rangle$ and the electromagnetic field in state $|0\rangle_{em}$ with no photon. Strictly speaking, the electrons in the system should be antisymmetrized with the electrons in the detector, but when they are far enough apart and one electron is detected, we can assume that it is distinguishible from electrons in the piece of material. The coupling of matter with electromagnetic field that produces this transition from initial to final state is $\mathbf{j} \cdot \mathbf{A}$ as we saw previously. Hence, the transition rate will be proportional to the square of the following matrix element

$$
\begin{aligned}
& -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \otimes \langle 0|_{em} \mathbf{j}_{\mathbf{k}'} \cdot \mathbf{A}_{-\mathbf{k}'} |m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em} . && (24.1) \\
= \quad & -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \mathbf{j}_{\mathbf{k}'} |m\rangle \otimes |0\rangle \cdot \langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle_{em} && (24.2)
\end{aligned}
$$

The vector potential is the analog of the position operator for harmonic vibration of the electromagnetic field. Hence, it is proportionnal to $a^{\dagger}_{-\mathbf{k}'} + a_{\mathbf{k}'}$ and $\mathbf{k}' = \mathbf{q}$ with the destruction operator will lead to a non-zero value of $\langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle$. For the range of energies of interest, the wave vector of the photon $\mathbf{k}' = \mathbf{q}$ can be considered in the center of the Brillouin zone. The current operator is a one-body operator. In the continuum, it is then given by

$$
\mathbf{j}_{\mathbf{k}'=\mathbf{0}} = \frac{e}{\mathcal{V}} \sum_{\mathbf{p}} \frac{\mathbf{p}}{m} c^{\dagger}_{\mathbf{p}} c_{\mathbf{p}}. \tag{24.3}
$$

The value $\mathbf{p} = \mathbf{k}_{||}$ will lead to a non-zero matrix element. Overall then, the matrix element is

$$
-\langle n| c_{\mathbf{k}_{||}} |m\rangle \left(\langle \mathbf{k}| c^{\dagger}_{\mathbf{k}_{||}} |0\rangle \frac{e}{\mathcal{V}^2} \frac{\mathbf{k}_{||}}{m} \cdot \langle 0|_{em} \mathbf{A}_{\mathbf{k}'=\mathbf{q}\sim\mathbf{0}} |1_{\mathbf{q}}\rangle_{em} \right). \tag{24.4}
$$

The term in large parenthesis is a matrix element that does not depend on the state of the system. Without going into more details of the assumptions going into the derivation then, Fermi's golden rule suggests, (see first section of Chapter 2) that the cross section for ejecting an electron of momentum $\mathbf{k}_{||}$ and energy ω (measured with respect to μ) is proportional to

$$
\begin{aligned}
\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \quad & \propto \quad \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega + \mu - (E_m - E_n)\right) && (24.5) \\
& \propto \quad \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega - (K_m - K_n)\right) && (24.6) \\
& \propto \quad \int dt e^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle . && (24.7)
\end{aligned}
$$

In the above equations, we have measured energies with respect to the chemical potential, defining $K_m = E_m - N_m \mu$. Since there is one more particle in state

$|m\rangle$ than in state $|n\rangle$, that explains the extra chemical potential. For the last line, we have followed van Hove and used the same steps as in the corresponding derivation for the cross section for electron scattering.8 In the latter case, there was a relation between the correlation function and the spectral weight that could be established with the fluctuation dissipation theorem. We will be able to achieve the same thing below in Sec. 28.4. More specifically, we will be able to rewrite this result in terms of the spectral weight $A\left(\mathbf{k}_{||},\omega\right)$ as follows,

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\propto f\left(\omega\right)A\left(\mathbf{k}_{||},\omega\right) \tag{24.8}$$

where $f\left(\omega\right)$ is the Fermi function.

24.2 Definition of the many-body G^R and link with the previous one

When the Hamiltonian is quadratic in creation-annihilation operators, in other words when we have a one-body problem, the retarded single-particle Green's function we are about to define does reduce to the Green's function we studied in the one-body Schrödinger equation. Its actual definition is however better suited for many-body problems as we shall see in the present section.

Consider the definition we had before

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)=-i\left\langle\mathbf{r}\right|e^{-iH\left(t-t'\right)}\left|\mathbf{r}'\right\rangle\theta\left(t-t'\right). \tag{24.9}$$

Since in second-quantization the operator $\psi^\dagger\left(\mathbf{r}\right)$ creates a particle at point $\mathbf{r}$, the following definition seems natural

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)=-i\left\langle GS\right|\psi\left(\mathbf{r}\right)e^{-iH\left(t-t'\right)}\psi^\dagger\left(\mathbf{r}'\right)\left|GS\right\rangle\theta\left(t-t'\right) \tag{24.10}$$

In this expression, $|GS\rangle$ is a many-body vacuum (ground-state). Choosing appropriately the zero of energy, $H\left|GS\right\rangle=0\left|GS\right\rangle=0$ the above result could be written

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)=-i\left\langle GS\right|\psi\left(\mathbf{r},t\right)\psi^\dagger\left(\mathbf{r}',t'\right)\left|GS\right\rangle\theta\left(t-t'\right). \tag{24.11}$$

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 $t=t'+0^+$

$$G^R\left(\mathbf{r},t+0^+;\mathbf{r}',t\right)=-i\delta\left(\mathbf{r}-\mathbf{r}'\right) \tag{24.12}$$

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. This means that $\left\langle GS\right|\psi\left(\mathbf{r},t\right)\psi^\dagger\left(\mathbf{r}',t\right)\left|GS\right\rangle$ 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.(24.12) 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:

$$G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)=-i\left\langle GS\right|\left\{\psi\left(\mathbf{r},t\right),\psi^\dagger\left(\mathbf{r}',t'\right)\right\}\left|GS\right\rangle\theta\left(t-t'\right)\quad;\quad\text{for}\quad\text{fermions} \tag{24.13}$$

$$G^R(\mathbf{r},t;\mathbf{r}',t') = -i\langle GS|\left[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')\right]|GS\rangle\,\theta(t-t') \quad ; \quad \text{for} \quad \text{bosons} \tag{24.14}$$

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 12

$$\boxed{G^R(\mathbf{r},t;\mathbf{r}',t') = -i\left\langle\left\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')\right\}\right\rangle\theta(t-t') \quad ; \quad \textit{for} \quad \textit{fermions}} \tag{24.15}$$

$$\boxed{G^R(\mathbf{r},t;\mathbf{r}',t') = -i\left\langle\left[\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t')\right]\right\rangle\theta(t-t') \quad ; \quad \textit{for} \quad \textit{bosons}} \tag{24.16}$$

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 81 *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 82 *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).*

24.3 Examples with quadratic Hamiltonians:

When the Hamiltonian is quadratic in creation-annihilation operators, the equation of motion obeyed by this Green's function is the same as in the one-body case. An example of quadratic Hamiltonian is that for free particles

$$\langle\mathbf{r}|H|\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m}\langle\mathbf{r}|\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m}\delta(\mathbf{r}-\mathbf{r}_1). \tag{24.17}$$

In the general second quantized case, we write

$$\widehat{H} = \int d\mathbf{r}_1\int d\mathbf{r}_2\psi^\dagger(\mathbf{r}_2,t)\langle\mathbf{r}_2|H|\mathbf{r}_1\rangle\psi(\mathbf{r}_1,t) \tag{24.18}$$

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, $\phi_n(\mathbf{r}) = \langle\mathbf{r}|n\rangle$, $\langle n'|H|n\rangle = E_n\delta_{n,n'}$

$$\psi(\mathbf{r},t) = \sum_n\langle\mathbf{r}|n\rangle a_n(t) = \sum_n e^{-iE_nt}\langle\mathbf{r}|n\rangle a_n = \sum_n e^{-iE_nt}\phi_n(\mathbf{r})a_n \tag{24.19}$$

$$\left\{\psi\left(\mathbf{r},t\right),\psi^{\dagger}\left(\mathbf{r}',0\right)\right\}=\sum_{n}\sum_{m}e^{-iE_{n}t}\phi_{n}\left(\mathbf{r}\right)\left\{a_{n},a_{m}^{\dagger}\right\}\phi_{m}^{*}\left(\mathbf{r}'\right)=\sum_{n}e^{-iE_{n}t}\phi_{n}\left(\mathbf{r}\right)\phi_{n}^{*}\left(\mathbf{r}'\right)\tag{24.20}$$

$$G^{R}\left(\mathbf{r},t;\mathbf{r}',0\right)=-i\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^{\dagger}\left(\mathbf{r}',0\right)\right\}\right\rangle\theta\left(t\right)=-i\sum_{n}e^{-iE_{n}t}\phi_{n}\left(\mathbf{r}\right)\phi_{n}^{*}\left(\mathbf{r}'\right)\theta\left(t\right)\tag{24.21}$$

$$G^{R}\left(\mathbf{r},\mathbf{r}';\omega\right)=\int dte^{i(\omega+i\eta)t}\left(-i\right)\sum_{n}e^{-iE_{n}t}\phi_{n}\left(\mathbf{r}\right)\phi_{n}^{*}\left(\mathbf{r}'\right)\theta\left(t\right)=\sum_{n}\frac{\phi_{n}\left(\mathbf{r}\right)\phi_{n}^{*}\left(\mathbf{r}'\right)}{\omega+i\eta-E_{n}}\tag{24.22}$$

Calculation from the equations of motion In general, the equation of motion can be obtained as follows

$$i\frac{\partial}{\partial t}G^{R}\left(\mathbf{r},t;\mathbf{r}',t'\right)=i\frac{\partial}{\partial t}\left[-i\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^{\dagger}\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right)\right]\tag{24.23}$$

$$=\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^{\dagger}\left(\mathbf{r}',t'\right)\right\}\right\rangle\delta\left(t-t'\right)+i\left\langle\left\{\left[\widehat{H},\psi\left(\mathbf{r},t\right)\right],\psi^{\dagger}\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right)\tag{24.24}$$

Following the steps analogous to those in Eq.(23.78) above, using the anticommutation relations Eqs.(23.42)(23.43a), or more directly recalling the commutator of the number operator with a creation or an annihilation operator, it is clear that

$$\left[\widehat{H},\psi\left(\mathbf{r},t\right)\right]=-\int d\mathbf{r}_{1}\left\langle\mathbf{r}\right|H\left|\mathbf{r}_{1}\right\rangle\psi\left(\mathbf{r}_{1},t\right)\tag{24.25}$$

so that

$$\begin{aligned}
&i\frac{\partial}{\partial t}G^{R}\left(\mathbf{r},t;\mathbf{r}',t'\right) &&(24.26)\\
&=\quad\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)-i\int d\mathbf{r}_{1}\left\langle\mathbf{r}\right|H\left|\mathbf{r}_{1}\right\rangle\left\langle\left\{\psi\left(\mathbf{r}_{1},t\right),\psi^{\dagger}\left(\mathbf{r}',t'\right)\right\}\right\rangle\theta\left(t-t'\right)\\
&=\quad\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)+\int d\mathbf{r}_{1}\left\langle\mathbf{r}\right|H\left|\mathbf{r}_{1}\right\rangle G^{R}\left(\mathbf{r}_{1},t;\mathbf{r}',t'\right) &&(24.27)
\end{aligned}$$

This last expression may be rewritten as

$$\begin{aligned}
\int d\mathbf{r}_{1}\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_{1}\right\rangle G^{R}\left(\mathbf{r}_{1},t;\mathbf{r}',t'\right)&=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) &&(24.28)\\
&=\left\langle\mathbf{r}\left|\mathbf{r}'\right.\right\rangle\delta\left(t-t'\right) &&(24.29)
\end{aligned}$$

where we recognize the equation (16.48) found in the previous Chapter. Formally then

$$\left\langle\mathbf{r}\right|\left(i\frac{\partial}{\partial t}-\widehat{H}\right)G^{R}\left(t-t'\right)\left|\mathbf{r}'\right\rangle=\left\langle\mathbf{r}\left|\mathbf{r}'\right.\right\rangle\delta\left(t-t'\right)\tag{24.30}$$

so that the operator form of the Green's function is the same as that found before, namely

$$\widehat{G}^{R}\left(t-t'\right)=\left(i\frac{\partial}{\partial t}-\widehat{H}\right)^{-1}\delta\left(t-t'\right)\tag{24.31}$$

It is convenient to rewrite the result for the equation of motion Eq.(24.28) in the following form that is more symmetrical in space and time.

$$\int d\mathbf{r}_{1}\int dt_{1}\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_{1}\right\rangle\delta\left(t-t_{1}\right)G^{R}\left(\mathbf{r}_{1},t_{1};\mathbf{r}',t'\right)=\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)\tag{24.32}$$

We may as well let time play a more important role since in the many-body case it will be essential, as we have already argued in the context of the frequency dependence of the self-energy. The inverse of the Green's function in this notation is just like above,

$$G^R\left(\mathbf{r},t;\mathbf{r}_1,t_1\right)^{-1}=\left\langle\mathbf{r}\right|i\frac{\partial}{\partial t}-\widehat{H}\left|\mathbf{r}_1\right\rangle\delta\left(t-t_1\right). \tag{24.33}$$

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 13 *The following short-hand notation is often used*

$$\boxed{G^R\left(1,1'\right)\equiv G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)} \tag{24.34}$$

$$\boxed{G^R\left(1,\overline{1}\right)^{-1}G^R\left(\overline{1},1'\right)=\delta\left(1-1'\right)} \tag{24.35}$$

where the index with the overbar stands for an integral.

25. INTERACTION REPRESENTATION, WHEN TIME ORDER MATTERS

Perturbation theory in the many-body case is less trivial than in the one-body case. Whereas the Lippmann-Schwinger equation was written down for a single frequency, in the many-body case time and frequency dependence are unavoidable. To construct perturbation theory we will follow the same steps as those used in the derivation of linear response theory in Chapter 10. 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

$$H = H_0 + V \tag{25.1}$$

where

$$[H_0, V] \neq 0 \tag{25.2}$$

Let us begin. We assume that H is time independent. Typical matrix elements we want to compute at finite temperature are of the form

$$\langle i| e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') |i\rangle \tag{25.3}$$

We do not write explicitly indices other than time to keep the notation simple. Recall the Heisenberg and Schrödinger picture

$$\psi_H(t) = e^{iHt} \psi_S e^{-iHt} \tag{25.4}$$

We define the time evolution operator

$$U(t,0) = e^{-iHt} \tag{25.5}$$

so that

$$\psi_H(t) = U(0,t)\, \psi_S U(t,0) \tag{25.6}$$

Because from now on we assume time-reversal symmetry, we will always make the replacement

$$U^\dagger(t,0) = U(0,t) \tag{25.7}$$

as we just did. The differential equation for the time-evolution operator is

$$i\frac{\partial U(t,0)}{\partial t} = HU(t,0) \tag{25.8}$$

With the initial condition $U(0,0) = 1$ it has $U(t,0) = e^{-iHt}$ as its solution. It obeys the semi-group property

$$U(t,t') = U(t,0)\, U(0,t') = e^{-iH(t-t')} \tag{25.9}$$

$$U^{-1}(t,0) = U(0,t) \tag{25.10}$$

$$U(t_0,t_0) = 1 \tag{25.11}$$

for arbitrary t_0

We are now ready to introduce the interaction representation. In this representation, the fields evolve with the unperturbed Hamiltonian

$$\boxed{\widehat{\psi}(t) = e^{iH_0t}\psi_S e^{-iH_0t}} \tag{25.12}$$

Note that we now use the caret (hat) to mean "interaction picture". We hope this change of notation causes no confusion. To introduce these interaction representation fields in a general matrix element,

$$\langle i|\, e^{-\beta H}\psi_H(t)\,\psi_H^\dagger(t')\,|i\rangle = \langle i|\, e^{-\beta H}U(0,t)\,\psi_S U(t,0)\,U(0,t')\,\psi_S^\dagger U(t',0)\,|i\rangle \tag{25.13}$$

it suffices to notice that it is easy to remove the extra e^{iH_0t} coming from the replacement of ψ_S by $e^{-iH_0t}\widehat{\psi}(t)\,e^{iH_0t}$ simply by including them in the definition of the evolution operator in the interaction representation

$$\widehat{U}(t,0) = e^{iH_0t}U(t,0) \tag{25.14}$$

$$\widehat{U}(0,t) = U(0,t)\,e^{-iH_0t} \tag{25.15}$$

$$\widehat{U}(t,0)\,\widehat{U}(0,t) = \widehat{U}(0,t)\,\widehat{U}(t,0) = 1 \tag{25.16}$$

With these definitions, we have that our general matrix element takes the form

$$\langle i|\, e^{-\beta H}\psi_H(t)\,\psi_H^\dagger(t')\,|i\rangle = \langle i|\, e^{-\beta H}\widehat{U}(0,t)\,\widehat{\psi}(t)\,\widehat{U}(t,0)\,\widehat{U}(0,t')\,\widehat{\psi}^\dagger(t')\,\widehat{U}(t',0)\,|i\rangle \tag{25.17}$$

The purpose of the exercise is evidently to find a perturbation expansion for the evolution operator in the interaction representation. It will be built starting from its equation of motion

$$i\frac{\partial\widehat{U}(t,0)}{\partial t} = e^{iH_0t}(-H_0+H)\,U(t,0) = e^{iH_0t}V \quad \left(e^{-iH_0t}e^{iH_0t}\right) \quad U(t,0) \tag{25.18}$$

Since a general operator is a product of ψ fields, it will also evolve with time in the same way so it is natural to define the interaction representation for V as well. Our final result for the equation of motion for $\widehat{U}(t,0)$ 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

$$\boxed{i\frac{\partial\widehat{U}(t,t_0)}{\partial t} = \widehat{V}(t)\,\widehat{U}(t,t_0)} \tag{25.19}$$

Remark 83 *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*

$$\frac{\partial}{\partial t}\ln\widehat{U}(t,t_0) = \lim_{\Delta t\to 0}\widehat{U}(t,t_0)^{-1}\left[\widehat{U}(t+\Delta t,t_0) - \widehat{U}(t,t_0)\right]/\Delta t$$

or

$$\lim_{\Delta t\to 0}\left[\widehat{U}\left(t+\Delta t,t_0\right)-\widehat{U}\left(t,t_0\right)\right]\widehat{U}\left(t,t_0\right)^{-1}/\Delta t\ ? \tag{25.20}$$

The two limits cannot be identical since in general

$$\lim_{\Delta t\to 0}\left[\widehat{U}\left(t+\Delta t,t_0\right),\widehat{U}\left(t,t_0\right)^{-1}\right]\neq 0. \tag{25.21}$$

because $\widehat{U}\left(t,t_0\right)$ *is made up of operators such as* V *and* e^{-iH_0t} *that do not commute with each other.*

To solve the equation for the evolution operator Eq.(25.19), it is more convenient to write the equivalent integral equation that is then solved by iteration. Integration on both sides of the equation and use of the initial condition Eq.(25.11) gives immediately

$$\int_{t_0}^{t}\frac{\partial\widehat{U}\left(t',t_0\right)}{\partial t'}dt'=-i\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\widehat{U}\left(t',t_0\right) \tag{25.22}$$

$$\widehat{U}\left(t,t_0\right)=1-i\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\widehat{U}\left(t',t_0\right) \tag{25.23}$$

Solving by iteration, we find

$$\widehat{U}\left(t,t_0\right)=1-i\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\widehat{U}\left(t',t_0\right)= \tag{25.24}$$

$$= \quad 1-i\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)+\left(-i\right)^2\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\int_{t_0}^{t'}dt''\widehat{V}\left(t''\right) \tag{25.25}$$

$$+\left(-i\right)^3\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\int_{t_0}^{t'}dt''\widehat{V}\left(t''\right)\int_{t_0}^{t"}dt'''\widehat{V}\left(t'''\right)+... \tag{25.26}$$

Suppose $t>t_0$ and consider a typical term in this series. By suitably defining a contour C and time-ordering operator along this contour T_c, it can be rearranged as follows

$$\left(-i\right)^3\int_{t_0}^{t}dt'\widehat{V}\left(t'\right)\int_{t_0}^{t'}dt''\widehat{V}\left(t''\right)\int_{t_0}^{t"}dt'''\widehat{V}\left(t'''\right) \tag{25.27}$$

$$=\left(-i\right)^3\frac{1}{3!}T_c\left[\int_C dt_1\widehat{V}\left(t_1\right)\int_C dt_2\widehat{V}\left(t_2\right)\int_C dt_3\widehat{V}\left(t_3\right)\right] \tag{25.28}$$

where

- C is a contour that is here just a real line segment going from t_0 to t.
- T_c is the "time-ordering operator". 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 lef-hand side of the last equation covers all possible times such that the operators with the time that is largest (latest) are to the left. The $\frac{1}{3!}$ comes from the fact that for a general $\widehat{V}\left(t_1\right)\widehat{V}\left(t_2\right)\widehat{V}\left(t_3\right)$ there are 3! ways of ordering the operators. All these possible orders appear in the integrals on the right-hand side of the last equation. The operator T_c always orders them in the order corresponding to the left-hand side, but this means that the integral on the left-hand side appears 3! times on the right-hand side, hence the overall factor of $\frac{1}{3!}$.

- A product of operators on which T_c acts is called a time-ordered product.

One also needs $\widehat{U}(0,t)$. 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

$$\widehat{U}(t,t_0)=\sum_{k=0}^{\infty}(-i)^k\frac{1}{k!}T_c\left[\left(\int_C dt_1\widehat{V}(t_1)\right)^k\right] \tag{25.29}$$

which we can in turn write in the convenient notation

$$\boxed{\widehat{U}(t,t_0)=T_c\left[\exp\left(-i\int_C dt_1\widehat{V}(t_1)\right)\right]} \tag{25.30}$$

where the contour is as defined above. In other words, operators are ordered right to left from t_0 to t whether t, as a real number, is larger or smaller than t_0.

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 84 *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_0t}. The only property of the exponential that we really use in the above derivation is the composition law obeyed by time-evolution operators in general, namely $U_0(t,t')U_0(t',t'')=U_0(t,t'')$.*

Remark 85 *The general case of time-dependent Hamiltonians: The problem we just solved for the time evolution in the interaction picture Eq.(25.19) is a much more general problem that poses itself whenever the Hamiltonian is time-dependent.*

26. 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

$$e^{-\beta H} = U\left(-i\beta, 0\right) = e^{-iH_0(-i\beta)}\widehat{U}\left(-i\beta, 0\right) = e^{-\beta H_0}\widehat{U}\left(-i\beta, 0\right) \tag{26.1}$$

The solution of the imaginary time evolution equation

$$i\frac{\partial \widehat{U}\left(it'', 0\right)}{\partial\left(it''\right)} = \widehat{V}\left(it''\right)\widehat{U}\left(it'', 0\right)$$

is then

$$\widehat{U}\left(-i\beta, 0\right) = T_c\left[\exp\left(-i\int_C d\left(it''\right)\widehat{V}\left(it''\right)\right)\right] \tag{26.2}$$

where

$$\boxed{t'' \equiv \mathrm{Im}\left(t\right)} \tag{26.3}$$

$$\widehat{V}\left(it''\right) = e^{-t''H_0}Ve^{t''H_0} \tag{26.4}$$

and the contour C now proceeds from $t'' = 0$ to $t'' = -\beta$.

Overall now, the matrix elements that we need to evaluate can be expressed in such a way that the trace will be performed over the unperturbed density matrix. Indeed, using our above results, we find

$$\left\langle i\right| e^{-\beta H}\psi_H\left(t\right)\psi_H^{+}\left(t'\right)\left|i\right\rangle = \left\langle i\right| e^{-\beta H_0}\widehat{U}\left(-i\beta, 0\right)\widehat{U}\left(0, t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t, 0\right)\widehat{U}\left(0, t'\right)\widehat{\psi}^{+}\left(t'\right)\widehat{U}\left(t', 0\right)\left|i\right\rangle \tag{26.5}$$

We want to take initial states at a time t_0 so that in practical calculations where the system is *out of equilibrium* we can choose $t_0 = -\infty$ where we can assume that the system is in equilibrium at this initial time. Hence, we are here considering a more general case than we really need but that is not more difficult so let us continue. Since we are evaluating a trace, we are free to take

$$\left|i\right\rangle = \widehat{U}\left(0, t_0\right)\left|i\left(t_0\right)\right\rangle \tag{26.6}$$

then we have

$$\left\langle i\right| e^{-\beta H} = \left\langle i\left(t_0\right)\right|\widehat{U}\left(t_0, 0\right)e^{-\beta H} = \left\langle i\left(t_0\right)\right|\left(e^{-\beta H_0}e^{\beta H_0}\right)\left(e^{iH_0t_0}e^{-iHt_0}\right)e^{-\beta H} \tag{26.7}$$

$$= \left\langle i\left(t_0\right)\right| e^{-\beta H_0}e^{iH_0(t_0-i\beta)}e^{-iH(t_0-i\beta)} = \left\langle i\left(t_0\right)\right| e^{-\beta H_0}\widehat{U}\left(t_0 - i\beta, 0\right) \tag{26.8}$$

This allows us to write an arbitrary matrix element entering the thermodynamic trace as the evolution along a contour in complex time

$$\left\langle i\right| e^{-\beta H}\psi_H\left(t\right)\psi_H^{\dagger}\left(t'\right)\left|i\right\rangle = \left\langle i\left(t_0\right)\right| e^{-\beta H_0}\widehat{U}\left(t_0 - i\beta, 0\right)\widehat{U}\left(0, t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t, 0\right)\widehat{U}\left(0, t'\right)\widehat{\psi}^{\dagger}\left(t'\right)\widehat{U}\left(t', 0\right)\left|i\right\rangle$$

$$= \langle i(t_0)|\, e^{-\beta H_0}\widehat{U}(t_0-i\beta,t_0)\,\widehat{U}(t_0,t)\,\widehat{\psi}(t)\,\widehat{U}(t,t')\,\widehat{\psi}^{\dagger}(t')\,\widehat{U}(t',t_0)\,|i(t_0)\rangle \tag{26.9}$$

How would we evaluate the retarded Green's function in practice using this approach? Take the case of fermions. It is convenient to define $G^{>}(t-t')$ and $G^{<}(t-t')$ by

$$\boxed{G^{>}(t-t') = -i\left\langle \psi_H(t)\,\psi_H^{\dagger}(t')\right\rangle} \tag{26.10}$$

$$\boxed{G^{<}(t-t') = i\left\langle \psi_H^{\dagger}(t')\,\psi_H(t)\right\rangle} \tag{26.11}$$

in such a way that

$$G^{R}(t-t') = -i\left\langle\left\{\psi_H(t)\,,\psi_H^{\dagger}(t')\right\}\right\rangle\theta(t-t') \equiv \left[G^{>}(t-t') - G^{<}(t-t')\right]\theta(t-t') \tag{26.12}$$

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.(26-1). 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.

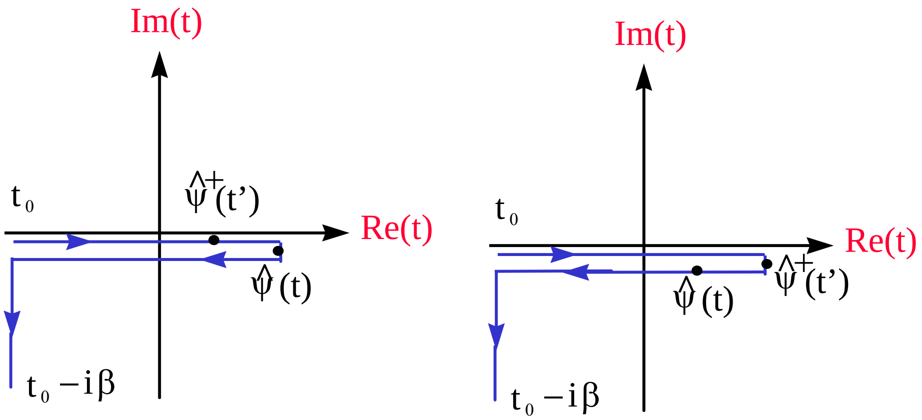

Figure 26-1 Kadanoff-Baym contour to compute $G^{>}(t-t')$.

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.(26.9). In practice this greatly simplifies the calculations since the contour, illustrated in Fig.(26-2), is such that integrals always go from $-\infty$ to ∞. To specify if a given creation or annihilation operator is on the upper or the lower contour, a simple 2×2 matrix suffices since there are only four possibilities..

In equilibrium, the analog of the fluctuation dissipation theorem in the form of Eq.(11.100) for correlation functions, allows us to relate $G^{>}$ and $G^{<}$, which

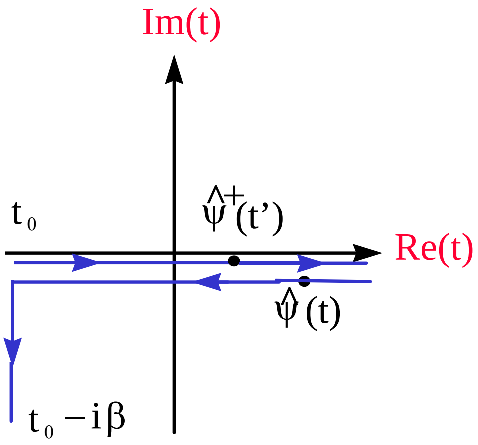

Figure 26-2 Keldysh-Schwinger contour.

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.

27. 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.(27-1) below. This slight generalization of the Green's function is a mathematical device that is simple, elegant and extremely convenient since the integration contour is now simple. In a sense, we take advantage of the fact that we are free to define Green functions as we wish, as long as we connect them to observable quantities in at the end of the calculation. This is similar to what we did for correlation function. All the information about the system was in $\chi''(\mathbf{k},\omega)$, now it is all in the spectral weight $A(\mathbf{k},\omega)$,so that as long as we can extract the single-particle spectral weight we do not loose information.

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 producs 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. We have already seen this with the Matsubara representation for correlation functions.11.9 The same tricks apply not only to Green's functions but also to these correlation function.

After introducing the so-called Matsubara Green's function itself, we will study its properties. First, using essentially the same trick as for the fluctuation-dissipation theorem for correlation functions, we prove that 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.

27.1 Definition

The Matsubara Green's function is defined by

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right)=-\left\langle T_\tau\psi\left(\mathbf{r},\tau\right)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle} \tag{27.1}$$

$$=-\left\langle\psi\left(\mathbf{r},\tau\right)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle\theta\left(\tau-\tau'\right)+\left\langle\psi^\dagger\left(\mathbf{r}',\tau'\right)\psi\left(\mathbf{r},\tau\right)\right\rangle\theta\left(\tau'-\tau\right) \tag{27.2}$$

The definition of Ref.([3]) has an overall minus sign difference with the definition given here.

Definition 14 *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

$$\langle\mathcal{O}\rangle\equiv\frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]} \tag{27.3}$$

with μ the chemical potential and N is the total number of particle operator, while the time evolution of the operators is defined by

$$\boxed{\psi\left(\mathbf{r},\tau\right)\equiv e^{\tau(H-\mu N)}\psi_S\left(\mathbf{r}\right)e^{-\tau(H-\mu N)}} \tag{27.4}$$

$$\boxed{\psi^\dagger\left(\mathbf{r},\tau\right)\equiv e^{\tau(H-\mu N)}\psi_S^+\left(\mathbf{r}\right)e^{-\tau(H-\mu N)}} \tag{27.5}$$

For convenience, it is useful to define

$$\boxed{K\equiv H-\mu N} \tag{27.6}$$

Several points should attract our attention:

- The correspondence with the real time evolution operators e^{-iHt} is done by noting that
$$\tau=-\operatorname{Im}\left(t\right) \tag{27.7}$$
or, in general for complex time
$$\boxed{\tau=it}$$
- Strictly speaking, we should use $\psi\left(\mathbf{r},-i\tau\right)$ if we want the symbol $\psi\left(\mathbf{r},t\right)$ for t complex to mean the same thing as before. That is why several authors write $\widehat{\psi}\left(\mathbf{r},\tau\right)$ for the Matsubara field operator. We will stick with $\psi\left(\mathbf{r},\tau\right)$ 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 $f\left(\mathbf{k}\right)$ to denote the Fourier transform of $f\left(\mathbf{r}\right)$.

- $\psi^{\dagger}(\mathbf{r},\tau)$ 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 $\psi^{\dagger}$: namely $\psi^{\dagger}$ to the left of ψ and $\psi^{\dagger}$ to the right of ψ. Both possibilities appear in G^R. If we had only $\tau > 0$, only one possibility would appear in the Matsubara Green's function. We will see however in the next section that, in practice, antiperiodicity allows us to trivially take into account what happens in the interval $-\beta \leq \tau \leq 0$ if we know what happens in the interval $0 \leq \tau \leq \beta$.
- 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 $(\mathrm{Im}(t) = -\beta) > (\mathrm{Im}(t') = \beta)$ which corresponds to $(\tau = \beta) > (\tau' = -\beta)$. The present contour is illustrated in Fig.(27-1).

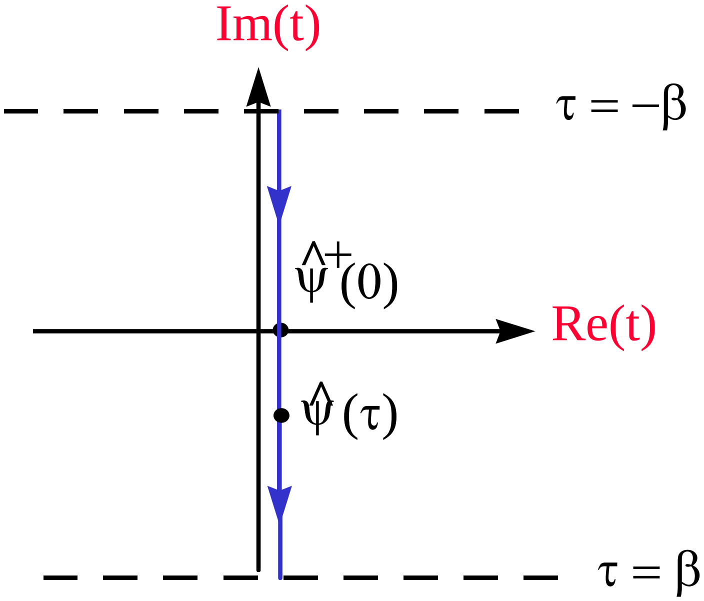

Figure 27-1 Contour for time ordering in imaginary time. Only the time difference is important. The contour is translated slightly along the real-time axis for clarity.

Remark 86 *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* $(\psi^{+}\psi)$ *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.*

27.2 Time ordered product in practice

Suppose I want to compute

$$\left\langle T_{\tau}\psi\left(\tau_{1}\right)\psi^{\dagger}\left(\tau_{3}\right)\psi\left(\tau_{2}\right)\psi^{\dagger}\left(\tau_{4}\right)\right\rangle . \tag{27.8}$$

We drop space indices to unclutter the equations. The time ordered product for fermions keeps tract of permutations, so if I exchange the first two operators for example, I find

$$\left\langle T_{\tau}\psi\left(\tau_{1}\right)\psi^{\dagger}\left(\tau_{3}\right)\psi\left(\tau_{2}\right)\psi^{\dagger}\left(\tau_{4}\right)\right\rangle = -\left\langle T_{\tau}\psi^{\dagger}\left(\tau_{3}\right)\psi\left(\tau_{1}\right)\psi\left(\tau_{2}\right)\psi^{\dagger}\left(\tau_{4}\right)\right\rangle \tag{27.9}$$

I need not worry about delta functions at equal time or anything but the number of fermion exchanges. Indeed, whichever of the above two expressions I start with, if $\tau_1 < \tau_2 < \tau_3 < \tau_4$, I will find at the end that

$$\left\langle T_{\tau}\psi\left(\tau_{1}\right)\psi^{\dagger}\left(\tau_{3}\right)\psi\left(\tau_{2}\right)\psi^{\dagger}\left(\tau_{4}\right)\right\rangle = -\left\langle \psi^{\dagger}\left(\tau_{4}\right)\psi^{\dagger}\left(\tau_{3}\right)\psi\left(\tau_{2}\right)\psi\left(\tau_{1}\right)\right\rangle . \tag{27.10}$$

We cannot, however, have two of the times equal. We have to specify that one is infinitesimally larger or smaller than the other to know in which order to place the operators.

27.3 Antiperiodicity and Fourier expansion (Matsubara frequencies)

Suppose $\tau < 0$. Then

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = \left\langle \psi^{+}\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},\tau\right)\right\rangle \tag{27.11}$$

Using the cyclic property of the trace twice, as in the demonstration of the fluctuation-dissipation theorem it is easy to show that

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = -\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right) \quad ; \quad \tau < 0} \tag{27.12}$$

This boundary condition is sometimes known as the Kubo-Martin-Schwinger (KMS) boundary condition.

Proof: Let

$$e^{-\beta\Omega} \equiv \mathrm{Tr}\left[e^{-\beta K}\right] \tag{27.13}$$

then

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) = e^{\beta\Omega}\,\mathrm{Tr}\left[e^{-\beta K}\psi^{+}\left(\mathbf{r}'\right)\psi\left(\mathbf{r},\tau\right)\right] \tag{27.14}$$

The cyclic property of the trace then tells us that

$$\begin{aligned}
\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) &= e^{\beta\Omega}\,\mathrm{Tr}\left[\psi\left(\mathbf{r},\tau\right)e^{-\beta K}\psi^{+}\left(\mathbf{r}'\right)\right] && (27.15)\\
&= e^{\beta\Omega}\,\mathrm{Tr}\left[\left(e^{-\beta K}e^{\beta K}\right)\left(e^{K\tau}\psi\left(\mathbf{r}\right)e^{-K\tau}\right)e^{-\beta K}\psi^{+}\left(\mathbf{r}'\right)\right] && (27.16)\\
&= \left\langle\psi\left(\mathbf{r},\tau+\beta\right)\psi^{+}\left(\mathbf{r}',0\right)\right\rangle && (27.17)\\
&= -\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right) && (27.18)
\end{aligned}$$

The last line follows because given that $-\beta<\tau$, we necessarily have $\tau+\beta>0$ so that the other θ function must be used in the definition of the Matsubara Green's function.

If $\tau>0$, the above arguments can be repeated to yield

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\beta\right)=-\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)\quad;\quad\tau>0} \qquad (27.19)$$

However, for $\tau>0$ note that

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)\neq-\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right)\quad;\quad\tau>0 \qquad (27.20)$$

While $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right)$ 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

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)=\tfrac{1}{\beta}\sum_{n=-\infty}^{\infty}e^{-ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)} \qquad (27.21)$$

where the so-called Matsubara frequencies for fermions are odd, namely

$$\boxed{k_n=\left(2n+1\right)\pi T=\tfrac{(2n+1)\pi}{\beta}}\quad;\quad n\quad\text{integer} \qquad (27.22)$$

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

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=\int_0^{\beta}d\tau e^{ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)} \qquad (27.23)$$

Note that only the $\tau>0$ region of the domain of definition is needed, as promised.

Remark 87 *Domain of definition of the Matsubara Green's function: The value of $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ given by the Fourier series (27.21) for τ outside the interval $-\beta<\tau<\beta$, is in general different from the actual value of Eq.(27.1) $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right)=-\left\langle T_\tau\psi\left(\mathbf{r},\tau\right)\psi^{+}\left(\mathbf{r}',\tau'\right)\right\rangle$. Indeed, to define a Fourier series one extends the function defined in the interval $-\beta<\tau<\beta$ so that it is periodic in τ outside this interval with a period 2β. The true function $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right)=-\left\langle T_\tau\psi\left(\mathbf{r},\tau\right)\psi^{+}\left(\mathbf{r}',\tau'\right)\right\rangle$ has an envelope that is, instead, exponential outside the original interval. We will see an explicit example in the case of the free particles. In perturbation expansions, we never need $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ 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.*

27.4 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

$$G^R(\mathbf{r},\mathbf{r}';t) = -i\left\langle\left\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',0)\right\}\right\rangle\theta(t) \tag{27.24}$$

but this time, the evolution operator is defined to take into account the fact that we will work in the grand-canonical ensemble. By analogy with the definition of the Matsubara operators, we now have

$$K = H - \mu N$$

$$\psi(\mathbf{r},t) \equiv e^{itK}\psi_S(\mathbf{r})e^{-itK} \tag{27.25}$$

$$\psi^\dagger(\mathbf{r},t) \equiv e^{itK}\psi_S^+(\mathbf{r})e^{-itK} \tag{27.26}$$

We now proceed by analogy with the response functions. On the left we show the definitions for response functions, and on the right the analogous definitions for response functions. Let

$$G^R(\mathbf{r},\mathbf{r}';t) = -iA(\mathbf{r},\mathbf{r}';t)\theta(t) \quad ; \quad \chi_{ij}^R(t) = 2i\chi_{ij}''(t)\theta(t) \tag{27.27}$$

where the *spectral weight* is defined by

$$\boxed{A(\mathbf{r},\mathbf{r}';t) \equiv \left\langle\left\{\psi(\mathbf{r},t),\psi^+(\mathbf{r}',0)\right\}\right\rangle} \quad ; \quad \chi_{ij}''(t) = \frac{1}{2}\left\langle\left[A_i(\mathbf{r},t),A_j(\mathbf{r}',0)\right]\right\rangle \tag{27.28}$$

Then taking the Fourier transform, one obtains the spectral representation

$$\boxed{G^R(\mathbf{r},\mathbf{r}';\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'}} \quad ; \quad \chi_{ij}^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi_{ij}''(\omega')}{\omega'-(\omega+i\eta)}. \tag{27.29}$$

The spectral weight will obey sum-rules, like χ'' did. For example

$$\boxed{\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A(\mathbf{r},\mathbf{r}';\omega') = \left\langle\left\{\psi(\mathbf{r},0),\psi^+(\mathbf{r}',0)\right\}\right\rangle = \delta(\mathbf{r}-\mathbf{r}')} \tag{27.30}$$

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

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) = -\left\langle\psi(\mathbf{r},\tau)\psi^+(\mathbf{r}',0)\right\rangle\theta(\tau) + \left\langle\psi^+(\mathbf{r}',0)\psi(\mathbf{r},\tau)\right\rangle\theta(-\tau) \tag{27.31}$$

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) \tag{27.32}$$

$$= \int_0^\beta d\tau e^{ik_n\tau}\left[-\left\langle\psi(\mathbf{r},\tau)\psi^+(\mathbf{r}',0)\right\rangle\right] \tag{27.33}$$

Assume that $k_n > 0$. Then, as illustrated in Fig.(27-2), we can deform the contour of integration within the domain of analyticity along $\mathrm{Re}\,(t) = \mathrm{Im}\,(\tau) > 0$. (The analyticity of $\left\langle \psi\left(\mathbf{r},\tau\right)\psi^+\left(\mathbf{r}',0\right)\right\rangle$ in that domain comes from $e^{-\beta H}$ in the trace. You will be able to prove this later by calculating $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ with the help of the spectral representation Eq.(27.40) and tricks for evaluating sums on Matsubara frequencies. For $\mathrm{Im}\,(\tau) = \infty$ there will be no contribution from the small segment since $e^{ik_n\tau}$ becomes a decaying exponential. The integral becomes

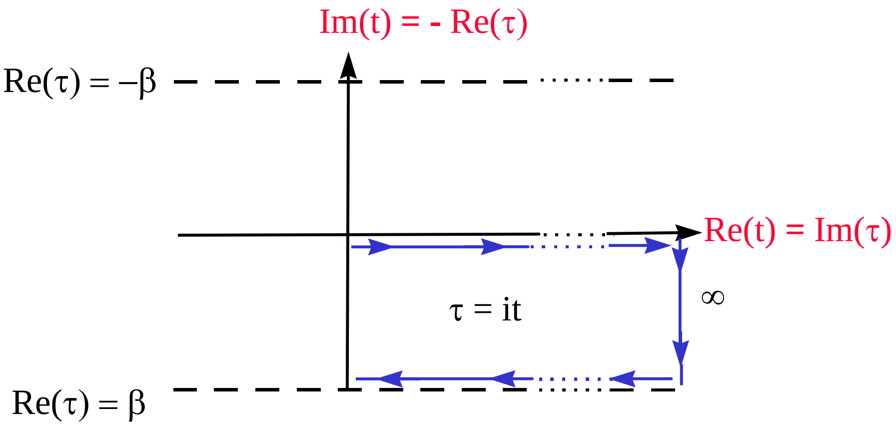

Figure 27-2 Deformed contour used to relate the Matsubara and the retarded Green's functions.

$$\begin{aligned} &\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \\ &\int_{t=0}^{t=\infty} d\left(it\right)\left[-\left\langle \psi\left(\mathbf{r},t\right)\psi^+\left(\mathbf{r}'\right)\right\rangle\right]e^{ik_n(it)} \\ &+\int_{t=\infty}^{t=0} d\left(it\right)\left[-\left\langle \psi\left(\mathbf{r},t-i\beta\right)\psi^+\left(\mathbf{r}'\right)\right\rangle\right]e^{(ik_n)i(t-i\beta)} \end{aligned} \tag{27.34}$$

In the last integral, we then use the results

$$e^{(ik_n)i(-i\beta)} = e^{(ik_n)\beta} = -1 \tag{27.35}$$

$$\int_\infty^0 = -\int_0^\infty \tag{27.36}$$

$$\begin{aligned} -\left\langle \psi\left(\mathbf{r},t-i\beta\right)\psi^+\left(\mathbf{r}'\right)\right\rangle &= \\ \left[-\left\langle e^{iK(t-i\beta)}\psi_S\left(\mathbf{r}\right)e^{-iK(t-i\beta)}\psi_S^\dagger\left(\mathbf{r}'\right)\right\rangle\right] &= \left[-\left\langle e^{\beta K}e^{iKt}\psi_S\left(\mathbf{r}\right)e^{-iKt}e^{-\beta K}\psi_S^\dagger\left(\mathbf{r}'\right)\right\rangle\right] \end{aligned} \tag{27.37}$$

It then suffices to cancel the left most $e^{\beta K}$ with the density matrix and to use the cyclic property of the trace to obtain for the integrand of the last integral,

$$= \left[-\left\langle \psi^\dagger\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},t\right)\right\rangle\right]. \tag{27.38}$$

Overall then, the integral in Eq.(27.34) is equal to

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = -i\int_0^\infty dt\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^\dagger\left(\mathbf{r}',0\right)\right\}\right\rangle e^{i(ik_n)t} \tag{27.39}$$

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n-\omega'}} \tag{27.40}$$

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(27.29), we see that analytic continuation is possible.

$$\boxed{G^R(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{ik_n \rightarrow \omega + i\eta} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n)} \tag{27.41}$$

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 88 *Connectedness: For a general bosonic correlation function, similar spectral representations can also be defined for connected functions (see below). As an example of connected function,* $\langle A(\tau) B\rangle - \langle A(\tau)\rangle \langle B\rangle$ *is connected. The subtracted term allows the combination of correlation functions to behave as a response function and appears naturally in the functional derivative approach. If* $\langle A(\tau)\rangle$ *has a piece that is independent of* τ*, the subtraction allows the integral on the contour at infinity on the above figure to vanish even at zero Matsubara frequency. Otherwise, that would not be the case.*

27.5 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.(27.40)

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{ik_n - \omega'} \tag{27.42}$$

The spectral weight $A(\mathbf{r}, \mathbf{r}'; \omega')$ was discussed just in the previous subsection (See also Eq.(28.6) for the Lehman representation).

The Matsubara Green's function and the retarded functions are special case of a more general function defined in the complex frequency plane by

$$\boxed{G(\mathbf{r}, \mathbf{r}'; z) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{r}, \mathbf{r}'; \omega')}{z - \omega'}} \tag{27.43}$$

This function is analytic everywhere except on the real axis. Physically interesting special cases are

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) = G(\mathbf{r}, \mathbf{r}'; ik_n)$$

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\eta \rightarrow 0} G(\mathbf{r}, \mathbf{r}'; \omega + i\eta) \tag{27.44}$$

$$G^A(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\eta \rightarrow 0} G(\mathbf{r}, \mathbf{r}'; \omega - i\eta) \tag{27.45}$$

The function $G(\mathbf{r}, \mathbf{r}'; z)$ has a jump on the real axis given by

$$\boxed{A(\mathbf{r}, \mathbf{r}'; \omega) = i \lim_{\eta \rightarrow 0} \left[G(\mathbf{r}, \mathbf{r}'; \omega + i\eta) - G(\mathbf{r}, \mathbf{r}'; \omega - i\eta)\right]} \tag{27.46}$$

$$A(\mathbf{r}, \mathbf{r}'; \omega) = i \left[G^R(\mathbf{r}, \mathbf{r}'; \omega) - G^A(\mathbf{r}, \mathbf{r}'; \omega)\right]$$

In the special case where $A(\mathbf{r},\mathbf{r}';\omega)$ is real (which is almost always the case in practice since we consider $\mathbf{r}=\mathbf{r}'$ or $\mathbf{k}=\mathbf{k}'$), we have

$$A(\mathbf{r},\mathbf{r}';\omega)=-2\operatorname{Im}G^{R}(\mathbf{r},\mathbf{r}';\omega) \tag{27.47}$$

like we have often used in the one-body case.

The previous results are summarized in Fig.(27-3) which displays the analytic structure of $G(\mathbf{r},\mathbf{r}';z)$. This function is analytical everywhere except on the real axis where it has a branch cut leading to a jump Eq.(27.46) in the value of the function as we approach the real axis from either the upper or lower complex half-plane. The limit as we come from the upper half-plane is equal to $G^{R}(\mathbf{r},\mathbf{r}';\omega)$ whereas from the lower half-plane it is equal to $G^{A}(\mathbf{r},\mathbf{r}';\omega)$. The Matsubara Green's function is defined only on a discrete but infinite set of points along the imaginary frequency axis.

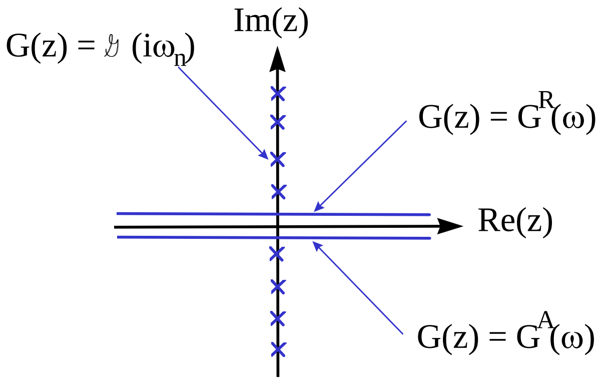

Figure 27-3 Analytical structure of $G(z)$ in the complex frequency plane. $G(z)$ reduces to either $G^{R}(\omega)$, $G^{A}(\omega)$ or $\mathcal{G}(i\omega_n)$ depending on the value of the complex frequency z. There is a branch cut along the real axis.

The problem of finding $G^{R}(\mathbf{r},\mathbf{r}';\omega)$ along the real-time axis from the knowledge of the Matsubara Green's function is a problem of analytical continuation. Unfortunately, $G(z=ik_n)$ does not have a unique analytical continuation because there is an infinite number of analytical functions that have the same value along this discrete set of points. For example, suppose we know $G(z=ik_n)$, then $G(z)\left(1+\left(e^{\beta z}+1\right)\right)$ has the same value as $G(z)$ for all points $z=ik_n$ because $e^{ik_n\beta}+1=0$. Baym and Mermin[5], using results from the theory of complex functions, have obtained the following result.

Theorem 15 *If*

1. $G(z)$ is analytical in the upper half-plane
2. $G(z)=\mathcal{G}(ik_n)$ for all Matsubara frequencies
3. $\lim_{z\to\infty} zG(z)=cst$

then the analytical continuation is unique and

$$G^{R}(\mathbf{r},\mathbf{r}';\omega)=\lim_{ik_n\to\omega+i\eta}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) \tag{27.48}$$

The key point is the third one on the asymptotic behavior at high frequency. That this is the correct asymptotic behavior at high frequency follows trivially from the spectral representation Eq.(27.43) as long as we remember that the spectral weight is bounded in frequency. The non-trivial statement is that this asymptotic behavior suffices to make the analytical continuation unique. In practice this rarely poses a problem. The simple replacement $ik_n \rightarrow \omega + i\eta$ 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 (29.1).

27.6 Matsubara Green's function in the 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. Let us first show explicitly what we mean by Green's function in momentum space. We expect $\mathcal{G}\left(\mathbf{k};\tau-\tau'\right) = -\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right) c_{\mathbf{k}}^{\dagger}\left(\tau'\right)\right\rangle$ but let us see this in detail.

With our definition of momentum and real space second quantized operators, and our normalization for momentum eigenstates Eq.(23.35) we have

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right) = -\left\langle T_\tau \psi\left(\mathbf{r},\tau\right)\psi^{\dagger}\left(\mathbf{r}',\tau'\right)\right\rangle = -\left\langle T_\tau \sum_{\mathbf{k}} \left\langle \mathbf{r}\mid\mathbf{k}\right\rangle c_{\mathbf{k}}\left(\tau\right) \sum_{\mathbf{k}'} c_{\mathbf{k}'}^{\dagger}\left(\tau'\right)\left\langle \mathbf{k}'\mid\mathbf{r}'\right\rangle\right\rangle \tag{27.49}$$

$$\left\langle \mathbf{r}\mid\mathbf{k}\right\rangle\left\langle \mathbf{k}'\mid\mathbf{r}'\right\rangle = \frac{1}{\mathcal{V}}e^{i\mathbf{k}\cdot\mathbf{r}-i\mathbf{k}'\cdot\mathbf{r}'} = \frac{1}{\mathcal{V}}e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)+i\left(\frac{\mathbf{k}+\mathbf{k}'}{2}\right)\cdot\left(\mathbf{r}-\mathbf{r}'\right)}. \tag{27.50}$$

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

$$\frac{1}{\mathcal{V}}\int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)} = \frac{1}{\mathcal{V}}\left(2\pi\right)^{3}\delta\left(\mathbf{k}-\mathbf{k}'\right) = \delta_{\mathbf{k},\mathbf{k}'} \tag{27.51}$$

we are left with

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right) = -\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}\left(\tau\right)c_{\mathbf{k}'}^{\dagger}\left(\tau'\right)e^{i\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\right\rangle \tag{27.52}$$

$$\mathcal{G}\left(\mathbf{k};\tau-\tau'\right) = \int d\left(\mathbf{r}-\mathbf{r}'\right)e^{-i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\left[-\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}\left(\tau\right)c_{\mathbf{k}'}^{\dagger}\left(\tau'\right)e^{i\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\right\rangle\right] \tag{27.53}$$

$$\boxed{\mathcal{G}\left(\mathbf{k};\tau-\tau'\right) = -\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right)c_{\mathbf{k}}^{\dagger}\left(\tau'\right)\right\rangle} \tag{27.54}$$

which could have been guessed from the start! Our definitions of Fourier transforms just make this work.

Remark 89 *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.*

The above is a general result for a translationally invariant system. Let us specialize to non-interacting particles, namely to quadratic diagonal Hamiltonian

$$K_0 = \sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} - \mu\right) c_{\mathbf{k}}^{+} c_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c_{\mathbf{k}}^{+} c_{\mathbf{k}} \tag{27.55}$$

The result for the Green's function may be obtained either directly by calculating the spectral weight and integrating, or from the definition or by integrating the equations of motion. The three ways of obtaining the simple result

$$\boxed{\mathcal{G}_0\left(\mathbf{k}; ik_n\right) = \frac{1}{ik_n - \zeta_{\mathbf{k}}}} \tag{27.56}$$

are instructive, so we will do all of them below. Assuming for one moment that the above result is correct, our rules for analytic continuation then immediately give us the retarded function

$$\boxed{G^R\left(\mathbf{k}; \omega\right) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}}} \tag{27.57}$$

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 $\zeta_{\mathbf{k}}$.

27.6.1 $\mathcal{G}_0\left(\mathbf{k}; \tau\right)$ and $\mathcal{G}_0\left(\mathbf{k}; ik_n\right)$ from the definition

To evaluate the Green's function from its definition, we need $c_{\mathbf{k}}\left(\tau\right)$. That quantity may be obtained by solving the Heisenberg equations of motion,

$$\frac{\partial c_{\mathbf{k}}}{\partial \tau} = \left[K_0, c_{\mathbf{k}}\right] = -\zeta_{\mathbf{k}} c_{\mathbf{k}} \tag{27.58}$$

The anticommutator was easy to evaluate using our standard trick Eq.(23.77). The resulting differential equation is easy to integrate given the initial condition on Heisenberg operators. We obtain,

$$c_{\mathbf{k}}\left(\tau\right) = e^{-\zeta_{\mathbf{k}}\tau} c_{\mathbf{k}} \tag{27.59}$$

so that substituting in the definition,

$$\mathcal{G}_0\left(\mathbf{k}; \tau\right) = -\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right) c_{\mathbf{k}}^{+}\right\rangle = -e^{-\zeta_{\mathbf{k}}\tau}\left[\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^{+}\right\rangle \theta\left(\tau\right) - \left\langle c_{\mathbf{k}}^{+} c_{\mathbf{k}}\right\rangle \theta\left(-\tau\right)\right] \tag{27.60}$$

using the standard result from elementary statistical mechanics,

$$\left\langle c_{\mathbf{k}}^{+} c_{\mathbf{k}}\right\rangle = f\left(\zeta_{\mathbf{k}}\right) = \frac{1}{e^{\beta\zeta_{\mathbf{k}}} + 1} \tag{27.61}$$

and $\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^{+}\right\rangle = 1 - \left\langle c_{\mathbf{k}}^{+} c_{\mathbf{k}}\right\rangle$ we obtain

$$\boxed{\mathcal{G}_0\left(\mathbf{k}; \tau\right) = -e^{-\zeta_{\mathbf{k}}\tau}\left[\left(1 - f\left(\zeta_{\mathbf{k}}\right)\right)\theta\left(\tau\right) - f\left(\zeta_{\mathbf{k}}\right)\theta\left(-\tau\right)\right]}. \tag{27.62}$$

Remark 90 *Inadequacy of Matsubara representation outside the domain of definition: We see here clearly that if $\tau < 0$ the equality*

$$\mathcal{G}_0\left(\mathbf{k}; \tau + \beta\right) = -\mathcal{G}_0\left(\mathbf{k}; \tau\right) \tag{27.63}$$

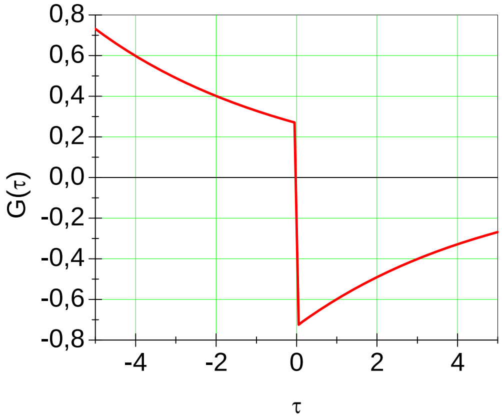

Figure 27-4 $\mathcal{G}_0(\mathbf{p}, \boldsymbol{\tau})$ for a value of momentum above the Fermi surface.

is satisfied because $e^{-\zeta_{\mathbf{k}}\beta}(1 - f(\zeta_{\mathbf{k}})) = f(\zeta_{\mathbf{k}})$. *On the other hand,*

$$\mathcal{G}_0(\mathbf{k}; \tau + 3\beta) \neq \mathcal{G}_0(\mathbf{k}; \tau + \beta) \tag{27.64}$$

as we might have believed if we had trusted the expansion

$$\mathcal{G}_0(\mathbf{k}; \tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-ik_n\tau} \mathcal{G}_0(\mathbf{k}; ik_n)$$

outside its domain of validity! The conclusion is that as long as the Matsubara frequency representation is used to compute functions inside the domain $-\beta < \tau < \beta$, *it is correct. The perturbation expansion of the interaction picture does not force us to use Green's functions outside this domain, so the Matsubara representation is safe!*

Remark 91 *Alternate evaluation of time evolution: We could have obtained the time evolution also by using the identity*

$$e^A C e^A = C + [A, C] + \frac{1}{2!}[A, [A, C]] + \frac{1}{3!}[A, [A, [A, C]]] + \ldots \tag{27.65}$$

that follows from expanding the exponential operators. This is less direct.

Remark 92 *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.(27-4) to (27-6). Note that the jump at* $\tau = 0$ *is always unity, reflecting the anticommutation relations. What is meant by antiperiodicity also becomes clear. The extremal values near* $\pm\beta$ *and* ± 0 *are simply related to the occupation number, independently of interactions.*

Let us continue with the derivation of the Matsubara frequency result $\mathcal{G}_0(\mathbf{k}; ik_n)$.

$$\mathcal{G}_0(\mathbf{k}; ik_n) = \int_0^\beta d\tau e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau) = -(1 - f(\zeta_{\mathbf{k}})) \int_0^\beta d\tau e^{ik_n\tau} e^{-\zeta_{\mathbf{k}}\tau} \tag{27.66}$$

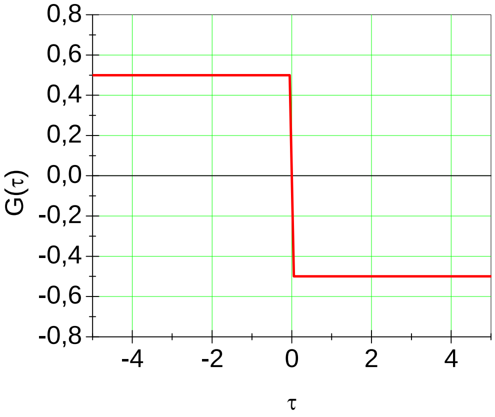

Figure 27-5 $\mathcal{G}_0(\mathbf{p}, \boldsymbol{\tau})$ for a value of momentum at the Fermi surface.

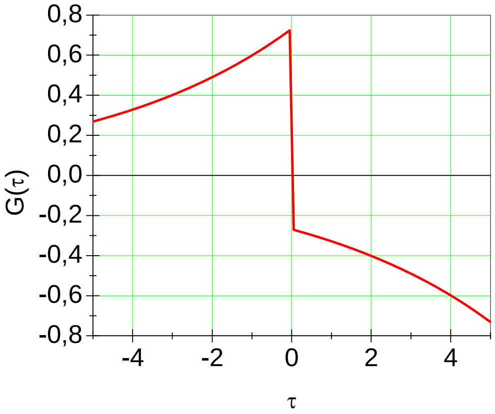

Figure 27-6 $\mathcal{G}_0(\mathbf{p}, \boldsymbol{\tau})$ for a value of momentum below the Fermi surface.

$$= -\left(1 - f\left(\zeta_{\mathbf{k}}\right)\right) \frac{e^{ik_n\beta} e^{-\zeta_{\mathbf{k}}\beta} - 1}{ik_n - \zeta_{\mathbf{k}}} \tag{27.67}$$

$$= -\left(1 - f\left(\zeta_{\mathbf{k}}\right)\right) \frac{-e^{-\zeta_{\mathbf{k}}\beta} - 1}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{27.68}$$

The last equality follows because

$$\left(1 - f\left(\zeta_{\mathbf{k}}\right)\right) = \frac{e^{\zeta_{\mathbf{k}}\beta}}{e^{\zeta_{\mathbf{k}}\beta} + 1} = \frac{1}{e^{-\zeta_{\mathbf{k}}\beta} + 1} \tag{27.69}$$

We thus have our final result Eq.(27.56) for non-interacting particles.

27.6.2 $\mathcal{G}_0\left(\mathbf{k};\tau\right)$ and $\mathcal{G}_0\left(\mathbf{k};ik_n\right)$ from the equations of motion

In complete analogy with the derivation in subsection (24.3) we can obtain the equations of motion in the quadratic case.

$$\frac{\partial}{\partial\tau}\mathcal{G}_0\left(\mathbf{k};\tau\right) = -\frac{\partial}{\partial\tau}\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right) c_{\mathbf{k}}^\dagger\right\rangle \tag{27.70}$$

$$= -\delta\left(\tau\right)\left\langle\left\{c_{\mathbf{k}}\left(\tau\right), c_{\mathbf{k}}^\dagger\right\}\right\rangle - \left\langle T_\tau\left(\frac{\partial}{\partial\tau}c_{\mathbf{k}}\left(\tau\right)\right) c_{\mathbf{k}}^\dagger\right\rangle \tag{27.71}$$

Using the equal-time anticommutation relations as well as the Heisenberg equations of motion for free particles Eq.(27.58) the above equation becomes,

$$\frac{\partial}{\partial\tau}\mathcal{G}_0\left(\mathbf{k};\tau\right) = -\delta\left(\tau\right) + \zeta_{\mathbf{k}}\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right) c_{\mathbf{k}}^\dagger\right\rangle \tag{27.72}$$

so that the equation of motion for the Matsubara propagator is

$$\boxed{\left(\tfrac{\partial}{\partial\tau} + \zeta_{\mathbf{k}}\right)\mathcal{G}_0\left(\mathbf{k};\tau\right) = -\delta\left(\tau\right)} \tag{27.73}$$

To obtain the Matsubara-frequency result, we only need to integrate on both sides using the general expression to obtain Fourier coefficients Eq.(27.23)

$$\int_{0^-}^{\beta^-}\left[\left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}}\right)\mathcal{G}_0\left(\mathbf{k};\tau\right)\right] e^{ik_n\tau} d\tau = -1 \tag{27.74}$$

so that integrating by parts,

$$e^{ik_n\tau}\left.\mathcal{G}_0\left(\mathbf{k};\tau\right)\right|_{0^-}^{\beta^-} - ik_n\mathcal{G}_0\left(\mathbf{k};ik_n\right) + \zeta_{\mathbf{k}}\mathcal{G}_0\left(\mathbf{k};ik_n\right) = -1 \tag{27.75}$$

Note that we had to specify that the domain of integration includes 0. The integrated term disappears because of the KMS boundary conditions (antiperiodicity) $e^{ik_n\tau}\left.\mathcal{G}_0\left(\mathbf{k};\tau\right)\right|_{0^-}^{\beta^-}$ Eq.(27.12). Indeed, antiperiodicity implies that

$$e^{ik_n\tau}\left.\mathcal{G}_0\left(\mathbf{k};\tau\right)\right|_{0^-}^{\beta^-} = -\mathcal{G}_0\left(\mathbf{k};\beta^-\right) - \mathcal{G}_0\left(\mathbf{k};0^-\right) = 0 \tag{27.76}$$

Eq.(27.75) for the Matsubara Green's function then immediately gives us the desired result Eq.(27.56).

27.7 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

$$T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{27.77}$$

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

$$\mathcal{G}\left(\mathbf{k};\tau\right) = T\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} \tag{27.78}$$

We already know that the Green's function has a jump at $\tau = 0$. In other words,

$$\left[\lim_{\tau\to 0^+} \mathcal{G}\left(\mathbf{k};\tau\right) = -\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \right\rangle\right] \neq \left[\lim_{\tau\to 0^-} \mathcal{G}\left(\mathbf{k};\tau\right) = \left\langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \right\rangle\right] \tag{27.79}$$

This inequality in turn means that

$$T\sum_n \frac{e^{-ik_n0^-}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{e^{-ik_n0^+}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{27.80}$$

The sum does not converge uniformly in the interval including $\tau = 0$ because the $1/n$ decrease for $n \to \infty$ is too slow. Even if we can obtain a finite limit for the last sum by combining positive and negative Matsubara frequencies, what makes physical sense is only one or the other of the two limits $\tau \to 0^\pm$.

Remark 93 Remark 94 *The jump,* $\lim_{\tau\to 0^-} \mathcal{G}\left(\mathbf{k};\tau\right) - \lim_{\tau\to 0^+} \mathcal{G}\left(\mathbf{k};\tau\right)$ *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* $\left(ik_n\right)^{-1}$ *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

$$\boxed{T\sum_n \frac{e^{-ik_n0^-}}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{e^{\beta\zeta_{\mathbf{k}}}+1} = f\left(\zeta_{\mathbf{k}}\right) = \mathcal{G}_0\left(\mathbf{k};0^-\right)} \tag{27.81}$$

$$\boxed{T\sum_n \frac{e^{-ik_n0^+}}{ik_n - \zeta_{\mathbf{k}}} = \frac{-1}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -1 + f\left(\zeta_{\mathbf{k}}\right) = \mathcal{G}_0\left(\mathbf{k};0^+\right)} \tag{27.82}$$

Obviously, the non-interacting Green's function has the correct jump $\mathcal{G}_0\left(\mathbf{k};0^-\right) - \mathcal{G}_0\left(\mathbf{k};0^+\right) = 1$.In addition, since $\mathcal{G}_0\left(\mathbf{k};0^-\right) = \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle$ and $\mathcal{G}_0\left(\mathbf{k};0^+\right) = -\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle$ the above results just tell us that $\left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle = f\left(\zeta_{\mathbf{k}}\right)$ that we know from elementary statistical mechanics. The anticommutation relations immediately give $-\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle = -1 + f\left(\zeta_{\mathbf{k}}\right)$ .So these sums over Matsubara frequencies better behave as advertized.

Proof: [6]To perform the sum over Matsubara frequencies, the standard trick is to go to the complex plane. The following function

$$-\beta\frac{1}{e^{\beta z}+1} \tag{27.83}$$

has poles for z equal to any fermionic Matsubara frequency: $z = ik_n$. Its residue at these poles is unity since for

$$z = ik_n + \delta z \tag{27.84}$$

we have

$$-\beta\frac{1}{e^{\beta z}+1} = -\beta\frac{1}{e^{ik_n\beta+\beta\delta z}+1} = -\beta\frac{1}{-1e^{\beta\delta z}+1} \tag{27.85}$$

$$\lim_{z-ik_n\to 0}\delta z\left[-\beta\frac{1}{e^{\beta z}+1}\right] = 1 \tag{27.86}$$

Similarly the following function has the same poles and residues:

$$\lim_{z-ik_n\to 0}\delta z\left[\beta\frac{1}{e^{-\beta z}+1}\right] = 1 \tag{27.87}$$

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.(27.86) this allows us to establish the equality

$$\frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = -\frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{\beta z}+1}\frac{e^{-z\tau}}{z-\zeta_{\mathbf{k}}} \tag{27.88}$$

This contour can be deformed, as illustrated in Fig.(27-7), into C_2+C_3 (going through C_1') with no contribution from the semi-circles at $\mathrm{Re}\,(z) = \pm\infty$ because $\frac{1}{e^{\beta z}+1}$ insures convergence when $\mathrm{Re}\,(z) > 0$ despite $e^{-z\tau}$ in the numerator, and $e^{-z\tau}$ insures convergence when $\mathrm{Re}\,(z) < 0$, $\tau < 0$. With the deformed contour $C_2 + C_3$, only the contribution from the pole in the clockwise direction is left so that we have

$$\boxed{\frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = \frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{\beta\zeta_{\mathbf{k}}}+1} = e^{-\zeta_{\mathbf{k}}\tau} f\left(\zeta_{\mathbf{k}}\right)} \tag{27.89}$$

which agrees with the value of $\mathcal{G}_0\left(\mathbf{k};\tau\right)$ in Eq.(27.62) when $\tau < 0$. In particular, when $\tau = 0^-$ we have proven the identity (27.82) . To evaluate the $\tau > 0$ case we use the same contour but with the other form of auxiliary function Eq.(27.87). We then obtain,

$$\frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = \lim_{\eta\to 0^+}\frac{1}{2\pi i}\int_{C_1}\frac{dz}{e^{-\beta z}+1}\frac{e^{-z\tau}}{z-\zeta_{\mathbf{k}}} \tag{27.90}$$

This contour can be deformed into $C_2 + C_3$ with no contribution from the semi-circles at $\mathrm{Re}\,(z) = \pm\infty$ because this time $e^{-z\tau}$ insures convergence when $\mathrm{Re}\,(z) > 0$, $\tau > 0$ and $\frac{1}{e^{-\beta z}+1}$ ensures convergence when $\mathrm{Re}\,(z) < 0$ 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

$$\boxed{\frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n-\zeta_{\mathbf{k}}} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}e^{\beta\zeta_{\mathbf{k}}}}{e^{\beta\zeta_{\mathbf{k}}}+1} = -e^{-\zeta_{\mathbf{k}}\tau}\left(1-f\left(\zeta_{\mathbf{k}}\right)\right)} \tag{27.91}$$

which agrees with the value of $\mathcal{G}_0\left(\mathbf{k};\tau\right)$ in Eq.(27.62) when $\tau < 0$. In particular, when $\tau = 0^+$ we have proven the identity (27.81).

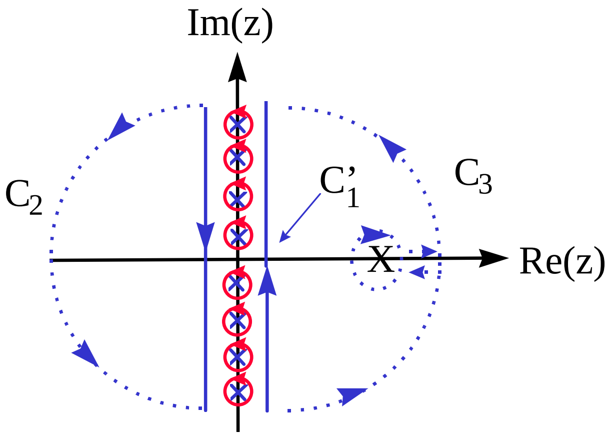

Figure 27-7 Evaluation of fermionic Matsubara frequency sums in the complex plane.

27.8 Exercices

27.8.1 $\mathcal{G}_0\left(\mathbf{k}; ik_n\right)$ from the spectral weight and analytical continuation

Find $\mathcal{G}_0\left(\mathbf{k}; ik_n\right)$ starting from the spectral weight for non-interacting particles and analytical continuation.

27.8.2 Représentation de Lehman et prolongement analytique

Soit la définition habituelle à l’aide d’un commutateur pour la susceptibilité de charge retardée

$$\chi_{\rho\rho}^{R}\left(\mathbf{q};t-t'\right)=i\theta\left(t-t'\right)\left\langle\left[\rho\left(\mathbf{q},t\right),\rho\left(-\mathbf{q},t'\right)\right]\right\rangle \tag{27.92}$$

Soit aussi la susceptibilité de charge correspondante de Matsubara

$$\begin{aligned}\chi_{\rho\rho}\left(\mathbf{q};\tau-\tau'\right) &= \left\langle T_\tau\rho\left(\mathbf{q},\tau\right)\rho\left(-\mathbf{q},0\right)\right\rangle && (27.93)\\ &= \theta\left(\tau\right)\left\langle\rho\left(\mathbf{q},\tau\right)\rho\left(-\mathbf{q},0\right)\right\rangle+\theta\left(-\tau\right)\left\langle\rho\left(-\mathbf{q},0\right)\rho\left(\mathbf{q},\tau\right)\right\rangle && (27.94)\end{aligned}$$

Les moyennes sont prises dans l’ensemble grand-canonique.

a) Trouvez les conditions de périodicité en temps imaginaire pour la fonction de Matsubara et déduisez-en un développement en fréquences discrètes.

b) Trouvez la représentation de Lehman pour chacune de ces deux fonctions de réponse et déduisez-en la règle permettant de faire le prolongement analytique d’une fonction à l’autre.

c) Vérifiez à partir de la représentation de Lehman que le poids spectral satisfait à la condition $\omega\chi_{\rho\rho}''\left(\mathbf{q},\omega\right)>0$.

d) Pourquoi n’a-t-on pas besoin d’un facteur de convergence pour calculer $\sum_{n=-\infty}^{\infty}\chi_{\rho\rho}\left(\mathbf{q};i\omega_n\right)$

27.8.3 Fonction de Green pour les bosons

Soient $a_{\lambda k}$ et $a^{+}_{\lambda k}$ les opérateurs de destruction et de création pour des phonons (statistiques de Bose) de polarisation λ et de nombre d'onde k. L'amplitude quantifiée correspondante est

$$Q_{\lambda,k} = \frac{1}{\sqrt{2\omega_{\lambda k}}}\left(a_{\lambda,k} + a^{+}_{\lambda,-k}\right)$$

$(\hbar = 1)$. Definissons le propagateur de phonon de Matsubara par:

$$D_{\lambda\lambda'}(k,k';\tau-\tau') = -2\sqrt{\omega_{\lambda k}\omega_{\lambda' k'}} < T_\tau\left[Q_{\lambda,k}\left(\tau\right)Q_{\lambda',-k'}\left(\tau'\right)\right] > .$$

Notez que pour les quantités bosoniques il n'y a pas de changement de signe lorsqu'on réordonne les opérateurs avec le produit chronologique.

a)

-Prouvez que $D_{\lambda\lambda'}(k,k';\tau-\tau')$ ne dépend que de $\tau-\tau'$.

- Dérivez la condition de périodicité en temps imaginaire.

- Donnez le développement de $D_{\lambda\lambda'}(k,k';\tau-\tau')$ en fréquences discrètes.

b) Soit

$$H = \sum_{k,\lambda}\omega_{\lambda k}[a^{+}_{\lambda,k}a_{\lambda,k} + \frac{1}{2}]$$

- Calculez le $D_\lambda(k,i\omega_n) \equiv D_{\lambda\lambda}\left(k,k;i\omega_n\right)$ correspondant.

- Trouvez le poids spectral.

- Montrez que le poids spectral s'annule à fréquence nulle. (Ceci est le cas général pour les bosons. Ceci permet de faire le prolongement analytique de la représentation spectrale sans rencontrer de problèmes avec la fréquence de Matsubara nulle.)

- Faites le prolongement analytique pour obtenir la fonction de Green retardée correspondante.

- Utilisez un contour dans le plan complexe et la formule de Cauchy pour évaluer

$$\sum_{n=-\infty}^{\infty} D_{\lambda\lambda}\left(k,k;i\omega_n\right)e^{i\omega_n 0^{\pm}} \tag{27.95}$$

Pourquoi le résultat ne dépend-t-il pas du facteur de convergence choisi, $e^{i\omega_n 0^{+}}$ ou $e^{i\omega_n 0^{-}}$?

27.8.4 Oscillateur harmonique en contact avec un réservoir

Un oscillateur harmonique de fréquence Ω interagissant avec un réservoir d'oscillateurs de fréquences ω_i est décrit par l'hamiltonien

$$H = \Omega a^{+}a + \sum_i \omega_i b_i^{+}b_i + \sum_i g_i\left(a^{+}b_i + ab_i^{+}\right)$$

Définissons les propagateurs de Matsubara suivants:

$$D\left(\tau\right) = - < T_\tau[a\left(\tau\right)a^{+}(0)] >$$

$$F_i\left(\tau\right) = - < T_\tau[b_i\left(\tau\right)a^{+}(0)] >$$

a) Ecrivez les equations du mouvement pour ces propagateurs.

b) Prenez la transformée de Fourier pour obtenir les équations du mouvement pour $D(i\omega_n)$ et $F_i(i\omega_n)$ et résolvez ces équations.

c) Faites le prolongement analytique pour obtenir les propagateurs retardés.

d) Décrivez la structure analytique de $D^R(\omega)$ dans le plan complexe, en montrant où sont les pôles et autres singularités. Vous pouvez aussi supposer que i peut prendre les valeurs de 1 à N et montrer que $D^R(\omega)$ s'écrit comme le rapport de deux polynômes, un de degré N au numérateur et un de degré $N+1$ au dénominateur.

e) Tracez un shéma du dénominateur de $D^R(\omega)$ pour montrer comment obtenir graphiquement comment le réservoir donne de nouveaux pôles. Pour simplifier la discussion, supposez qu'il n'y a que deux oscillateurs dans le réservoir et trouvez ce qui arrive si Ω est plus petit, plus grand, ou entre les deux fréquences des oscillateurs du réservoir.

27.8.5 Limite du continuum pour le réservoir, et irréversibilité

Continuons le problème précédent. Supposons que le nombre d'oscillateurs du réservoir augmente sans limite de telle sorte que la fonction

$$\Gamma(\omega) \equiv \sum_i g_i^2 \delta(\omega - \omega_i)$$

devienne continue

a) Montrez que si Γ et ses dérivées sont petites, la partie imaginaire du pôle de $D^R(\omega)$ est à $-i\pi\Gamma(\Omega)$. Donnez une expression intégrale pour le déplacement de la fréquence (encore une fois à l'ordre dominant en Γ).

b) Montrez que $D^R(t)$ décroît exponentiellement dans le temps. La fréquence d'oscillation est-elle déplacée? Dans cette limite nous avons un oscillateur quantique amorti! Pourquoi ce résultat est-il si différent de celui du problème précédent? Que se passe-t-il si le nombre d'oscillateurs est grand mais pas infini? Discutez la façon dont l'irréversibilité est apparue dans le problème, en particulier notez que la limite du volume infini (nombre d'oscillateurs infini) est prise avant $\eta \to 0$.

c) Si $\Gamma(\omega)$ est donné par

$$\Gamma(\omega) = \frac{\epsilon}{1 + \omega^2\tau^2}$$

trouvez, à l'ordre dominant en ϵ, la fréquence renormalisée et l'amortissement.

28. 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.

28.1 Spectral weight for non-interacting particles

The general result for the spectral weight in terms of the Green's function Eq.(27.46) gives us for non-interacting particles

$$\begin{aligned} A_0(\mathbf{k},\omega) &= i\left[\frac{1}{\omega+i\eta-\zeta_{\mathbf{k}}}-\frac{1}{\omega-i\eta-\zeta_{\mathbf{k}}}\right] && (28.1)\\ &= 2\pi\delta\left(\omega-\zeta_{\mathbf{k}}\right) && (28.2)\end{aligned}$$

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

28.2 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.(24.22),

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

and also in Sec. 11.6 on correlation functions.

Let us consider the more general many-body case, starting from the Matsubara Green's function. It suffices to insert a complete set of energy eigenstates between each field operator in the expression for the spectral weight

$$\begin{aligned}A(\mathbf{r},\mathbf{r}';t) &\equiv \left\langle\left\{\psi(\mathbf{r},t),\psi^+(\mathbf{r}',0)\right\}\right\rangle \qquad (28.3)\\ &= e^{\beta\Omega}\sum_{m,n}\Big[\langle n|\,e^{-\beta K}e^{iKt}\psi_S(\mathbf{r})\,e^{-iKt}\,|m\rangle\,\langle m|\,\psi_S^\dagger(\mathbf{r}')\,|n\rangle\\ &\quad+\langle n|\,e^{-\beta K}\psi_S^\dagger(\mathbf{r}')\,|m\rangle\,\langle m|\,e^{iKt}\psi_S(\mathbf{r})\,e^{-iKt}\,|n\rangle\Big]\end{aligned}$$

We now use $e^{-iKt}|n\rangle=e^{-iK_nt}|n\rangle$ 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 $\int dte^{i\omega' t}$ we have

$$\begin{aligned}A(\mathbf{r},\mathbf{r}';\omega') &= e^{\beta\Omega}\times \qquad (28.4)\\ &\sum_{mn}\Big[e^{-\beta K_n}\langle n|\,\psi_S(\mathbf{r})\,|m\rangle\,\langle m|\,\psi_S^\dagger(\mathbf{r}')\,|n\rangle\,2\pi\delta(\omega'-(E_m-\mu-E_n))\\ &+e^{-\beta K_n}\langle n|\,\psi_S^\dagger(\mathbf{r}')\,|m\rangle\,\langle m|\,\psi_S(\mathbf{r})\,|n\rangle\,2\pi\delta(\omega'-(E_n-\mu-E_m))\Big]\end{aligned}$$

One can interpret physically the spectral weight as follows. It has two pieces, the first one for excited states with one more particle, and the second one for excited states with one more hole. Photoemission experiments (See Einstein's Nobel prize) access this last piece of the spectral weight, while Bremsstrahlung inverse spectroscopy (BIS) experiments measure the first piece.[1] Excited particle states contribute to positive frequencies ω' if their excitation energy is larger than the chemical potential, $E_m-E_n>\mu$ and to negative frequencies otherwise. Zero frequency means that the excitation energy is equal to the chemical potential. In other words, every excited single-particle or single-hole state corresponds to a delta function in the spectral weight whose weight depends on the overlap between initial states with one more particle at $\mathbf{r}'$ or one more hole at $\mathbf{r}$, and the true excited states.

Remark 95 *At zero temperature, we have*

$$\begin{aligned}A(\mathbf{r},\mathbf{r}';\omega') &= \sum_m\Big[\langle 0|\,\psi_S(\mathbf{r})\,|m\rangle\,\langle m|\,\psi_S^\dagger(\mathbf{r}')\,|0\rangle\,2\pi\delta(\omega'+\mu-(E_m-E_0))\\ &\quad+\langle 0|\,\psi_S^\dagger(\mathbf{r}')\,|m\rangle\,\langle m|\,\psi_S(\mathbf{r})\,|0\rangle\,2\pi\delta(\omega'+\mu-(E_0-E_m))\Big] \qquad (28.5)\end{aligned}$$

In the first term, E_m is the energy of an eigenstate with one more particle than the ground state. The minimal energy to add a particle is μ, hence, $E_m-E_0\geq\mu$ and the delta function contributes to positive frequencies. In the second term however, E_m is the energy with one less particle so $0\leq E_0-E_m\leq\mu$ since we can remove a particle, or create a hole, below the Fermi surface. Hence the second term contributes to negative frequencies.

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[1] To be more specific, these experiments add or remove particles in momentum, not position eigenstates. The only change that this implies in the discussion above is that $\psi_S^{(\dagger)}(\mathbf{r})$ should be replaced by $c_{\mathbf{p}}^{(\dagger)}$.

Remark 96 *By using $K = H - \mu N$ instead of H as time evolution operator, we have adopted a convention where the frequency ω represents the energy of single-particle excitations above or below the chemical potential. If we had used H as evolution operator, only ω instead of the combination $\omega + \mu$ would have appeared in the delta functions above.*

The spectral representation Eq.(27.40) immediately tells us that the poles of the single-particle Green's functions are at the same position as delta functions in the spectral weight, in other words they are at the excited single-particle or single-hole states. Doing changes of dummy summation indices we can arrange so that it is always $\langle n|$ that has one less particle. Then,

$$\boxed{A\left(\mathbf{r},\mathbf{r}';\omega'\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n}+e^{-\beta K_m}\right)\langle n|\,\psi_S\left(\mathbf{r}\right)|m\rangle\,\langle m|\,\psi_S^{\dagger}\left(\mathbf{r}'\right)|n\rangle\,2\pi\delta\left(\omega'-\left(K_m-K_n\right)\right)} \tag{28.6}$$

Substituting in the spectral representation Eq.(27.40) we have,

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\frac{\langle n|\psi_S(\mathbf{r})|m\rangle\langle m|\psi_S^{\dagger}(\mathbf{r}')|n\rangle}{ik_n-(E_m-E_n-\mu)}} \tag{28.7}$$

This is the Lehman representation. It tells us how to interpret the poles of the analytically continued $\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)$.

Remark 97 *Standard way of proving analytical continuation formula: The standard way of proving that $G^R\left(\omega\right) = \lim_{ik_n\rightarrow\omega+i\eta}\mathcal{G}\left(ik_n\right)$ is to first find the Lehman representation for both quantities.*

28.3 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.(28.6)

$$\boxed{A\left(\mathbf{k},\omega'\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\left|\langle n|\,c_{\mathbf{k}}\,|m\rangle\right|^2 2\pi\delta\left(\omega'-\left(K_m-K_n\right)\right).} \tag{28.8}$$

The overlap matrix element $\left|\langle n|\,c_{\mathbf{k}}\,|m\rangle\right|^2$ that gives the magnitude of the delta function contribution to the spectral weight represents the overlap between the initial state with one more particle or hole in a momentum eigenstate and the true excited one-particle or one-hole state. The last equation clearly shows that $A\left(\mathbf{k},\omega'\right)/\left(2\pi\right)$ is positive and we already know that it is normalized to unity,

$$\int\frac{d\omega'}{2\pi}A\left(\mathbf{k},\omega'\right) = \left\langle\left\{c_{\mathbf{k}},c_{\mathbf{k}}^{\dagger}\right\}\right\rangle = 1. \tag{28.9}$$

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 98 *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 99 *Physical reason for high-frequency fall-off: The explicit expression for the spectral weight Eq.(28.8) suggests why the spectral weight falls off fast at large frequencies for a given $\mathbf{k}$,as we have discussed in Subsection (29.1). 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.*

28.4 Analog of the fluctuation dissipation theorem

We have seen in Eq.(C.10) the fluctuation dissipation theorem for correlation functions, (with $\hbar = 1$)

$$S_{A_iA_j}(\omega) = 2(1 + n_B(\omega))\chi''_{A_iA_j}(\omega) \tag{28.10}$$

where $n_B(\omega)$ is the Bose function. That can also be written in the form

$$\int dte^{i\omega t} \langle A_i(t) A_j \rangle = (1 + n_B(\omega)) \int dte^{i\omega t} \langle [A_i(t), A_j] \rangle . \tag{28.11}$$

It would be nice to find the analog for the Green's function because we saw, when we discussed ARPES in Sec. 24.1, that the cross section for angle-resolved photoemission measures $\int dte^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle$,which looks like one piece of the anticommutator.

The key is the real time version of the antiperiodicity that we discussed for Matsubara Green's functions in Sec. 27.4. We will demonstrate that

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \int dte^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle = f(\omega) A\left(\mathbf{k}_{||}, \omega\right) . \tag{28.12}$$

Proof: The most direct and simple proof is from the Lehman representation Eq.(28.8). To get a few more general results about $G^<\left(\mathbf{k}_{||}, \omega\right) = i \int dte^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle$ and $G^>\left(\mathbf{k}_{||}, \omega\right) = -i \int dte^{i\omega t} \left\langle c_{\mathbf{k}_{||}}(t) c^{\dagger}_{\mathbf{k}_{||}} \right\rangle$ we present the following alternate proof. The cross section is proportional to the Fourier transform of $G^<\left(\mathbf{k}_{||}, \omega\right)$ as defined in Eq.(26.11).

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \int dte^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle \equiv -iG^<\left(\mathbf{k}_{||}, \omega\right) \tag{28.13}$$

One can relate $G^<$ and $G^>$ to the spectral weight in a very general way through the Fermi function. This is done using the usual cyclic property of the trace (fluctuation-dissipation theorem). From

$$\begin{aligned}
\left\langle c_{\mathbf{k}_{||}}(t)\, c^\dagger_{\mathbf{k}_{||}}\right\rangle &= Z^{-1}\mathrm{Tr}\left[e^{-\beta K}\left(e^{iKt}c_{\mathbf{k}_{||}}e^{-iKt}\right)c^\dagger_{\mathbf{k}_{||}}\right] && (28.14)\\
&= Z^{-1}\mathrm{Tr}\left[\left(e^{\beta K}e^{-\beta K}\right)c^\dagger_{\mathbf{k}_{||}}e^{-\beta K}\left(e^{iKt}c_{\mathbf{k}_{||}}e^{-iKt}\right)\right] && (28.15)\\
&= \left\langle c^\dagger_{\mathbf{k}_{||}}c_{\mathbf{k}_{||}}(t+i\beta)\right\rangle && (28.16)
\end{aligned}$$

one finds by simple use of definitions and change of integration variables,

$$\begin{aligned}
A\left(\mathbf{k}_{||},\omega\right) &= \int dt e^{i\omega t}\left\langle c^\dagger_{\mathbf{k}_{||}}c_{\mathbf{k}_{||}}(t)+c_{\mathbf{k}_{||}}(t)\,c^\dagger_{\mathbf{k}_{||}}\right\rangle && (28.17)\\
&= \int dt e^{i\omega t}\left\langle c^\dagger_{\mathbf{k}_{||}}c_{\mathbf{k}_{||}}(t)\right\rangle + \int dt e^{i\omega(t+i\beta-i\beta)}\left\langle c^\dagger_{\mathbf{k}_{||}}c_{\mathbf{k}_{||}}(t+i\beta)\right\rangle\\
&= \left(1+e^{\beta\omega}\right)\int dt e^{i\omega t}\left\langle c^\dagger_{\mathbf{k}_{||}}c_{\mathbf{k}_{||}}(t)\right\rangle && (28.18)\\
&= f(\omega)^{-1}\left(-iG^<\left(\mathbf{k}_{||},\omega\right)\right) && (28.19)
\end{aligned}$$

Substituting in Eq.(28.13) proves Eq.(28.12). Note that since from the definitions in Eqs.(26.10) and (26.11) the spectral weight is obtained from

$$A\left(\mathbf{k}_{||},\omega\right) = -i\left[G^<\left(\mathbf{k}_{||},\omega\right) - G^>\left(\mathbf{k}_{||},\omega\right)\right] \tag{28.20}$$

we also have the result

$$iG^>\left(\mathbf{k}_{||},\omega\right) = \left(1-f(\omega)\right)A\left(\mathbf{k}_{||},\omega\right) \tag{28.21}$$

28.5 Some experimental results from ARPES

The state of technology and historical coincidences have conspired so that the first class of layered (quasi-two-dimensional) compounds that became available for ARPES study around 1990 were high temperature superconductors. These materials have properties that make them non-conventional materials that are not yet understood using standard approaches of solid-state Physics. Hence, people started to look for two-dimensional materials that would behave as expected from standard models. Such a material, semimetallic $TiTe_2$ was finally found around 1992. For our purposes, quasi-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.(28-1).

We have to remember that the incident photon energy is $21.2eV$ while the variation of ω is on a scale of $200meV$ so that, for all practical purposes, the momentum vector in Fig.(24-1) is a fixed length vector. Hence, the angle with respect to the incident photon suffices to define the value of $\mathbf{k}_{||}$. Each curve in Fig.(28-1) is for a given $\mathbf{k}_{||}$, in other words for a given angle measured from the direction of incidence of the photon. The intensity is plotted as a function of the energy of the outgoing electron. The zero corresponds to an electron extracted from the Fermi level. Electrons with a smaller kinetic energy come from states with larger binding energy. In other words, each of the curves above is basically a plot of the hole-like part of $A\left(\mathbf{k}_{||},\omega\right)$,or if you want $f(\omega)A\left(\mathbf{k}_{||},\omega\right)$. From band

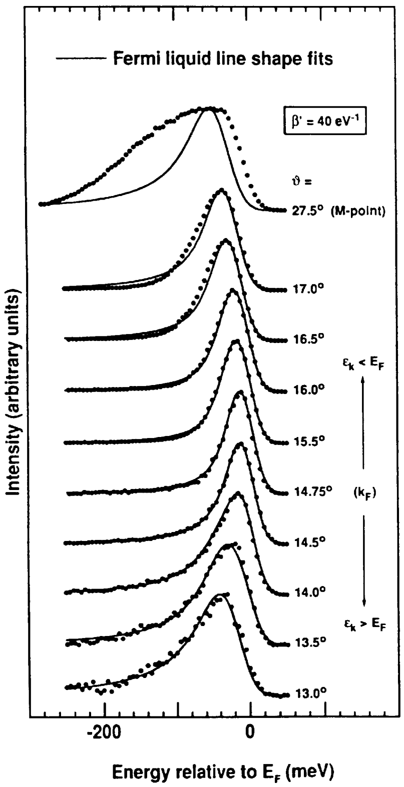

Figure 28-1 ARPES spectrum of $1-T-TiTe_2$, after R. Claessen, R.O. Anderson, J.W. Allen, C.G. Olson, C. Janowitz, W.P. Ellis, S. Harm, M. Kalning, R. Manzke, and M. Skibowski, Phys. Rev. Lett **69**, 808 (1992).

structure calculations, one knows that the angle $\theta = 14.75^0$ corresponds to the Fermi level (marked k_F on the plot) of a $Ti - 3d$ derived band. It is for this scattering angle that the agreement between experiment and Fermi liquid theory is best (see Sec.(28.7) below). The plots for angles $\theta < 14.75^0$ corresponds to wave vectors above the Fermi level. There, the intensity is *much* smaller than for the other peaks. For $\theta = 13^0$, the experimental results are scaled up by a factor 16. The intensity observed for wave-vectors above $\omega = 0$ comes from the Fermi function and also from the non-zero projection of the state with a given $\mathbf{k}$ on several values of ω in the spectral weight.

The energy resolution is $35meV$. Nevertheless, it is clear that the line shapes are larger than the energy resolution: Clearly the spectral weight is not a delta function and the electrons in the system are not free particles. Nevertheless, there is a definite maximum in the spectra whose position changes with $\mathbf{k}_{||}$. It is tempting to associate the width of the line to a lifetime. In other words, a natural explanation of these spectra is that the electrons inside the system are "quasiparticles" whose energy disperses with wave vector and that have a lifetime. We try to make these concepts more precise below.

28.6 Quasiparticles[9]

The intuitive notions we may have about lifetime and effective mass of an electron caused by interactions in a solid can all be extracted from the self-energy, as we will see. For a general interacting system, the one-particle Green's function takes the form,

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \sum^R(\mathbf{k},\omega)} \tag{28.22}$$

The corresponding spectral weight is,

$$\begin{aligned} A(\mathbf{k},\omega) &= -2\,\mathrm{Im}\,G^R(\mathbf{k},\omega) & (28.23)\\ &= \frac{-2\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{\left(\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\sum^R(\mathbf{k},\omega)\right)^2 + \left(\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2} & (28.24)\end{aligned}$$

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, at fixed $\mathbf{k}$,there is a value of ω that satisfies

$$\boxed{\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega) = 0} \tag{28.25}$$

We assume the solution of this equation exists. Let $E_{\mathbf{k}} - \mu$ be the value of ω for which this equation is satisfied. $E_{\mathbf{k}}$ is the so-called *quasiparticle energy*. This energy is clearly in general different from the results of band structure calculations that are usually obtained by neglecting the frequency dependence of the self-energy. Expanding $\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$ around $\omega = E_{\mathbf{k}} - \mu$ where $A(\mathbf{k},\omega)$ is a maximum, we find

$$\begin{aligned} \omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega) &\approx 0 + \frac{\partial}{\partial\omega}\left[\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\right]_{\omega=E_{\mathbf{k}}-\mu}(\omega - E_{\mathbf{k}} + \mu) + \dots \\ &\approx \left(1 - \left.\frac{\partial\,\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)}{\partial\omega}\right|_{E_{\mathbf{k}}-\mu}\right)(\omega - E_{\mathbf{k}} + \mu) + \dots & (28.26)\end{aligned}$$

If we define the "quasiparticle weight" or square of the wave function renormalization by

$$\boxed{Z_{\mathbf{k}} = \frac{1}{1-\frac{\partial}{\partial\omega}\operatorname{Re}\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}}} \tag{28.27}$$

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

$$A(\mathbf{k},\omega) \approx 2\pi Z_{\mathbf{k}}\frac{1}{\pi}\frac{-Z_{\mathbf{k}}\operatorname{Im}\sum^R(\mathbf{k},\omega)}{(\omega-E_{\mathbf{k}}+\mu)^2+\left(Z_{\mathbf{k}}\operatorname{Im}\sum^R(\mathbf{k},\omega)\right)^2}+inc \tag{28.28}$$

$$= 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega-E_{\mathbf{k}}+\mu)^2+(\Gamma_{\mathbf{k}}(\omega))^2}\right]+inc \tag{28.29}$$

The last equation needs some explanation. First, it is clear that we have defined the scattering rate

$$\boxed{\Gamma_{\mathbf{k}}(\omega) = -Z_{\mathbf{k}}\operatorname{Im}\Sigma^R(\mathbf{k},\omega)} \tag{28.30}$$

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

$$Z_{\mathbf{k}} \leq 1 \tag{28.31}$$

and that there are additional contributions to the spectral weight that we have denoted *inc* in accord with the usual terminology of "incoherent background". The equality in the last equation holds only if the real part of the self-energy is frequency independent.

It is also natural to ask how the quasiparticle disperses, in other words, what is its effective Fermi velocity compared with that of the bare particle. Let us define the bare velocity by

$$v_{\mathbf{k}} = \nabla_{\mathbf{k}}\zeta_{\mathbf{k}} \tag{28.32}$$

and the renormalized velocity by

$$v_{\mathbf{k}}^* = \nabla_{\mathbf{k}}E_{\mathbf{k}} \tag{28.33}$$

Then the relation between both quantities is easily obtained by taking the gradient of the quasiparticle equation Eq.(28.25)

$$\nabla_{\mathbf{k}}\left[E_{\mathbf{k}}-\mu-\zeta_{\mathbf{k}}-\operatorname{Re}\Sigma^R(\mathbf{k},E_{\mathbf{k}}-\mu)=0\right] \tag{28.34}$$

$$v_{\mathbf{k}}^*-v_{\mathbf{k}}-\nabla_{\mathbf{k}}\operatorname{Re}\Sigma^R(\mathbf{k},E_{\mathbf{k}}-\mu)-\left.\frac{\partial\operatorname{Re}\Sigma^R(\mathbf{k},\omega)}{\partial\omega}\right|_{E_{\mathbf{k}}-\mu}v_{\mathbf{k}}^*=0 \tag{28.35}$$

where $\nabla_{\mathbf{k}}$ in the last equation acts only on the first argument of $\operatorname{Re}\Sigma^R(\mathbf{k},E_{\mathbf{k}}-\mu)$. The last equation is easily solved if we can write that $\mathbf{k}$ dependence of Σ^R as a function of $\zeta_{\mathbf{k}}$ instead, something that is always possible for spherical Fermi surfaces. In such a case, we have

$$\boxed{v_{\mathbf{k}}^* = v_{\mathbf{k}}\frac{1+\frac{\partial}{\partial\zeta_{\mathbf{k}}}\operatorname{Re}\Sigma^R(\mathbf{k},E_{\mathbf{k}}-\mu)}{1-\frac{\partial}{\partial\omega}\operatorname{Re}\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}}} \tag{28.36}$$

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

$$\boxed{\frac{m}{m^*} = \lim_{\mathbf{k}\to\mathbf{k}_F} \frac{1+\frac{\partial}{\partial\zeta_{\mathbf{k}}} \operatorname{Re}\Sigma^R(\mathbf{k},E_{\mathbf{k}}-\mu)}{1-\frac{\partial}{\partial\omega} \operatorname{Re}\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}}} \tag{28.37}$$

28.7 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.(28.29) 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

$$\Sigma^R = \Sigma' + i\Sigma'' \tag{28.38}$$

Our two hypothesis imply that Σ'' has the Taylor expansion

$$\Sigma''(\mathbf{k}_F;\omega) = \alpha\omega - \gamma\omega^2 + \dots \tag{28.39}$$

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.(28.22). 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.(19.1), (Sec.29.2) or from the spectral representation,

$$
\begin{aligned}
\lim_{\omega\rightarrow small}\left[\Sigma'\left(\mathbf{k}_F;\omega\right)-\Sigma'\left(\mathbf{k}_F;\infty\right)\right] &= \lim_{\omega\rightarrow small}\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\Sigma''\left(\mathbf{k}_F;\omega'\right)}{\omega'-\omega} && (28.40)\\
&= \mathcal{P}\int\frac{d\omega'}{\pi}\frac{-\gamma\left(\omega'^2-\omega^2+\omega^2\right)}{\omega'-\omega} && (28.41)\\
&= \mathcal{P}\int\frac{d\omega'}{\pi}\frac{-\gamma\left(\omega'-\omega\right)\left(\omega'+\omega\right)}{\omega'-\omega}+O\left(\omega^2\right) && (28.42)\\
&= -\gamma\mathcal{P}\int\frac{d\omega'}{\pi}\omega'-\gamma\omega\mathcal{P}\int\frac{d\omega'}{\pi}+O\left(\omega^3\right) && (28.43)
\end{aligned}
$$

We assume cutoffs in the integrals that can be different at low and high frequency. 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 $\Sigma'\left(\mathbf{k}_F;\infty\right)$ does not suffice to evaluate the chemical potential). The second term in the last equation tells us that

$$
\left.\frac{\partial}{\partial\omega}\Sigma'\left(\mathbf{k}_F,\omega\right)\right|_{\omega=0}=-\gamma\mathcal{P}\int\frac{d\omega'}{\pi}=\left[\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\Sigma''\left(\mathbf{k}_F;\omega'\right)}{\left(\omega'\right)^2}\right] \qquad (28.44)
$$

Since $\Sigma''=-\gamma\omega^2$ the integral exists and is negative (if we assume a frequency cutoff as discussed below), hence

$$
\left.\frac{\partial}{\partial\omega}\Sigma'\left(\mathbf{k},\omega\right)\right|_{\omega=0}<0 \qquad (28.45)
$$

This in turn means that the corresponding value of Z_{k_F} is less than unity, as we had concluded in Eqs.(28.27) and (28.31) above. In summary, the analyticity hypothesis along with the vanishing of $\Sigma''(0)$ implies the existence of quasiparticles.

Remark 100 *Warning: there are subtleties. The above results assume that there is a cutoff to* $\Sigma''\left(\mathbf{k}_F;\omega'\right)$. *The argument just mentioned in Eq.(28.44) fails when the integral diverges. Then, the low frequency expansion for the self-energy in Eq.(28.41) 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,* $\Sigma''\left(\mathbf{k}_F;\omega\right)\sim\omega^2+\left(\pi T\right)^2$ *so that the* $\left(\pi T\right)^2$ *appears to lead to a divergent integral in Eq.(28.44). Returning to the original Kramers-Krönig expression fo* Σ' *however, the principal part integral shows that the constant term* $\left(\pi T\right)^2$ *for* $\Sigma''\left(\mathbf{k}_F;\omega\right)$ *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.(28-1) 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.(28.30)

$$
\Gamma_{k_F}\left(\omega\right)=Z_{k_F}\gamma\omega^2=\gamma'\omega^2. \qquad (28.46)
$$

Contrary to E_k, the damping parameter γ' is the same for all curves. The solid-line fits are obtained with $\gamma'=40eV^{-1}$ (β' on the figure). The fits become increasingly worse as one moves away from the Fermi surface, as expected. It is important to

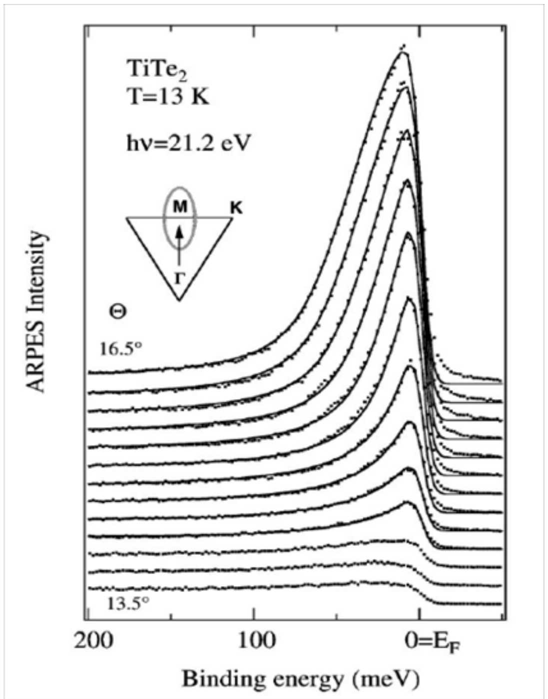

Figure 28-2 Figure 1 from Ref.[19] for the ARPES spectrum of 1*T*-TiTe$_2$ measured near the Fermi surface crossing along the high-symmetry ΓM direction ($\theta = 0$ is normal emission). The lines are results of Fermi liquid fits and the inset shows a portion of the Brillouin zone with the relevant ellipsoidal electron pocket.

notice, however, that even the small left-over weight for wave-vectors above the Fermi surface $\left(\theta < 14.75^0\right)$ can be fitted with the same value of γ. This weight is the tail of a quasiparticle that could be observed at positive frequencies in inverse photoemission experiments (so-called BIS). The authors compared the results of their fits to the theoretical estimate,[12] $\gamma = 0.067\omega_p/\varepsilon_F^2$. Using $\omega_p = 18.2eV$, $\varepsilon_F = 0.3eV$ and the extrapolated value of Z_{k_F} obtained by putting[2] $r_s = 10$ 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. (28-2). 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 $\hbar v_F = 0.73 \pm 0.1 eV\ \dot{A}$ close to band structure calculations, $\hbar v_F = 0.68\ eV\ \dot{A}$ and γ' that varies between 0.5 eV^{-1} (16^0) and 0.9 eV^{-1} (14.5^0). The Fermi liquid fit is just as good, but the interpretation of the origin of the broadening terms is different. This shows that there is much uncertainty still in the interpretation of ARPES data, even for Fermi liquids.

Theoretical estimates for high-temperature superconductors are two orders of magnitude smaller than the observed result [11].

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[2] r_s is the average electron spacing expressed in terms of the Bohr radius.

Remark 101 *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 102 *Failure of Fermi liquid at high-frequency: Clearly the Fermi liquid expression for the self-energy fails at large frequencies since we know from its spectral representation that the real-part of the self-energy goes to a frequency-independent constant at large frequency, the first correction being proportional to* $1/\omega$ *as discussed below in subsection (29.1). 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 103 *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.(28.44). When* $\Sigma''(\omega)$ *vanishes slower than* ω^2, *then Eq.(28.44) for the slope of the real part is not valid. The integral does not converge uniformly and it is not possible to interchange the order of differentiation and integration. In such a case it is possible to have the opposite inequality for the slope of the real part* $\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k},\omega)\big|_{\omega=0} > 0$. *This does not lead to any contradiction, such as* $Z_{k_F} > 1$, *because there is no quasiparticle solution at* $\omega = 0$ *in this case. This situation occurs for example in two dimensions when classical thermal fluctuations create a pseudogap in the normal state before a zero-temperature phase transition is reached [14].*

28.8 Momentum distribution in an interacting system

In an interacting system, momentum is not a good quantum number so $\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle$ is *not* equal to the Fermi distribution. On the other hand, $\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle$ can be computed from the spectral weight. By taking the Fourier transform of Eq.(28.12) $\int dt e^{i\omega t}\left\langle c^\dagger_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t)\right\rangle = f(\omega) A\left(\mathbf{k}_{||},\omega\right)$ one finds

$$\boxed{\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle = \lim_{\tau\to 0^-}\mathcal{G}(\mathbf{k},\tau) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi} f(\omega') A(\mathbf{k},\omega')}. \tag{28.47}$$

Alternate derivation

$$\begin{aligned}\left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle &= \lim_{\tau\to 0^-}\left[-\left\langle T_\tau c_{\mathbf{k}}(\tau) c^\dagger_{\mathbf{k}}\right\rangle\right] \\ &= \lim_{\tau\to 0^-}\mathcal{G}(\mathbf{k},\tau)\end{aligned} \tag{28.48}$$

> To compute the latter quantity from the spectral weight, it suffices to use the spectral representation Eq.(27.40)
>
> $$\begin{aligned} \lim_{\tau\to 0^-}\mathcal{G}(\mathbf{k},\tau) &= T\lim_{\tau\to 0^-}\sum_{n=-\infty}^{\infty}e^{-ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) \\ &= T\lim_{\tau\to 0^-}\sum_{n=-\infty}^{\infty}e^{-ik_n\tau}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{k},\omega')}{ik_n-\omega'} \end{aligned} \quad (28.49)$$
>
> Using the result Eq.(27.81) found above for the sum over Matsubara frequencies, we are left with the desired result.

Our result means that the momentum distribution is a Fermi-Dirac distribution only if the spectral weight is a delta function. This occurs for free particles or, more generally if the real-part of the self-energy is frequency independent since, in this case, the Kramers-Kronig relations imply that the imaginary part of the self-energy vanishes so that Eq.(28.24) for the spectral weight gives us a delta function.

Remark 104 *Jump of the momentum distribution at the Fermi level: Even if* $\left\langle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}\right\rangle$ *is no-longer a Fermi-Dirac distribution in an interacting system, nevertheless at zero-temperature in a system subject only to electron-electron interaction, there is a jump in* $\left\langle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}\right\rangle$ *at the Fermi level. The existence of this jump can be seen as follows. At zero temperature, our last result gives us*

$$\left\langle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}\right\rangle = \int_{-\infty}^{0}\frac{d\omega'}{2\pi}A(\mathbf{k},\omega') \quad (28.50)$$

Let us take the quasiparticle form Eq.(28.29) of the spectral weight with the Fermi liquid expression Eq.(28.46) for the scattering rate. The incoherent background varies smoothly with $\mathbf{k}$ *and hence cannot lead to any jump in occupation number. The quasiparticle piece on the other hand behaves when* $k\to k_F$, *or in other words when* $E_{\mathbf{k}}-\mu\to 0$, *as* $Z_{k_F}\delta(\omega)$. *At least crudely speaking. When* $E_{\mathbf{k}}-\mu\to 0^-$, *this delta function is inside the integration domain hence it contributes to the integral, while when* $E_{\mathbf{k}}-\mu\to 0^+$ *the delta function is outside and does not contribute to the integral. This means that there is a big difference between these two nearby wave vectors, namely*

$$\lim_{\mathbf{k}\to\mathbf{k}_f^-}\left\langle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}\right\rangle - \lim_{\mathbf{k}\to\mathbf{k}_f^+}\left\langle c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}\right\rangle = Z_{k_F} \quad (28.51)$$

In the above argument, we have done as if $\Gamma_{\mathbf{k}}(\omega)$ *was frequency independent and infinitesimally small in Eq.(28.29). 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 105 *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.(28-3). 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.*

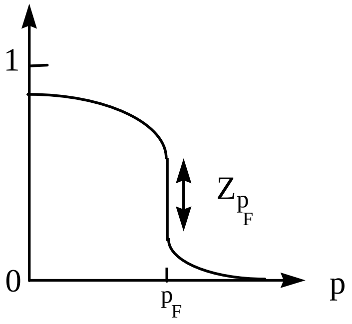

Figure 28-3 Qualitative sketch of the zero-temperature momentum distribution in an interacting system.

Remark 106 *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.*

29. 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.

29.1 Asymptotic behavior of $\mathcal{G}\left(\mathbf{k};ik_n\right)$ and $\Sigma\left(\mathbf{k};ik_n\right)$

As usual, the high-frequency asymptotic properties of the Green's function are determined by sum rules. From the spectral representation(27.40), we obtain, for the general interacting case

$$\lim_{ik_n\rightarrow\infty}\mathcal{G}\left(\mathbf{k};ik_n\right)=\lim_{ik_n\rightarrow\infty}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{k};\omega'\right)}{ik_n-\omega'} \tag{29.1}$$

$$=\lim_{ik_n\rightarrow\infty}\frac{1}{ik_n}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)=\lim_{ik_n\rightarrow\infty}\frac{1}{ik_n}\left\langle\left\{c_{\mathbf{k}},c_{\mathbf{k}}^{+}\right\}\right\rangle=\lim_{ik_n\rightarrow\infty}\frac{1}{ik_n} \tag{29.2}$$

Defining the self-energy as usual

$$\mathcal{G}\left(\mathbf{k};ik_n\right)=\frac{1}{ik_n-\zeta_{\mathbf{k}}-\Sigma\left(\mathbf{k},ik_n\right)} \tag{29.3}$$

the correct asymptotic behavior for the Green's function implies that the self-energy at high frequency cannot diverge: It must go to a constant independent of frequency

$$\lim_{ik_n\rightarrow\infty}\Sigma\left(\mathbf{k},ik_n\right)=cst. \tag{29.4}$$

We will see later that the value of this constant is in fact given correctly by the Hartree-Fock approximation.

The converse of the above result [10] for the Green's function, is that if

$$\lim_{ik_n\rightarrow\infty}\mathcal{G}\left(\mathbf{k};ik_n\right)=\lim_{ik_n\rightarrow\infty}\frac{1}{ik_n}$$

then that is all that is needed to obtain an approximation for the Green's function which obeys the anticommutation relation:

$$\mathcal{G}\left(\mathbf{k};0^{-}\right)-\mathcal{G}\left(\mathbf{k};0^{+}\right)=\left\langle c_{\mathbf{k}}^{+}c_{\mathbf{k}}\right\rangle+\left\langle c_{\mathbf{k}}c_{\mathbf{k}}^{+}\right\rangle=1 \tag{29.5}$$

Proof :It suffices to notice that

$$\mathcal{G}\left(\mathbf{k};0^-\right)-\mathcal{G}\left(\mathbf{k};0^+\right)=\frac{1}{\beta}\sum_n\left[e^{-ik_n0^-}-e^{-ik_n0^+}\right]\mathcal{G}\left(\mathbf{k};ik_n\right) \tag{29.6}$$

We can add and subtract the asymptotic behavior to obtain,

$$\frac{1}{\beta}\sum_n\left[\left(e^{-ik_n0^-}-e^{-ik_n0^+}\right)\left(\mathcal{G}\left(\mathbf{k};ik_n\right)-\frac{1}{ik_n}\right)\right]+\frac{1}{\beta}\sum_n\left(e^{-ik_n0^-}-e^{-ik_n}\right)\frac{1}{ik_n} \tag{29.7}$$

In the first sum, $\mathcal{G}\left(\mathbf{k};ik_n\right)-\frac{1}{ik_n}$ decays faster than $\frac{1}{ik_n}$ so that the convergence factors are not needed for the sum to converge. This means that this first sum vanishes. The last sum gives unity, as we easily see from the previous section. This proves our assertion.

Remark 107 *High-frequency expansion for the Green's function and sum-rules: The coefficients of the high-frequency expansion of* $\mathcal{G}\left(\mathbf{k};ik_n\right)$ *in powers of* $1/ik_n$ *are obtained from sum rules on the spectral weight, in complete analogy with what we have found in previous chapters. The fact that* $A\left(\mathbf{k},\omega\right)$ *falls fast enough to allow us to expand under the integral sign follows from the fact that all frequency moments of* $A\left(\mathbf{k},\omega\right)$ *, namely* $\int d\omega\omega^n A\left(\mathbf{k},\omega\right)$ *, exist and are given by equal-time commutators. Explicit expressions for* $A\left(\mathbf{k},\omega\right)$ *in terms of matrix elements, as given in Subsection(28.3) above, show physically why* $A\left(\mathbf{k},\omega\right)$ *falls so fast at large frequencies. As an example, to show that the coefficient of the* $1/ik_n$ *term in the high frequency expansion is equal to* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)$ *it is sufficient that* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|\omega' A\left(\mathbf{k};\omega'\right)\right|$ *exists.[8] This can be seen as follows,*

$$\begin{aligned}
ik_n\mathcal{G}\left(\mathbf{k};ik_n\right)-\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)\left(\frac{ik_n}{ik_n-\omega'}-1\right) && (29.8)\\
&= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)\frac{\omega'}{ik_n-\omega'} && (29.9)\\
&\leq \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|A\left(\mathbf{k};\omega'\right)\frac{\omega'}{ik_n-\omega'}\right| && (29.10)\\
&\leq \left|\frac{1}{ik_n}\right|\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left|A\left(\mathbf{k};\omega'\right)\omega'\right| && (29.11)
\end{aligned}$$

If the integral exists then, it is a rigorous result that

$$\lim_{ik_n\to\infty}ik_n\mathcal{G}\left(\mathbf{k};ik_n\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right) \tag{29.12}$$

This is an important result. It suggests that approximate theories that give 1 *as the coefficient of* $\left(ik_n\right)^{-1}$ *in the high frequency expansion have a normalized spectral weight. However[8] the above proof assumes that there is indeed a spectral representation for* $\mathcal{G}\left(\mathbf{k};ik_n\right)$*. A Green's function for a theory that is not causal fails to have a spectral representation. If a spectral representation is possible, the analytically continued approximate* $G^R\left(\mathbf{k},\omega\right)$ *is necessarily causal. Approximate theories may not be causal. This failure of causality may reflect a phase transition, as we will see later, or may simply be a sign that the approximation is bad. As an example, suppose that we obtain* $\mathcal{G}\left(\mathbf{k};ik_n\right)=\left(ik_n-ia\right)^{-1}$*. This has the correct high-frequency behavior but its analytical continuation does not satisfy causality. It has no spectral representation. On the other hand,* $\mathcal{G}\left(\mathbf{k};ik_n\right)=\left(ik_n+\left(k_n/\left|k_n\right|\right)ia\right)^{-1}$ *has a Lorentzian as a spectral weight and is causal. It may also occur that the approximate theory may have* $\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A\left(\mathbf{k};\omega'\right)=1$ *but* $A\left(\mathbf{k};\omega'\right)<0$ *for some range of* ω'*. This unphysical result may again signal that the approximate theory fails because of a phase transition or because it is a bad approximation.*

29.2 Implications of causality for G^R and Σ^R

Consider the retarded Green function as a matrix in $\mathbf{r},\mathbf{r}'$. We will show that the real and imaginary parts of G^R and of Σ^R are each Hermitian matrices. in addition, $\operatorname{Im} G^R$ and $\operatorname{Im}\Sigma^R$ are both negative definite (except in the special case of non-interacting particles where $\operatorname{Im}\Sigma^R = 0$).

In analogy with the Matsubara Green function Eq.(28.7) G^R has the Lehman representation

$$G^R\left(\mathbf{r},\mathbf{r}';\omega\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\frac{\langle n|\,\psi_S\left(\mathbf{r}\right)|m\rangle\,\langle m|\,\psi_S^{\dagger}\left(\mathbf{r}'\right)|n\rangle}{\omega+i\eta-\left(E_m-E_n-\mu\right)}. \tag{29.13}$$

In a basis where the matrix $\operatorname{Im} G^R\left(\mathbf{r},\mathbf{r}';\omega\right)$ is diagonal, say for quantum number α, then

$$\begin{aligned}\operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right) &= -\pi\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\langle n|\,c_{\boldsymbol{\alpha}}\,|m\rangle\,\langle m|\,c_{\boldsymbol{\alpha}}^{\dagger}\,|n\rangle\,\delta\left(\omega-\left(E_m-E_n-\mu\right)\right)\\ &= -\pi\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\left|\langle n|\,c_{\boldsymbol{\alpha}}\,|m\rangle\right|^2\delta\left(\omega-\left(E_m-E_n-\mu\right)\right) \quad (29.14)\end{aligned}$$

which proves that the matrix for the imaginary part is negative definite. The negative sign comes from the $+i\eta$ in the original formula and is clearly a consequence of causality. In that same diagonal basis,

$$\operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m}+e^{-\beta K_n}\right)\frac{\left|\langle n|\,c_{\boldsymbol{\alpha}}\,|m\rangle\right|^2}{\omega-\left(E_m-E_n-\mu\right)}. \tag{29.15}$$

When we change to an arbitrary basis with the unitary transformation U, we find, using also $\operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right) = \operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right)^*$ and $\operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right) = \operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right)^*$ that

$$\begin{aligned}G^R\left(\mathbf{r},\mathbf{r}';\omega\right) &= U\left(\mathbf{r},\boldsymbol{\alpha}\right)G^R\left(\boldsymbol{\alpha};\omega\right)U^{\dagger}\left(\boldsymbol{\alpha},\mathbf{r}'\right) && (29.16)\\ &= U\left(\mathbf{r},\boldsymbol{\alpha}\right)\operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right)U^{\dagger}\left(\boldsymbol{\alpha},\mathbf{r}'\right)+iU\left(\mathbf{r},\boldsymbol{\alpha}\right)\operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right)U^{\dagger}\left(\boldsymbol{\alpha},\mathbf{r}'\right)\\ &\equiv X\left(\mathbf{r},\mathbf{r}';\omega\right)+iY\left(\mathbf{r},\mathbf{r}';\omega\right) && (29.17)\\ G^R\left(\mathbf{r},\mathbf{r}';\omega\right)^* &= X\left(\mathbf{r},\mathbf{r}';\omega\right)^*-iY\left(\mathbf{r},\mathbf{r}';\omega\right)^* && (29.18)\\ &= U^*\left(\mathbf{r},\boldsymbol{\alpha}\right)\operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right)U\left(\mathbf{r}',\boldsymbol{\alpha}\right)-iU^*\left(\mathbf{r},\boldsymbol{\alpha}\right)\operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right)U\left(\mathbf{r}',\boldsymbol{\alpha}\right)\\ &= U\left(\mathbf{r}',\boldsymbol{\alpha}\right)\operatorname{Re} G^R\left(\boldsymbol{\alpha};\omega\right)U^{\dagger}\left(\boldsymbol{\alpha},\mathbf{r}\right)-iU\left(\mathbf{r}',\boldsymbol{\alpha}\right)\operatorname{Im} G^R\left(\boldsymbol{\alpha};\omega\right)U^{\dagger}\left(\boldsymbol{\alpha},\mathbf{r}\right)\\ &= X\left(\mathbf{r}',\mathbf{r};\omega\right)-iY\left(\mathbf{r}',\mathbf{r};\omega\right) && (29.19)\end{aligned}$$

where there is an implicit sum over $\boldsymbol{\alpha}$. This means that in arbitrary canonical basis, we can write $G^R = X - iY$ and $G^A = X + iY$ where both X and Y are hermitian matrices.

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

$$\frac{1}{A\pm iB} = X\mp iY \tag{29.20}$$

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

$$\frac{1}{A\pm iB} = B^{-1/2}\frac{1}{B^{-1/2}AB^{-1/2}\pm iI}B^{-1/2}. \tag{29.21}$$

Since $B^{-1/2}AB^{-1/2}$ is Hermitian as well, we can diagonalize it by a unitary transformation $B^{-1/2}AB^{-1/2} = UcU^\dagger$ where c is a diagonal matrix. Thus,

$$\frac{1}{A \pm iB} = B^{-1/2}U\frac{1}{c \pm iI}U^\dagger B^{-1/2} = B^{-1/2}U\frac{c \mp iI}{c^2+1}U^\dagger B^{-1/2} = X \mp iY \quad (29.22)$$

with X and Y Hermitians since $\left(U^\dagger B^{-1/2}\right)^\dagger = B^{-1/2}U$. In addition, Y is positive definite since in the diagonal basis $Y \to \left(c^2+1\right)^{-1}$. Now, define $\left(G^R\right)^{-1} = (A - iB)^{-1} = X + iY$ and $\left(G_0^R\right)^{-1} = (A_0 - iB_0)^{-1} = X_0 + iY_0$ so that

$$\left(G^R\right)^{-1} = X + iY = \left(G_0^R\right)^{-1} - \Sigma^R = X_0 + iY_0 - \operatorname{Re}\Sigma^R - i\operatorname{Im}\Sigma^R. \quad (29.23)$$

Then, given that X, Y and X_0, Y_0 are Hermitians, we have that $\operatorname{Re}\Sigma^R$ and $\operatorname{Im}\Sigma^R$ are Hermitians. In addition, $\operatorname{Im}\Sigma^R$ 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).

30. THREE GENERAL THEOREMS

Risking to wear your patience out, we still have to go through three general theorems used repeatedly in Many-Body theory. Wick's theorem forms the basis ot the diagram technique in many-body theory. The linked-cluster theorems, or cumulant expansions, are much more general theorems that are also necessary to set up the machinery of diagrams. Finally, we prove a variational principle for the free energy that allows us to give a physical meaning to Hartree-Fock theory as the best one-body Hamiltonian for any given problem. This variational principle is useful for ordinary system, but also becomes indispensable when there is a broken symmetry.

30.1 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

$$\mathcal{G}(\tau)=-\frac{Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{U}(\beta,\tau)\,\widehat{\psi}(\tau)\,\widehat{U}(\tau,0)\,\widehat{\psi}^\dagger(0)\right)\right]}{Tr\left[e^{-\beta H_0}T_\tau\widehat{U}(\beta,0)\right]} \tag{30.1}$$

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

$$\boxed{\mathcal{G}(\tau)=-\frac{Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{U}(\beta,0)\widehat{\psi}(\tau)\widehat{\psi}^\dagger(0)\right)\right]}{Tr\left[e^{-\beta H_0}T_\tau\widehat{U}(\beta,0)\right]}} \tag{30.2}$$

More specifically the evolution operator is,

$$\boxed{\widehat{U}(\beta,0)=T_\tau\left[\exp\left(-\int_0^\beta d\tau_1\widehat{V}(\tau_1)\right)\right]} \tag{30.3}$$

Expanding this evolution operator to first order in the numerator of the Green's function one obtains

$$-Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{\psi}(\tau)\,\widehat{\psi}^\dagger(0)\right)\right]+\int_0^\beta d\tau_1 Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{V}(\tau_1)\,\widehat{\psi}(\tau)\,\widehat{\psi}^\dagger(0)\right)\right] \tag{30.4}$$

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,

$$\left\langle a_i(\tau_i)\,a_j(\tau_j)\,a_k^\dagger(\tau_k)\,a_l^\dagger(\tau_l)\right\rangle_0 \tag{30.5}$$

as long as the density matrix $e^{-\beta H_0}$ is that of a quadratic Hamiltonian.

Note that since quadratic Hamiltonians conserve the number of particles, expectation values vanish when the number of creation operators does not match the number of destruction operators.

Lemma 16 *If* $H_0 = \varepsilon_1 a_1^\dagger a_1 + \varepsilon_2 a_2^\dagger a_2$ *then* $\left\langle a_1 a_1^\dagger a_2 a_2^\dagger \right\rangle = \left\langle a_1 a_1^\dagger \right\rangle \left\langle a_2 a_2^\dagger \right\rangle$.

Proof: To understand what is going on, it is instructive to study first the problem where a single fermion state can be occupied. Then

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{Tr\left[e^{-\beta H_0} a_1 a_1^\dagger\right]}{Tr\left[e^{-\beta H_0}\right]} \tag{30.6}$$

$$= \frac{\langle 0| a_1 a_1^\dagger |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right) a_1 a_1^\dagger \left(a_1^\dagger |0\rangle\right)}{\langle 0| |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right)\left(a_1^\dagger |0\rangle\right)} = \frac{1}{1+e^{-\beta\epsilon_1}} \tag{30.7}$$

For two fermion states $1, 2$, then the complete set used to evaluate the trace is

$$|0\rangle |0\rangle\,, \quad a_1^\dagger |0\rangle |0\rangle\,, \quad |0\rangle a_2^\dagger |0\rangle\,, \quad a_1^\dagger |0\rangle a_2^\dagger |0\rangle \tag{30.8}$$

so that

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1+e^{-\beta\epsilon_2}}{1+e^{-\beta\epsilon_2}} = \frac{1}{1+e^{-\beta\epsilon_1}}. \tag{30.9}$$

The easiest way to understand the last result is to recall that $\left(1+a_1^\dagger\right)\left(1+a_2^\dagger\right)|0\rangle$ will generate the trace so that we can factor each subspace. The last result will remain true for an arbitrary number of fermion states, in other words

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}} = \frac{1}{1+e^{-\beta\epsilon_1}}. \tag{30.10}$$

Furthermore,

$$\left\langle a_1 a_1^\dagger a_2 a_2^\dagger \right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \frac{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}} \tag{30.11}$$

$$= \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \tag{30.12}$$

$$= \left\langle a_1 a_1^\dagger \right\rangle \left\langle a_2 a_2^\dagger \right\rangle \tag{30.13}$$

Theorem 17 *Any expectation value such as* $\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0$ *calculated with a density matrix* $e^{-\beta K_0}$ *that is quadratic in field operators can be computed as the sum of all possible products of the type* $\left\langle a_j(\tau_j)\, a_k^\dagger(\tau_k) \right\rangle_0 \left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \right\rangle_0$ *that can be formed by pairing creation an 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)

$$\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l) \right\rangle_0 = \tag{30.14}$$

$$\langle i|\,\alpha\rangle\,\langle j|\,\beta\rangle\left\langle a_\alpha\left(\tau_i\right)a_\beta\left(\tau_j\right)a_\gamma^\dagger\left(\tau_k\right)a_\delta^\dagger\left(\tau_l\right)\right\rangle_0\langle\gamma|\,k\rangle\,\langle\delta|\,l\rangle \tag{30.15}$$

We already know from Eq.(27.59) that

$$a_\alpha\left(\tau_i\right)=e^{-\zeta_\alpha\tau_i}a_\alpha\quad;\quad a_\alpha^\dagger\left(\tau_i\right)=a_\alpha^\dagger e^{\zeta_\alpha\tau_i} \tag{30.16}$$

so that

$$\left\langle a_i\left(\tau_i\right)a_j\left(\tau_j\right)a_k^\dagger\left(\tau_k\right)a_l^\dagger\left(\tau_l\right)\right\rangle_0 \tag{30.17}$$

$$=\langle i|\,\alpha\rangle\,e^{-\zeta_\alpha\tau_i}\,\langle j|\,\beta\rangle\,e^{-\zeta_\beta\tau_j}\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 e^{\zeta_\gamma\tau_k}\,\langle\gamma|\,k\rangle\,e^{\zeta_\delta\tau_l}\,\langle\delta|\,l\rangle \tag{30.18}$$

What we need to evaluate then are expectation values of the type

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0. \tag{30.19}$$

Evaluating the trace in the diagonal basis, we see that we will obtain a non-zero value only if indices of creation and annihilation operators match two by two or are all equal. Suppose $\beta=\gamma$, $\alpha=\delta$ and $\alpha\neq\beta$. Then, as in the lemma

$$\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0=\left\langle a_\alpha a_\alpha^\dagger\right\rangle_0\left\langle a_\beta a_\beta^\dagger\right\rangle_0 \tag{30.20}$$

If instead, $\beta=\delta$, $\alpha=\gamma$ and $\alpha\neq\beta$, then

$$\left\langle a_\alpha a_\beta a_\alpha^\dagger a_\beta^\dagger\right\rangle_0=-\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0=-\left\langle a_\alpha a_\alpha^\dagger\right\rangle_0\left\langle a_\beta a_\beta^\dagger\right\rangle_0. \tag{30.21}$$

The last case to consider is $\alpha=\beta$, $\beta=\delta$, $\alpha=\gamma$

$$\left\langle a_\alpha a_\alpha a_\alpha^\dagger a_\alpha^\dagger\right\rangle_0=0. \tag{30.22}$$

All these results, Eqs.(30.20)(30.21) and the last equation can be combined into one formula

$$\begin{aligned}\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 &= \left\langle a_\alpha a_\alpha^\dagger\right\rangle_0\left\langle a_\beta a_\beta^\dagger\right\rangle_0\left(\delta_{\alpha,\delta}\delta_{\beta,\gamma}-\delta_{\alpha,\gamma}\delta_{\beta,\delta}\right) &(30.23)\\ &= \left\langle a_\alpha a_\delta^\dagger\right\rangle_0\left\langle a_\beta a_\gamma^\dagger\right\rangle_0-\left\langle a_\alpha a_\gamma^\dagger\right\rangle_0\left\langle a_\beta a_\delta^\dagger\right\rangle_0 &(30.24)\end{aligned}$$

which is easiest to remember as follows,

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle=\left\langle \overset{\downarrow}{a_\alpha}\underset{\uparrow}{a_\beta}\underset{\uparrow}{a_\gamma^\dagger}\overset{\downarrow}{a_\delta^\dagger}\right\rangle+\left\langle \overset{\downarrow}{a_\alpha}\underset{\uparrow}{a_\beta}\overset{\downarrow}{a_\gamma^\dagger}\underset{\uparrow}{a_\delta^\dagger}\right\rangle \tag{30.25}$$

in other words, all possible pairs of creation and annihilation operators must be paired ("contracted") in all possible ways. There is a minus sign if an odd number of operator exchanges (transpositions) is necessary to bring the contracted operators next to each other on the right-hand side (In practice, just count one minus sign every time two operators are permuted). Substituting Eq.(30.24) back into the expression for the original average expressed in the diagonal basis Eq.(30.18) we have

$$\begin{aligned}&\left\langle a_i\left(\tau_i\right)a_j\left(\tau_j\right)a_k^\dagger\left(\tau_k\right)a_l^\dagger\left(\tau_l\right)\right\rangle_0 &(30.26)\\ =\;&\left\langle a_i\left(\tau_i\right)a_l^\dagger\left(\tau_l\right)\right\rangle_0\left\langle a_j\left(\tau_j\right)a_k^\dagger\left(\tau_k\right)\right\rangle_0-\left\langle a_i\left(\tau_i\right)a_k^\dagger\left(\tau_k\right)\right\rangle_0\left\langle a_j\left(\tau_j\right)a_l^\dagger\left(\tau_l\right)\right\rangle_0\end{aligned}$$

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 18 *Contraction: In the context of Wick's theorem, we call each factor* $\left\langle a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right\rangle_0$ *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

$$\boxed{\left\langle T_\tau\left[a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^{\dagger}\left(\tau_k\right) a_l^{\dagger}\left(\tau_l\right)\right]\right\rangle_0=} \tag{30.27}$$

$$\boxed{\left\langle T_\tau\left[a_i\left(\tau_i\right) a_l^{\dagger}\left(\tau_l\right)\right]\right\rangle_0\left\langle T_\tau\left[a_j\left(\tau_j\right) a_k^{\dagger}\left(\tau_k\right)\right]\right\rangle_0-\left\langle T_\tau\left[a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right]\right\rangle_0\left\langle T_\tau\left[a_j\left(\tau_j\right) a_l^{\dagger}\left(\tau_l\right)\right]\right\rangle_0}. \tag{30.28}$$

The only simplification that occurs with time-ordered products is the following. Note that, given the definition of time-ordered product, we have

$$\left\langle T_\tau\left[a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right]\right\rangle_0=-\left\langle T_\tau\left[a_k^{\dagger}\left(\tau_k\right) a_i\left(\tau_i\right)\right]\right\rangle_0 \tag{30.29}$$

Indeed, the left-hand side and right-hand side of the above equation are, respectively

$$\begin{aligned}
\left\langle T_\tau\left[a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right]\right\rangle_0 &= \left\langle a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right\rangle_0 \theta\left(\tau_i-\tau_k\right) && (30.30)\\
&\quad -\left\langle a_k^{\dagger}\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \theta\left(\tau_k-\tau_i\right) && (30.31)\\
-\left\langle T_\tau\left[a_k^{\dagger}\left(\tau_k\right) a_i\left(\tau_i\right)\right]\right\rangle_0 &= -\left\langle a_k^{\dagger}\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \theta\left(\tau_k-\tau_i\right) && (30.32)\\
&\quad +\left\langle a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right\rangle_0 \theta\left(\tau_i-\tau_k\right) && (30.33)
\end{aligned}$$

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

$$\left\langle a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right\rangle_0 \neq-\left\langle a_k^{\dagger}\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \tag{30.34}$$

as we can easily verify by looking at the special case $\tau_k=\tau_i$ or by going to a diagonal basis. We can anticommute operators at will to do the "contractions" but they cannot be permuted *inside* a contraction $\left\langle a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right)\right\rangle_0$.

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.

Exemple 19 *To make the example of Wick's theorem Eq.(30.28) more plausible, we give a few examples, Suppose first that the time order to the left of Eq.(30.28) is such that the destruction operators are inverted. Then,*

$$\left\langle T_\tau\left[a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^{\dagger}\left(\tau_k\right) a_l^{\dagger}\left(\tau_l\right)\right]\right\rangle_0=-\left\langle a_j\left(\tau_j\right) a_i\left(\tau_i\right) a_k^{\dagger}\left(\tau_k\right) a_l^{\dagger}\left(\tau_l\right)\right\rangle_0 \tag{30.35}$$

which means that since i and j have exchanged roles, in doing the contractions as above there is one more permutation to do, which gets rid of the extra minus sign and reproduces the right-hand side of Eq.(30.28). More explicitly, to do the *contractions as above, we have to change i for j on both the right- and the left-hand side of Eq.(30.26). Doing this and substituting above, we obtain*

$$\left\langle a_j(\tau_j)\, a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l)\right\rangle_0 = \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l)\right\rangle_0 \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\right\rangle_0 - \left\langle a_j(\tau_j)\, a_k^\dagger(\tau_k)\right\rangle_0 \langle a_i(\tau_i)\, a_l^\dagger(\tau_l) \tag{30.36}$$

which we substitute in the previous equation to obtain exactly what the right-hand side of Eq.(30.28) would have predicted. To take another example, suppose that the time orders are such that

$$\left\langle T_\tau\left[a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l)\right]\right\rangle_0 = -\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_j(\tau_j)\, a_l^\dagger(\tau_l)\right\rangle_0 . \tag{30.37}$$

Then, to do the contractions we proceed as above, being careful not to permute creation and annihilation operators within an expectation value

$$\begin{aligned} & -\left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\, a_j(\tau_j)\, a_l^\dagger(\tau_l)\right\rangle_0 \\ = & -\left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l)\right\rangle_0 \left\langle a_k^\dagger(\tau_k)\, a_j(\tau_j)\right\rangle_0 - \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\right\rangle_0 \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l)\right\rangle_0 \qquad (30.38) \end{aligned}$$

The right-hand side of Eq.(30.28) gives us

$$\begin{aligned} & \left\langle T_\tau\left[a_i(\tau_i)\, a_l^\dagger(\tau_l)\right]\right\rangle_0 \left\langle T_\tau\left[a_j(\tau_j)\, a_k^\dagger(\tau_k)\right]\right\rangle_0 - \left\langle T_\tau\left[a_i(\tau_i)\, a_k^\dagger(\tau_k)\right]\right\rangle_0 \left\langle T_\tau\left[a_j(\tau_j)\, a_l^\dagger(\tau_l)\right]\right\rangle_0 \qquad (30.39) \\ = & -\left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l)\right\rangle_0 \left\langle a_k^\dagger(\tau_k)\, a_j(\tau_j)\right\rangle_0 - \left\langle a_i(\tau_i)\, a_k^\dagger(\tau_k)\right\rangle_0 \left\langle a_j(\tau_j)\, a_l^\dagger(\tau_l)\right\rangle_0 \qquad (30.40) \end{aligned}$$

with the minus sign in the first term because we had to exchange the order in one of the time-ordered products.

30.2 Linked cluster theorems

Suppose we want to evaluate the Green's function by expanding the time-ordered product in the evolution operator Eq.(30.3). The expansion has to be done both in the numerator and in the denominator of the general expression for the average Eq.(30.1). This is a very general problem that forces us to introduce the notion of connected graphs. A generalization of this problem also occurs if we want to compute the free-energy from

$$\begin{aligned} \ln Z &= \ln\left(Tr\left[e^{-\beta H_0}\widehat{U}(\beta,0)\right]\right) = \ln\left(Z_0\left\langle\widehat{U}(\beta,0)\right\rangle_0\right) && (30.41) \\ &= \ln\left(\left\langle T_\tau\left[\exp\left(-\int_0^\beta d\tau_1 \widehat{V}(\tau_1)\right)\right]\right\rangle_0\right) + \ln Z_0 && (30.42) \end{aligned}$$

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.

30.2.1 Linked cluster theorem for normalized averages

Consider the calculation of

$$\frac{\left\langle e^{-f(\mathbf{x})}A\left(\mathbf{x}\right)\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} \tag{30.43}$$

where the expectation $\langle\rangle$ is computed over a multivariate probability distribution function for the variables collectively represented by $\mathbf{x}$. The function $f\left(\mathbf{x}\right)$ is arbitrary, as is the function $A\left(\mathbf{x}\right)$. Expanding the exponential, we may write

$$\frac{\left\langle e^{-f(\mathbf{x})}A\left(\mathbf{x}\right)\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle}=\frac{\sum_{n=0}^{\infty}\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}A\left(\mathbf{x}\right)\right\rangle}{\sum_{n=0}^{\infty}\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}\right\rangle} \tag{30.44}$$

When computing a term of a given order n, such as $\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}A\left(\mathbf{x}\right)\right\rangle$, we may always write

$$\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}A\left(\mathbf{x}\right)\right\rangle=\sum_{\ell=0}^{\infty}\sum_{m=0}^{\infty}\delta_{n,m+\ell}\frac{1}{n!}\frac{n!}{\ell!m!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}A\left(\mathbf{x}\right)\right\rangle_{c}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{m}\right\rangle \tag{30.45}$$

where the subscript c on the average means that none of the terms in $\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}A\left(\mathbf{x}\right)\right\rangle_{c}$ can be factored into lower order correlation functions, such as for example $\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}\right\rangle\left\langle A\left(\mathbf{x}\right)\right\rangle$ or $\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell-1}\right\rangle\left\langle\left(-f\left(\mathbf{x}\right)\right)A\left(\mathbf{x}\right)\right\rangle$ etc... The combinatorial factor corresponds to the number of ways the $\left(-f\left(\mathbf{x}\right)\right)^{n}$ can be grouped into a group of ℓ terms and a group of $n-\ell$ terms, the $\delta_{n,m+\ell}$ Kronecker delta function ensuring that indeed $m=n-\ell$. Using the last equation in the previous one, the sum over n is now trivially performed with the help of $\delta_{n,m+\ell}$ and one is left with

$$\frac{\left\langle e^{-f(\mathbf{x})}A\left(\mathbf{x}\right)\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle}=\frac{\sum_{\ell=0}^{\infty}\sum_{m=0}^{\infty}\frac{1}{m!\ell!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}A\left(\mathbf{x}\right)\right\rangle_{c}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{m}\right\rangle}{\sum_{n=0}^{\infty}\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{n}\right\rangle} \tag{30.46}$$

The numerator can now be factored so as to cancel the denominator which proves the theorem

Theorem 20 *Linked cluster theorem for normalized averages:*

$$\boxed{\frac{\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle}=\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^{\ell}A\left(\mathbf{x}\right)\right\rangle_{c}=\left\langle e^{-f(\mathbf{x})}A\left(\mathbf{x}\right)\right\rangle_{c}} \tag{30.47}$$

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 $\left(-f\left(\mathbf{x}\right)\right)$, namely $\left(-\int_{0}^{\beta}d\tau\widehat{V}\left(\tau\right)\right)$ can be moved within the T_{τ} product without costing any additional minus sign.

30.2.2 Linked cluster theorem for characteristic functions or free energy

We now wish to show the following general theorem for a multivariate probability distribution.

Theorem 21 *Linked cluster theorem (cumulant expansion).*

$$\boxed{\ln\left\langle e^{-f(\mathbf{x})}\right\rangle = \sum_{n=1}^{\infty}\frac{1}{n!}\left\langle\left(-f\left(\mathbf{x}\right)\right)^n\right\rangle_c = \left\langle e^{-f(\mathbf{x})}\right\rangle_c - 1} \tag{30.48}$$

The proof is inspired by Enz[16]. When $f\left(\mathbf{x}\right) = i\mathbf{k}\cdot\mathbf{x}$, the quantity $\left\langle e^{-i\mathbf{k}\cdot\mathbf{x}}\right\rangle$ is called the characteristic function of the probability distribution. It is the generating function for the moments. The quantities on the right-hand side, which as above are connected averages, are usually called *cumulants* in ordinary probability theory and $\ln\left\langle e^{-i\mathbf{k}\cdot\mathbf{x}}\right\rangle$ is the generating function for the cumulant averages.

Proof: To prove the theorem, we introduce first an auxiliary variable λ

$$\frac{\partial}{\partial\lambda}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle = \left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle \tag{30.49}$$

We can apply to the right-hand side the theorem we just proved

$$\left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle = \left\langle e^{-\lambda f(\mathbf{x})}\left[-f\left(\mathbf{x}\right)\right]\right\rangle_c \left\langle e^{-\lambda f(\mathbf{x})}\right\rangle \tag{30.50}$$

so that

$$\frac{1}{\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle}\frac{\partial}{\partial\lambda}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle = \left\langle\frac{\partial}{\partial\lambda}e^{-\lambda f(\mathbf{x})}\right\rangle_c . \tag{30.51}$$

Integrating both sides from 0 to 1, we obtain

$$\ln\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle|_0^1 = \left\langle e^{-f(\mathbf{x})}\right\rangle_c - 1 \tag{30.52}$$

QED

Exemple 22 *It is instructive to check the meaning of the above result explicitly to second order*

$$\ln\left\langle e^{-\lambda f(x)}\right\rangle \approx \ln\left\langle 1-\lambda f\left(x\right)+\frac{1}{2}\left(\lambda f\left(x\right)\right)^2\right\rangle \approx \left(-\left\langle\lambda f\left(x\right)\right\rangle + \frac{1}{2}\left\langle\left(\lambda f\left(x\right)\right)^2\right\rangle\right) - \frac{1}{2}\left\langle\lambda f\left(x\right)\right\rangle^2 \tag{30.53}$$

$$\left\langle e^{-\lambda f(x)}\right\rangle_c - 1 \approx -\left\langle\lambda f\left(x\right)\right\rangle_c + \frac{1}{2}\left\langle\left(\lambda f\left(x\right)\right)^2\right\rangle_c \tag{30.54}$$

so that equating powers of λ, we find as expected,

$$\left\langle\left(f\left(\mathbf{x}\right)\right)^2\right\rangle_c = \left\langle\left(f\left(\mathbf{x}\right)\right)^2\right\rangle - \left\langle f\left(\mathbf{x}\right)\right\rangle^2 . \tag{30.55}$$

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,

$$F = -T\ln\left[Z_0\left\langle T_\tau\left[e^{-\int_0^\beta d\tau\widehat{V}(\tau)}\right]\right\rangle_0\right] = -T\sum_{n=1}^{\infty}\frac{1}{n!}\left\langle T_\tau\left[-\int_0^\beta d\tau\widehat{V}\left(\tau\right)\right]^n\right\rangle_{0c} - T\ln Z_0 \tag{30.56}$$

$$\boxed{F = -T\ln Z = -T\left[\left\langle T_\tau\left[e^{-\int_0^\beta d\tau\widehat{V}(\tau)}\right]\right\rangle_{0c} - 1\right] - T\ln Z_0.} \tag{30.57}$$

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.

30.3 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.

30.3.1 Thermodynamic variational principle for classical systems

One can base the thermodynamic variational principle for classical systems on the inequality

$$\boxed{e^x \geq 1 + x} \tag{30.58}$$

which is valid for all x, whether $x > 0$, or $x < 0$. This inequality is a convexity inequality which appears obvious when the two functions are plotted. We give two proofs.

Proof 1: e^x is a convex function, *i.e.* $d^2e^x/d^2x \geq 0$ for all values of x. At $x = 0$ the functions e^x and $1+x$ as well as their first derivatives are equal. Since a straight line tangent to a convex curve at a point cannot intersect it anywhere else, the theorem is proven. *QED*

Algebraically, the proof goes as follows.

Proof 2: The 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

$$\sum_{n=2}^{\infty} \frac{1}{n!} x^n \geq 0. \tag{30.59}$$

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 (30.59) survives. *QED*

Moving back to our initial purpose, let $\widetilde{H}_0$ be a trial Hamiltonian. Then take $e^{-\beta\left(\widetilde{H}_0-\mu N\right)}/Z_0$ as the trial density matrix corresponding to averages $\langle\rangle_{\widetilde{0}}$. We will use the above inequality Eq.(30.58) to prove that

$$\boxed{-T \ln Z \leq -T \ln Z_{\widetilde{0}} + \left\langle H - \widetilde{H}_0 \right\rangle_{\widetilde{0}}} \tag{30.60}$$

This inequality is a variational principle because $\widetilde{H}_0$ is arbitrary, meaning that we are free to parametrize it and then to minimize with respect to the set of all parameters to find the best one-particle Hamiltonian in our Physically chosen space of Hamiltonians.

Proof Our general result for the free energy in terms of connected terms, Eq.(30.57), is obviously applicable to classical systems. The simplification that occurs there is that since all operators commute, we do not need to worry about the time-ordered product, thus with

$$\widetilde{V} = H - \widetilde{H}_0 \tag{30.61}$$

we have

$$F = -T \ln Z = -T \left[\left\langle e^{-\beta \widetilde{V}} \right\rangle_{\widetilde{0},c} - 1 \right] - T \ln Z_{\widetilde{0}}. \tag{30.62}$$

Using our basic inequality Eq.(30.58) for $e^{-\beta \widetilde{V}}$ we immediately obtain the desired result

$$F \leq -T \left\langle -\beta \widetilde{V} \right\rangle_{\widetilde{0},c} + F_{\widetilde{0}} \tag{30.63}$$

which is just another way of rewriting Eq.(30.60).

It is useful to note that in the language of density matrices, $\varrho_0 = e^{-\beta\left(\widetilde{H}_0 - \mu N\right)}/Z_0$ the variational principle Eq.(30.60) reads,

$$\boxed{-T \ln Z \leq \mathrm{Tr}\left[\varrho_0 \left(H - \mu N\right)\right] + T \mathrm{Tr}\left[\varrho_0 \ln \varrho_0\right]} \tag{30.64}$$

which looks as if we had the function $(E - \mu N) - TS$ to minimize, quite a satisfactory state of affairs.

30.3.2 Thermodynamic variational principle for quantum systems

The quantum proof is easiest if we start from the following inequality for the entropy[21]

$$\boxed{S = -\mathrm{Tr}\left[\varrho \ln \varrho\right] \leq -\mathrm{Tr}\left[\varrho \ln \varrho'\right].} \tag{30.65}$$

Proof Let $|m\rangle$ and $|m'\rangle$ be the basis that diagonalize respectively ϱ and ϱ'. Then by inserting the closure relation, and defining $p_m = \langle m| \varrho |m\rangle$ with the analogous definition for p'_m, we find

$$\begin{aligned} \mathrm{Tr}\left[-\varrho \ln \varrho + \varrho \ln \varrho'\right] &= -\sum_m p_m \ln p_m + \sum_{m,m'} p_m \langle m | m'\rangle \log p'_{m'} \langle m' | m\rangle \\ &= \sum_{m,m'} \langle m | m'\rangle \langle m' | m\rangle p_m \log \frac{p'_{m'}}{p_m}. \end{aligned} \tag{30.66}$$

In this sum, $\langle m | m'\rangle \langle m' | m\rangle p_m$ is positive or zero. We can now use $\ln y \leq y - 1$. (This inequality follows from the fact that the first derivative of $\ln y - y$ vanishes at $y = 1$ and that the second derivative, $-1/y^2$ is negative everywhere. Hence, $\ln y - y$ has a minimum at $y = 1$ and the value there is -1.) Using this inequality above, we find

$$\mathrm{Tr}\left[-\varrho \ln \varrho + \varrho \ln \varrho'\right] \leq \sum_{m,m'} \langle m | m'\rangle \langle m' | m\rangle \left(p'_m - p_m\right) = \mathrm{Tr}\left[\varrho'\right] - \mathrm{Tr}\left[\varrho\right] = 0. \tag{30.67}$$

The last equality follows from the fact that the trace of a density matrix is unity. The equality occurs only if $\langle m | m'\rangle = 0$ or if $p'_{m'}/p_m = 1$ for all possible choices of $|m\rangle$ and $|m'\rangle$.

To prove Feynmann's variational principle Eq.(30.64) it suffices to take $\varrho' = e^{-\beta(H-\mu N)}/Z$ and $\varrho = \varrho_0$.Then, the inequality for the entropy, Eq.(30.65) becomes $-\mathrm{Tr}\left[\varrho_0 \ln \varrho_0\right] \leq \beta \mathrm{Tr}\left[\varrho_0 \left(H - \mu N\right)\right] + \beta \ln Z$ which is the variational principle Eq.(30.64) found above, namely that the true free energy smaller than the free energy computed with a trial density matrix.

30.3.3 Application of the variational principle to Hartree-Fock theory

Writing down the most general one-body Hamiltonian with *orthonormal* eigenfunctions left as variational parameters, the above variational principle leads to the usual Hartree-Fock eigenvalue equation. Such a general one-body Hamiltonian would look like

$$\widetilde{H}_0 = \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}^{*}\left(\mathbf{x}\right)\left(-\frac{\nabla^2}{2m}\right)\phi_{\alpha}\left(\mathbf{x}\right) c_{\alpha}^{+} c_{\alpha} \tag{30.68}$$

with $\phi_{\alpha}\left(\mathbf{x}\right)$ 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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Part V

The Coulomb gas

The electron gas with long-range forces and a neutralizing background, also known as the jellium model, is probably the first challenge that was met by many-body theory in the context of Solid State physics. It is extremely important conceptually since it is crucial to understand how, in a solid, the long-range Coulomb force becomes effectively short-range, or screened, at low energy. Other models, such as the Hubbard model that we will discussed later on, have their foundation rooted in the physics of screening.

In this part, we assume that the uniform neutralizing background has infinite inertia. In a subsequent part of this book we will allow it to move, in other words to support sound waves, or phonons. We will consider electron-phonon interactions and see how these eventually lead to superconductivity.

The main physical phenomena to account for here in the immobile background, are screening and plasma oscillations, at least as far as collective modes are concerned. The surprises come in when one tries to understand single-particle properties. Hartree-Fock theory is a disaster since it predicts that the effective mass of the electron at the Fermi level vanishes. The way out of this paradox will indicate to us how important it is to take screening into account.

We will start by describing the source formalism due to the Schwinger-Martin school[1, 2] and then start to do calculations. The advantage of this approach is that it allows more easily to devise non-perturbative approximations and to derive general theorems. It gives a systematic algebraic way to formulate perturbation theory when necessary, without explicit use of Wick's theorem. With this formalism, so-called conserving approximations can also be formulated naturally. The source, or functional derivative formalism, is however less appealing than Feynman rules for the Feynmann diagram approach to perturbation theory. When these two competing approaches were invented, it was forbidden to the practitioners of the source approach to draw Feynamnn diagrams, but nothing really forbids it. The students, anyway, drew the forbidden pictures hidden in the basement. The two formalism are strictly equivalent.

After we introduce the formalism, we discuss first the density oscillations, where we will encounter screening and plasma oscillations. This will allow us to discuss the famous Random Phase Approximation (RPA). Then we move on to single particle properties and end with a general discussion of what would be needed to go beyond RPA. The electron gas is discussed in detail in a very large number of textbooks. The discussion here is brief and incomplete, its main purpose being to illustrate the physics involved.

31. THE FUNCTIONAL DERIVATIVE APPROACH

We basically want to compute correlation functions. In the first section below, we show, in the very simple context of classical statistical mechanics, how introducing artificial external fields (source fields) allows one to compute correlation functions of arbitrary order for the problem without external fields. This is one more example where enlarging the space of parameters of interest actually simplifies matters in the end. In the other section, we show how to obtain Green's functions with source fields and then give an impressionist's view of how we plan to use this idea for our problem.

31.1 External fields to compute correlation functions

In elementary statistical mechanics, we can obtain the magnetization by differentiating the free energy with respect to the magnetic field. To be more specific, let

$$Z_h = \mathrm{Tr}\left[e^{-\beta(K-hM)}\right] \tag{31.1}$$

then

$$\frac{\partial \ln Z_h}{\beta \partial h} = \frac{1}{Z_h}\mathrm{Tr}\left[e^{-\beta(K-hM)}M\right] = \langle M\rangle_h \,. \tag{31.2}$$

The indice h on $\langle M\rangle_h$ and Z_h reminds us that the magnetic field is non zero. We can obtain correlation fucntions of higher order by continuing the process

$$\begin{aligned} \frac{\partial^2 \ln Z_h}{\beta^2 \partial h^2} &= \langle MM\rangle_h - \mathrm{Tr}\left[e^{-\beta(K-hM)}M\right]\frac{1}{Z_h^2}\frac{\partial \mathrm{Tr}\left[e^{-\beta(K-hM)}\right]}{\beta\partial h} && (31.3)\\ &= \langle MM\rangle_h - \langle M\rangle_h \langle M\rangle_h \,. && (31.4)\end{aligned}$$

The second term clearly comes from the fact that Z_h in the denominator of the equation for $\langle M\rangle_h$ depends on h.One can clearly continue this process to find higher and higher order correlation functions. At the end, we can set $h = 0$. Clearly then, if one can compute $\langle M\rangle_h$ or Z_h,one can obtain higher order correlation functions just by differentiating.

Suppose now that we want for example $\langle M(\mathbf{x}_1) M(\mathbf{x}_2)\rangle - \langle M(\mathbf{x}_1)\rangle \langle M(\mathbf{x}_2)\rangle$ .That can still be achieved if we impose a position dependent-external field:

$$Z[h] = \mathrm{Tr}\left[e^{-\beta\left(K-\int d^3\mathbf{x}\, h(\mathbf{x})M(\mathbf{x})\right)}\right]. \tag{31.5}$$

It is as if at each position $\mathbf{x}$, there is an independent variable $h(\mathbf{x})$. The position is now just a label. The notation $Z[h]$ means that Z is a functional of $h(\mathbf{x})$ .It takes a function and maps it into a scalar. To obtain the magnetization at a single point, we intorduce the notion of functional derivative, which is just a simple generalization to the continuum of the idea of partial derivative. To be more specific,

$$\frac{\delta}{\delta h\left(\mathbf{x}_1\right)}\int d^3\mathbf{x}h\left(\mathbf{x}\right)M\left(\mathbf{x}\right) = \int d^3\mathbf{x}\frac{\delta h\left(\mathbf{x}\right)}{\delta h\left(\mathbf{x}_1\right)}M\left(\mathbf{x}\right) \tag{31.6}$$

$$= \int d^3\mathbf{x}\delta\left(\mathbf{x}_1-\mathbf{x}\right)M\left(\mathbf{x}\right) = M\left(\mathbf{x}_1\right). \tag{31.7}$$

In other words, the partial derivative for two independent variables y_1 and y_2

$$\frac{\partial y_1}{\partial y_2} = \delta_{1,2} \tag{31.8}$$

where $\delta_{1,2}$ is the Kroenecker delta, is replaced by

$$\frac{\delta h\left(\mathbf{x}\right)}{\delta h\left(\mathbf{x}_1\right)} = \delta\left(\mathbf{x}_1-\mathbf{x}\right). \tag{31.9}$$

Very simple.

Armed with this notion of functional derivative, one finds that

$$\frac{\delta\ln Z\left[h\right]}{\beta\delta h\left(\mathbf{x}_1\right)} = \left\langle M\left(\mathbf{x}_1\right)\right\rangle_h \tag{31.10}$$

and the quantity we want is obtained from one more funcitonal derivative

$$\frac{\delta^2\ln Z\left[h\right]}{\beta^2\delta h\left(\mathbf{x}_1\right)\delta h\left(\mathbf{x}_2\right)} = \left\langle M\left(\mathbf{x}_1\right)M\left(\mathbf{x}_2\right)\right\rangle_h - \left\langle M\left(\mathbf{x}_1\right)\right\rangle_h\left\langle M\left(\mathbf{x}_2\right)\right\rangle_h. \tag{31.11}$$

31.2 Green's functions and higher order correlations from functional derivatives

In our case, we are interested in correlation functions that depend not only on space but also on real or imaginary time. In addition, we know that time-ordered products are relevant. Hence, you will not be surprized to learn that we use as our partition function with source fields

$$Z\left[\phi\right] = \mathrm{Tr}\left[e^{-\beta K}T_\tau\exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\right] \tag{31.12}$$

where we used the short-hand

$$\left(1\right) = \left(\mathbf{x}_1,\tau_1;\sigma_1\right) \tag{31.13}$$

with the overbar indicating integrals over space-time coordinates and spin sums. More specifically,

$$\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right) =$$

$$\sum_{\sigma_1,\sigma_2}\int d^3\mathbf{x}_1\int_0^\beta d\tau_1\int d^3\mathbf{x}_2\int_0^\beta d\tau_2\psi^\dagger_{\sigma_1}\left(\mathbf{x}_1,\tau_1\right)\phi_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1,\mathbf{x}_2,\tau_2\right)\psi_{\sigma_2}\left(\mathbf{x}_2,\tau_2\right).$$

With the definition,

$$\mathcal{S}\left[\phi\right] = \exp\left(-\psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right) \tag{31.14}$$

we can write the Matsubara Green's function as a functional derivative of the generating function $\ln Z[\phi]$,

$$
\begin{aligned}
-\frac{\delta \ln Z[\phi]}{\delta \phi(2,1)} &= -\frac{\left\langle T_\tau \mathcal{S}[\phi]\, \psi(1)\, \psi^\dagger(2) \right\rangle}{\langle T_\tau \mathcal{S}[\phi] \rangle} \\
&= -\left\langle T_\tau \psi(1)\, \psi^\dagger(2) \right\rangle_\phi = \mathcal{G}(1,2)_\phi\,. \qquad (31.15)
\end{aligned}
$$

The functional derivative with respect to ϕ does not influence at all the time order so one can differentiate the exponential inside the time-ordered product. The thermal average on the first line is with respect to $e^{-\beta K}$ and in $\left\langle T_\tau \psi(1)\, \psi^\dagger(2) \right\rangle_\phi$ one does not write $\mathcal{S}[\phi]$ explicitly. Note the reversal in the order of indices in $\mathcal{G}$ and in ϕ.We have also used the fact that in a time ordered product we can displace operators as we wish, as long as we keep track of fermionic minus signs.

Higher order correlation functions can be obtained by taking further functional derivatives

$$
\begin{aligned}
\frac{\delta \mathcal{G}(1,2)_\phi}{\delta \phi(3,4)} &= -\frac{\delta}{\delta \phi(3,4)} \frac{\left\langle T_\tau \mathcal{S}[\phi]\, \psi(1)\, \psi^\dagger(2) \right\rangle}{\langle T_\tau \mathcal{S}[\phi] \rangle} \\
&= \frac{\left\langle T_\tau \mathcal{S}[\phi]\, \psi(1)\, \psi^\dagger(2)\, \psi^\dagger(3)\, \psi(4) \right\rangle}{\langle T_\tau \mathcal{S}[\phi] \rangle} - \frac{\left\langle T_\tau \mathcal{S}[\phi]\, \psi(1)\, \psi^\dagger(2) \right\rangle \left\langle T_\tau \mathcal{S}[\phi]\, \psi^\dagger(3)\, \psi(4) \right\rangle}{\langle T_\tau \mathcal{S}[\phi] \rangle^2} \\
&= \left\langle T_\tau \psi(1)\, \psi^\dagger(2)\, \psi^\dagger(3)\, \psi(4) \right\rangle_\phi + \mathcal{G}(1,2)_\phi\, \mathcal{G}(4,3)_\phi\,. \qquad (31.16)
\end{aligned}
$$

The first term is called a four-point correlation function. The last term comes from differentiating $\langle T_\tau \mathcal{S}[\phi] \rangle$ in the denominator. To figure out the minus signs in that last term note that there is one from $-1/Z^2$, one from the derivative of the argument of the exponential and one from ordering the field operators in the order corresponding to the definition of $\mathcal{G}_\sigma$. The latter is absorbed in the definition of $\mathcal{G}_\sigma$.

31.3 Source fields for Green's functions, an impressionist view

How can that formalism possibly be helpful. The reason is that the self-energy will be expressed in terms of a four point correlation function which in turn can be found from a functional derivative of $\mathcal{G}_\sigma(,)_\phi$. It will be possible to find this functional derivative if we know $\mathcal{G}_\sigma(,)_\phi$. We do have an expression for that quantity so that, in a sense, it closes the loop. We will see things are not so simple in practice, but at least that is a start.

How do we find $\mathcal{G}_\sigma(,)_\phi$? It suffices to write the equations of motion. What is different from the non-interacting case is the presence of ϕ and of interactions. When we compute $\frac{\partial \psi(1)}{\partial \tau_1} = [K, \psi(1)]$, there will be a term coming from the commutator of the interaction term with $\psi(1)$. That will be a term proportional to $V\psi^\dagger\psi\psi$ with V the potential energy. Using this result in the definition of $\mathcal{G}$, which has an extra $\psi^\dagger$tagged on the right, the equation of motion for $\mathcal{G}$ will read something like

$$
\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 - V\left\langle T_\tau \psi^\dagger \psi \psi \psi^\dagger \right\rangle. \qquad (31.17)
$$

Using our notion of irreducible self-energy, we define

$$\begin{aligned} \Sigma\mathcal{G} &= -V\left\langle T_\tau\psi^\dagger\psi\psi\psi^\dagger\right\rangle \\ \Sigma &= -V\left\langle T_\tau\psi^\dagger\psi\psi\psi^\dagger\right\rangle\mathcal{G}^{-1}. \end{aligned} \tag{31.18}$$

so that

$$\mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\phi-\Sigma. \tag{31.19}$$

which is equivalent to Dyson's equation

$$\mathcal{G}=\mathcal{G}_{0\phi}+\mathcal{G}_{0\phi}\Sigma\mathcal{G} \tag{31.20}$$

with $\mathcal{G}_{0\phi}=\left(\mathcal{G}_0^{-1}-\phi\right)^{-1}$.The four-point correlation function entering the definition of Σ is then obtained from a functional derivative of $\mathcal{G}$ since

$$\left\langle T_\tau\psi^\dagger\psi\psi\psi^\dagger\right\rangle=\frac{\delta\mathcal{G}}{\delta\phi}-\mathcal{G}\mathcal{G} \tag{31.21}$$

as we saw in the previous section.

To find that functional derivative we start from the equation of motion Eq.(31.17) which gave us Dyson's equation Eq.(31.19) which is easy to differentiate with respect to ϕ. Then, we can take advantage of this and $\mathcal{G}^{-1}\mathcal{G}=1$ to find the functional derivative of $\mathcal{G}$. Indeed,

$$\frac{\delta\left(\mathcal{G}^{-1}\mathcal{G}\right)}{\delta\phi}=\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}+\mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\phi}=0 \tag{31.22}$$

or, left multiplying by $\mathcal{G}$

$$\frac{\delta\mathcal{G}}{\delta\phi}=-\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} \tag{31.23}$$

which can be evaluated with the help of Dyson's equation Eq.(31.19)

$$\frac{\delta\mathcal{G}}{\delta\phi}=\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G}+\mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}. \tag{31.24}$$

We will see that we can write Σ as a functional of $\mathcal{G}$, at least in perturbation theory, and that there is no explicit dependence of Σ on ϕ. Hence, using the chain rule

$$\frac{\delta\Sigma}{\delta\phi}=\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi} \tag{31.25}$$

we have an integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$

$$\boxed{\tfrac{\delta\mathcal{G}}{\delta\phi}=\mathcal{G}\tfrac{\delta\phi}{\delta\phi}\mathcal{G}+\mathcal{G}\left(\tfrac{\delta\Sigma}{\delta\mathcal{G}}\tfrac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G}.} \tag{31.26}$$

If we can solve this, we can find $\mathcal{G}$ Eq.(31.17)

$$\boxed{\left(\mathcal{G}_0^{-1}-\phi\right)\mathcal{G}=1+\Sigma\mathcal{G}} \tag{31.27}$$

with the self-energy Eq.(31.18) written in terms of the four-point function Eq.(31.21)

$$\boxed{\Sigma=-V\left(\tfrac{\delta\mathcal{G}}{\delta\phi}-\mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1}.} \tag{31.28}$$

Since the integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$ requires that we know both $\mathcal{G}$ and $\frac{\delta\Sigma}{\delta\mathcal{G}}$ there will be some iteration process involved. The last three equations can be solved for $\phi=0$, since ϕ has played its role and is no longer necessary at that point.

One physical point that will become clearer when we put all indices back, is that the self-energy contains information about the fact that the medium is polarizable, i.e. it depends on the four-point correlation function $\frac{\delta\mathcal{G}}{\delta\phi}$ and hence on the density-density correlation function, or equivalently the longitudinal dielectric constant, as we shall verify.

We can also write an equation that looks as a closed functional equation for Σ by using the expression Eq.(31.24) relating $\frac{\delta\mathcal{G}}{\delta\phi}$ and $\frac{\delta\Sigma}{\delta\phi}$:

$$\begin{aligned}\Sigma &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G}+\mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}-\mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1}. \\ &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}+\mathcal{G}\frac{\delta\Sigma}{\delta\phi}-\mathcal{G}\right) \qquad (31.29)\end{aligned}$$

An alternate useful form that uses the fact that all the functional dependence of Σ on ϕ is implicit through its dependence on $\mathcal{G}$ is

$$\boxed{\Sigma = -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}-\mathcal{G}+\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)} \qquad (31.30)$$

Since Σ is already linear in V, it is tempting to use $\Sigma = -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}-\mathcal{G}\right)$ as a first approximation. This is the Hartree-Fock approximation.

Remark 108 $\frac{\delta\pm}{\delta\mathcal{G}}$ *in the equation for the functional derivative Eq.(31.26) is called the irreducible vertex in the particle-hole channel. The reason for this will become clear later. The term that contains this irreducible vertex is called a vertex correction. Note that* $\mathcal{G}\left(\frac{\delta\pm}{\delta\mathcal{G}}\right)\mathcal{G}$ *plays the role of a self-energy for the four-point function* $\frac{\delta\mathcal{G}}{\delta\phi}$. *For the same reason that it was profitable to resum infinite series for* $\mathcal{G}$ *by using the concept of a self-energy, it will be preferable to do the same here and use* $\mathcal{G}\left(\frac{\delta\pm}{\delta\mathcal{G}}\right)\mathcal{G}$ *as a self-energy instead of iterating the equation for* $\frac{\delta\mathcal{G}}{\delta\phi}$ *at some finite order.*

Remark 109 *If we had written an equation of motion for the four-point function, we would have seen that it depends on a six point function, and so on, so that is not the way to go. This would have been the analog of the so-called BBGKY hierarchy in classical transport theory.*

32. EQUATIONS OF MOTION TO FIND $\mathcal{G}$ IN THE PRESENCE OF SOURCE FIELDS

Here we try to do everything more rigorously with all the bells and whistles. It is clear that the first step is to derive the equations of motion for the Green's function. That begins with the Hamiltonian and equations for motion for $\psi_\sigma(1)$ which will enter the equation of motion for $\mathcal{G}$.

32.1 Hamiltonian and equations of motion for $\psi(1)$

The Hamiltonian we consider is the following. Note that we now introduce spin indices denoted by Greek indices:

$$\begin{aligned}
K &= H-\mu N = H_0+V+V_n-\mu N && (32.1)\\
H_0 &= \frac{1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \boldsymbol{\nabla}\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\cdot\boldsymbol{\nabla}\psi_{\sigma_1}(\mathbf{x}_1) && (32.2)\\
V &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1)\\
V_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n_0 && (32.3)
\end{aligned}$$

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

$$v(\mathbf{x}_1-\mathbf{x}_2)=\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|} \tag{32.4}$$

To derive the equations of motion for the Green's function, we first need those for the field operators.

$$\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau}=[K,\psi_\sigma(\mathbf{x},\tau)] \tag{32.5}$$

Using $[A,BC]=\{A,B\}C-B\{A,C\}$ and Eq.(32.1) for K we have

$$\begin{aligned}
\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} &= \frac{\nabla^2}{2m}\psi_\sigma(\mathbf{x},\tau)+\mu\psi_\sigma(\mathbf{x},\tau) && (32.6)\\
&\quad-\sum_{\sigma_2}\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\psi^\dagger_{\sigma_2}(\mathbf{x}_2,\tau)\psi_{\sigma_2}(\mathbf{x}_2,\tau)\psi_\sigma(\mathbf{x},\tau)
\end{aligned}$$

The last term does not have the 1/2 factor that appeared in the Hamiltonian because

$$\begin{aligned}\left[\psi_{\sigma_1}^{\dagger}(\mathbf{x}_1)\psi_{\sigma_2}^{\dagger}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1),\psi_{\sigma}(\mathbf{x})\right] &= \left[\psi_{\sigma_1}^{\dagger}(\mathbf{x}_1)\psi_{\sigma_2}^{\dagger}(\mathbf{x}_2),\psi_{\sigma}(\mathbf{x})\right]\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1)\\ &= -\delta_{\sigma_1,\sigma}\delta(\mathbf{x}-\mathbf{x}_1)\psi_{\sigma_2}^{\dagger}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1)\\ &\quad +\delta_{\sigma_2,\sigma}\delta(\mathbf{x}-\mathbf{x}_2)\psi_{\sigma_1}^{\dagger}(\mathbf{x}_1)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1).\end{aligned}$$

Anticommuting the destruction operators in the last term, substituting and changing dummy indices, the two contributions are identical.

The equation of motion can be rewritten in the more matrix-like form

$$\frac{\partial\psi(1)}{\partial\tau_1} = \frac{\nabla_1^2}{2m}\psi(1) + \mu\psi(1) - \psi^{\dagger}\left(\bar{2}\right)\psi\left(\bar{2}\right)V\left(\bar{2}-1\right)\psi(1) \tag{32.7}$$

if we define a time and spin dependent potential

$$\boxed{V(1,2) = V_{\sigma_1,\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) \equiv \tfrac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\delta(\tau_1-\tau_2).} \tag{32.8}$$

In reality the potential is independent of spin and is instantaneous but introducing these dependencies simplifies the notation.

Remark 110 *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*

$$+n_0\left[\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\right]\psi_{\sigma}(\mathbf{x},\tau) \tag{32.9}$$

The $\mathbf{q}=\mathbf{0}$ contribution of the potential in the above equation of motion gives on the other hand a contribution

$$-\left[\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\right]\left[\frac{1}{\mathcal{V}}\int d\mathbf{x}_2\sum_{\sigma_2}\psi_{\sigma_2}^{\dagger}(\mathbf{x}_2,\tau_2)\psi_{\sigma_2}(\mathbf{x}_2,\tau_2)\right]\psi_{\sigma}(\mathbf{x},\tau) \tag{32.10}$$

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.

32.2 Equations of motion for $\mathcal{G}_{\phi}$ and definition of Σ_{ϕ}

The equation of motion for $\mathcal{G}(1,2)_{\phi}$

$$\mathcal{G}(1,2)_{\phi} = -\frac{\left\langle T_{\tau}\mathcal{S}[\phi]\psi(1)\psi^{\dagger}(2)\right\rangle}{\left\langle T_{\tau}\mathcal{S}[\phi]\right\rangle}$$

is obtained by taking the time derivative. There will be three contributions. One from $\frac{\partial\psi(1)}{\partial\tau_1}$, that we found above, one from the time derivative of the $\theta(\tau_1-\tau_2)$

and $\theta(\tau_2 - \tau_1)$ entering the definition of the time-ordered product that gives the usual delta function, and one from the fact that terms in $\mathcal{S}[\phi]$ have to be orderd with respect to τ_1. The only unfamiliar contribution is the latter one. To understand how to compute it, we write explicitely the time integral associated with the creation operator in the exponential and order it properly:

$$\begin{aligned}\left\langle T_\tau \mathcal{S}[\phi]\,\psi(1)\,\psi^\dagger(2)\right\rangle &= \Big\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_1 \psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right) \\ &\qquad \psi(1)\exp\left(-\int_0^{\tau_1} d\tau_1 \psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\psi^\dagger(2)\Big\rangle\end{aligned}$$

Since we moved an even number of fermion operators, we do not need to worry about sign. We do not need to worry about the destruction operator in the exponential either since it anticommutes with $\psi(1)$: The time-ordered product will eventually take care of the proper order. So, in the end, we have a contribution to the time derivative with respect to τ_1 that reads

$$\begin{aligned}&\Big\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_1 \psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\int d^3\mathbf{x}_{1'}\left[\psi^\dagger\left(\mathbf{x}_{1'},\tau_1\right)\phi\left(\mathbf{x}_{1'},\tau_1,\overline{2}\right)\psi\left(\overline{2}\right),\psi\left(\mathbf{x}_1,\tau_1\right)\right] \\ &\exp\left(-\int_0^{\tau_1} d\tau_1 \psi^\dagger\left(\overline{1}\right)\phi\left(\overline{1},\overline{2}\right)\psi\left(\overline{2}\right)\right)\psi^\dagger(2)\Big\rangle \\ =\;& -\phi\left(1,\overline{2}\right)\left\langle T_\tau \mathcal{S}[\phi]\,\psi\left(\overline{2}\right)\psi^\dagger(2)\right\rangle\end{aligned}$$

Collecting the three contributions, we can write

$$\begin{aligned}\left(\frac{\partial}{\partial\tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\mathcal{G}(1,2)_\phi &= -\delta(1-2) + \left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)V\left(1-\overline{2}\right)\psi\left(\overline{2}\right)\psi(1)\,\psi^\dagger(2)\right]\right\rangle_\phi \\ &\quad -\phi\left(1,\overline{2}\right)\mathcal{G}\left(\overline{2},2\right)_\phi . \end{aligned} \tag{32.11}$$

Note that we had to specify$\psi^\dagger\left(\overline{2^+}\right)$ in the term with the potential energy. The superscrpt + specifies that the time in that field operator is later than the time in $\psi(1')$. In other words

$$2^+ \equiv \left(\mathbf{x}_2, \tau_2 + 0^+; \sigma_2\right)$$

Equal time does not mean anything in a time ordered product. The choice to take $\psi^\dagger\left(\overline{2^+}\right)$ keeps the field in the order it was in to begin with.

The equations of motion can be written in a compact form if we define

$$\boxed{\mathcal{G}_0^{-1}\left(1,\overline{2}\right) = -\left(\frac{\partial}{\partial\tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\delta\left(1-\overline{2}\right).} \tag{32.12}$$

With this definition, the equation of motion Eq.(32.11) takes the form

$$\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right) - \phi\left(1,\overline{2}\right)\right)\mathcal{G}\left(\overline{2},2\right)_\phi = \delta(1-2) - V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi(1)\,\psi^\dagger(2)\right]\right\rangle_\phi .$$

Comparing with Dyson's equation, we have an explicit form for the self-energy,

$$\boxed{\Sigma\left(1,\overline{2}\right)_\phi \mathcal{G}\left(\overline{2},2\right)_\phi = -V\left(1-\overline{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\overline{2}\right)\psi(1)\,\psi^\dagger(2)\right]\right\rangle_\phi .} \tag{32.13}$$

The equation of motion can then also be written as

$$\boxed{\left(\mathcal{G}_0^{-1}\left(1,\overline{2}\right) - \phi\left(1,\overline{2}\right) - \Sigma\left(1,\overline{2}\right)_\phi\right)\mathcal{G}\left(\overline{2},2\right)_\phi = \delta(1-2)}$$

which also reads

$$\boxed{\mathcal{G}^{-1}(1,2)_{\phi}=\mathcal{G}_0^{-1}(1,2)-\phi(1,2)-\Sigma(1,2)_{\phi}\,.} \tag{32.14}$$

Remark 111 *The self-energy is related to a four-point function and we note in passing that the trace of defining equation 32.13 is related to the potential energy. That can be seen as follows. In the limit $2\rightarrow 1^{+}$ the right-hand side becomes*

$$\left\langle T_{\tau}\left[\psi^{\dagger}\left(1^{+}\right)\psi^{\dagger}\left(\overline{1'^{+}}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(1\right)\right]\right\rangle .$$

Recalling the definition of the average potential energy

$$2\left\langle V\right\rangle=\sum_{\sigma_1}\int d^3\mathbf{x}_1\left\langle T_{\tau}\left[\psi^{\dagger}\left(1^{+}\right)\psi^{\dagger}\left(\overline{1'^{+}}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(1\right)\right]\right\rangle \tag{32.15}$$

this special case of our general formula gives

$$\sum_{\sigma_1}\int d^3\mathbf{x}_1\int_{1'}\Sigma\left(1,1'\right)\mathcal{G}\left(1',1^{+}\right)=2\left\langle V\right\rangle . \tag{32.16}$$

We have the freedom to drop the time-ordered product when we recall that the operators are all at the same time and in the indicated order. Using time-translational invariance the last result may also be written

$$\boxed{\Sigma\left(\overline{1},\overline{1'}\right)\mathcal{G}\left(\overline{1'},\overline{1^{+}}\right)=2\left\langle V\right\rangle\beta=\left\langle T_{\tau}\left[\psi^{\dagger}\left(\overline{1^{+}}\right)\psi^{\dagger}\left(\overline{1'^{+}}\right)V\left(\overline{1'}-1\right)\psi\left(\overline{1'}\right)\psi\left(\overline{1}\right)\right]\right\rangle} \tag{32.17}$$

Remark 112 *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.*

32.3 Four-point function from functional derivatives

Since we need a four-point function to compute the self-energy and we know $\mathcal{G}_{\phi}$ if we know the self-energy, let us find an equation for the four-point function in terms of functional derivatives as we saw at length in Eq.(31.16)

$$\frac{\delta\mathcal{G}(1,2)_{\phi}}{\delta\phi(3,4)}=\left\langle T_{\tau}\psi(1)\,\psi^{\dagger}(2)\,\psi^{\dagger}(3)\,\psi(4)\right\rangle_{\phi}+\mathcal{G}(1,2)_{\phi}\,\mathcal{G}(4,3)_{\phi}\,. \tag{32.18}$$

The equation for the functional derivative is then easy to find using $\mathcal{G}\mathcal{G}^{-1}=1$ and our matrix notation,

$$\begin{aligned}
\frac{\delta\left(\mathcal{G}\mathcal{G}^{-1}\right)}{\delta\phi} &= 0 && (32.19)\\
\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1}+\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi} &= 0 && (32.20)\\
\frac{\delta\mathcal{G}}{\delta\phi} &= -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}. && (32.21)
\end{aligned}$$

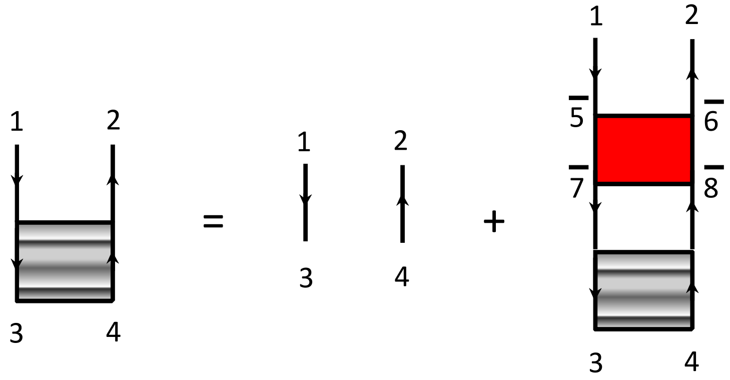


Figure 32-1 Diagrammatic representation of the integral equation for the four point function. The two lines on the right of the equal sign and on top of the last block are Green's function. The filled box is the functional derivative of the self-energy. It is called the particle-hole irreducible vertex. It plays, for the four-point function the role of the self-energy for the Green's function.

With Dyson's equation Eq. (32.14) for $\mathcal{G}^{-1}$ we find the right-hand side of that equation

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}. \tag{32.22}$$

Just to make sure what we mean, let us restore indices. This then takes the form

$$\begin{aligned}
\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,\overline{1}\right)_{\phi}\frac{\delta\phi\left(\overline{1},\overline{2}\right)}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{2},2\right)_{\phi} + \mathcal{G}\left(1,\overline{5}\right)_{\phi}\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{6},2\right)_{\phi} \\
&= \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi} + \mathcal{G}\left(1,\overline{5}\right)_{\phi}\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(3,4\right)}\mathcal{G}\left(\overline{6},2\right)_{\phi}.
\end{aligned} \tag{32.23}$$

We will see that Σ depends on ϕ only through its dependence on $\mathcal{G}$ so that this last equation can also be written in the form

$$\begin{aligned}
\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi} \\
&\quad + \mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(\frac{\delta\Sigma\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{7},\overline{8}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_{\phi}.
\end{aligned} \tag{32.24}$$

This general equation can also be written in short-hand notation

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\,\hat{}\,\mathcal{G} + \ \mathcal{G} \quad \begin{matrix}\frac{\delta\Sigma}{\delta\mathcal{G}} \\ \frac{\delta\mathcal{G}}{\delta\phi}\end{matrix} \quad \mathcal{G}\ \ , \tag{32.25}$$

where the caret $\hat{}$ reminds us that the indices adjacent to it are the same as those of ϕ and where the two terms on top of one another are matrix multiplied top down as well. Fig. 32-1 illustrates the equation with the indices.

32.4 Self-energy from functional derivatives

To compute the self-energy, according to Eq.(32.13), what we need is to obtain the self-energy is

$$\Sigma(1,3)_\phi = -V\left(1-\bar{2}\right)\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)\psi\left(\bar{2}\right)\psi(1)\psi^\dagger\left(\bar{4}\right)\right]\right\rangle_\phi \mathcal{G}_\phi^{-1}\left(\bar{4},3\right). \tag{32.26}$$

We write the four-point function with the help of the functional derivative Eq.(**??**) by replacing in the latter equation $3 \to 1'^+$, $4 \to 1'$, $1 \to 1$, $2 \to \bar{2}$ so that

$$\begin{aligned}\Sigma(1,3)_\phi &= -V\left(1-\bar{2}\right)\left[\frac{\delta\mathcal{G}\left(1,\bar{4}\right)_\phi}{\delta\phi\left(\overline{2^+},\bar{2}\right)} - \mathcal{G}\left(\bar{2},\overline{2^+}\right)_\phi \mathcal{G}\left(1,\bar{4}\right)_\phi\right]\mathcal{G}^{-1}\left(\bar{4},3\right)_\phi \\ &= -V\left(1-\bar{2}\right)\left[-\mathcal{G}\left(1,\bar{4}\right)_\phi \frac{\delta\mathcal{G}^{-1}\left(\bar{4},3\right)_\phi}{\delta\phi\left(\overline{2^+},\bar{2}\right)} - \mathcal{G}\left(\bar{2},\overline{2^+}\right)_\phi \delta(1-3)\right].\end{aligned}$$

where we used Eq.(32.20) $\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}$.This is the general expression that we need for Σ. Note that in $\delta\phi\left(\overline{2^+},\bar{2}\right)$ the spins are identical, in other words, in spin space that matrix is diagonal. This is not the only possibility but that is the only one that we need here as we can see from the four point correlation function that we need. This is the so-called longitudinal particle-hole channel. We will see why with diagrams later on.

Remark 113 *Mnemotechnic: The first index of the* $V\left(1-\bar{2}\right)$ *is the same as the first index of the upper line and is the same as the first indes on the left-hand side of the equation. The second index is summed over and is the same as the index on the second line. The two Green's function in* $\mathcal{G}\left(\bar{2},\overline{2^+}\right)_\phi \mathcal{G}\left(1,\bar{4}\right)_\phi$ *can be arranged on top of one another so that this rule is preserved.*

To begin to do approximations, we use the equation relating $\frac{\delta\mathcal{G}^{-1}}{\delta\phi}$ Eq.(32.22) to $\frac{\delta\Sigma}{\delta\phi}$ to obtain a closed set of equation for Σ that will lend itself to approximations in power series of the potential

$$\begin{aligned}\Sigma(1,3)_\phi &= -V\left(1-\bar{2}\right)\left[\mathcal{G}\left(1,\bar{4}\right)_\phi \frac{\delta\phi\left(\bar{4},3\right)_\phi}{\delta\phi\left(\overline{2^+},\bar{2}\right)} + \mathcal{G}\left(1,\bar{4}\right)_\phi \frac{\delta\Sigma\left(\bar{4},3\right)_\phi}{\delta\phi\left(\overline{2^+},\bar{2}\right)}\right. \\ &\qquad \left. -\mathcal{G}\left(\bar{2},\overline{2^+}\right)_\phi \delta(1-3)\right]\end{aligned} \tag{32.27}$$

$$\begin{aligned}&= -V(1-3)\,\mathcal{G}(1,3)_\phi + V\left(1-\bar{2}\right)\mathcal{G}\left(\bar{2},\overline{2^+}\right)_\phi \delta(1-3) \\ &\qquad -V\left(1-\bar{2}\right)\mathcal{G}\left(1,\bar{4}\right)_\phi \frac{\delta\Sigma\left(\bar{4},3\right)_\phi}{\delta\phi\left(\overline{2^+},\bar{2}\right)}.\end{aligned} \tag{32.28}$$

The first two terms are the Hartree-Fock contribution, that we will discuss in the next section and at length later on. The last term is the only one that will give a frequency dependence, and hence an imaginary part, to the self-energy.

In general, the functional dependence of Σ on ϕ will be through the dependence on $\mathcal{G}$, at least in weak coupling. Hence, using the chain rule, the above equation

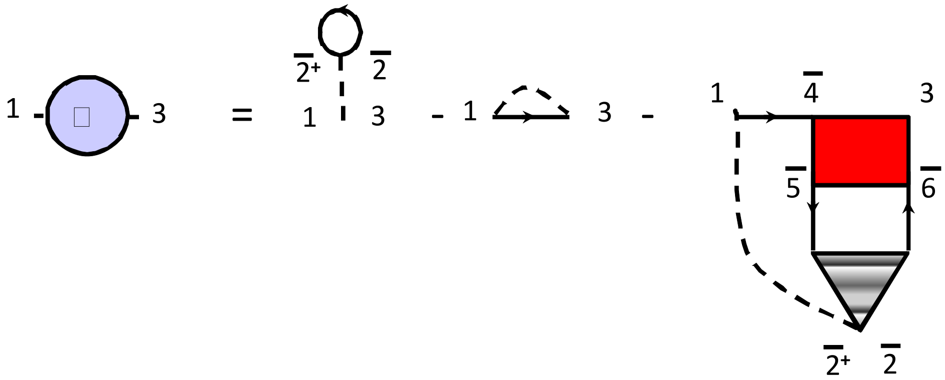


Figure 32-2 Diagrams for the self-energy. The dashed line represent the interaction. The first two terms are, respectively, the Hatree and the Fock contributions. The textured square appearing in the previous figure for the our-point function has been squeezed to a triangle to illustrate the fact that two of the indices (coordinates) are identical.

may be rewritten

$$\begin{aligned}\Sigma\left(1,3\right)_{\phi} &= -V\left(1-3\right)\mathcal{G}\left(1,3\right)_{\phi}+V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right)\\ &\quad -V\left(1-\overline{2}\right)\mathcal{G}\left(1,\overline{4}\right)_{\phi}\frac{\delta\Sigma\left(\overline{4},3\right)_{\phi}}{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}.\end{aligned}\tag{32.29}$$

The equation for the self-energy is represented schematically in Fig. 32-2. Note that the diagrams are one-particle irreducible, i.e. they cannot be cut in two seperate pieces by cutting a single propagator.

33. FIRST STEP WITH FUNCTIONAL DERIVATIVES: HARTREE-FOCK AND RPA

These are the two most famous approximations: Hartree-Fock for the self-energy and RPA for the density-density correlation function. We will see later on why these come out naturally from simple considerations, including the variational principle.

33.1 Equations in real space

Since Σ is already linear in external potential, it is tempting to drop the last term of the last equation of the previous section since that will be of second order at least. If we do this, we obtain

$$\Sigma\left(1,3\right)_{\phi}=-V\left(1-3\right)\mathcal{G}\left(1,3\right)_{\phi}+V\left(1-\overline{2}\right)\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta\left(1-3\right). \tag{33.1}$$

This is the Hartree-Fock approximation, on which we will comment much more later on. This can be used to compute $\frac{\delta\Sigma}{\delta\mathcal{G}}$ that appears both in the in the exact expression for the self-energy Eq.(32.29) and in the exact expression for the four-point function Eq.(32.24) that also appears in the self-energy. A look at the last two figures that we drew is helpful.

Refering to the exact expression for the four-point function Eq.(32.24), what we need is $\frac{\delta\Sigma(5,6)_{\phi}}{\delta\mathcal{G}(7,8)_{\phi}}$ which we evaluate from the the Hartree-Fock approximation Eq.(33.1),

$$\begin{aligned}\frac{\delta\Sigma\left(5,6\right)_{\phi}}{\delta\mathcal{G}\left(7,8\right)_{\phi}} &= V\left(5-\overline{9}\right)\delta\left(\overline{9}-7\right)\delta\left(\overline{9}-8\right)\delta\left(5-6\right)-V\left(5-6\right)\delta\left(7-5\right)\delta\left(8-6\right)\\ &= V\left(5-7\right)\delta\left(7-8\right)\delta\left(5-6\right)-V\left(5-6\right)\delta\left(7-5\right)\delta\left(8-6\right).\end{aligned}$$

It is easier to imagine the result by looking back at the illustration of the Hartree-Fock term in Fig. 32-1. The result of the functional derivative is illustrated in Fig. 33-1. When two coordinates are written on one end of the interaction line, it is because there is a delta function. For example, there is a $\delta\left(5-6\right)$ for the vertical line.

Substituting back in the equation for the exact found-point function $\frac{\delta\mathcal{G}}{\delta\phi}$ Eq.(32.24), we find

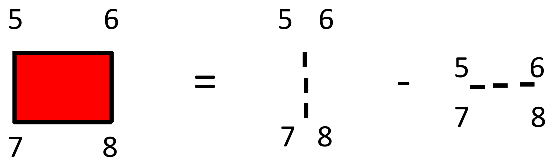


Figure 33-1 Expression for the irreducible vertex in the Hartree-Fock approximation. The labels on either side of the bare interaction represented by a dashed line are at the same point, in other words there is a delta function.

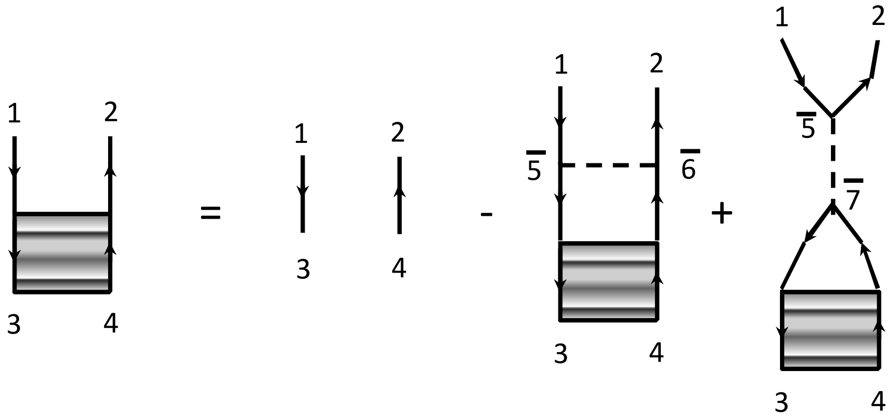


Figure 33-2 Integral equation for $\delta\mathcal{G}/\delta\phi$ in the Hartree-Fock approximation.

$$\begin{aligned}\frac{\delta\mathcal{G}\left(1,2\right)_{\phi}}{\delta\phi\left(3,4\right)} &= \mathcal{G}\left(1,3\right)_{\phi}\mathcal{G}\left(4,2\right)_{\phi} \\ &+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta\mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{5},2\right)_{\phi} \qquad (33.2) \\ &-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta\mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta\phi\left(3,4\right)}\right)\mathcal{G}\left(\overline{6},2\right)_{\phi}. \qquad (33.3)\end{aligned}$$

This expression is easy to deduce from the general diagrammatic representation of the general integral equation Fig. 32-1 by replacing the irreducible vertex by that in Fig. 33-1 that follows from the Hartree-Fock approximation. This is illustrated in Fig. 33-2.

To compute a better approximation for the self-energy we will need $\delta\phi\left(2^{+},2\right)$ instead of $\delta\phi\left(3,4\right)$, as can be seen from our exact result Eq.(32.29). Although one might guess it from symmetry, we will also see that all that we will need is, $\delta\mathcal{G}\left(1,1^{+}\right)$, although it is not obvious at this point. It is quite natural however that the density-density correlation function plays an important role since it is related to the dielectric constant. From the previous equation, that special case can be written

$$\begin{aligned} \frac{\delta \mathcal{G}\left(1,1^{+}\right)_{\phi}}{\delta \phi\left(2^{+},2\right)} &= \mathcal{G}\left(1,2\right)_{\phi} \mathcal{G}\left(2,1\right)_{\phi} && (33.4) \\ &+\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{7}\right)\frac{\delta \mathcal{G}\left(\overline{7},\overline{7}\right)_{\phi}}{\delta \phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{5},1\right)_{\phi} && (33.5) \\ &-\mathcal{G}\left(1,\overline{5}\right)_{\phi}\left(V\left(\overline{5}-\overline{6}\right)\frac{\delta \mathcal{G}\left(\overline{5},\overline{6}\right)_{\phi}}{\delta \phi\left(2^{+},2\right)}\right)\mathcal{G}\left(\overline{6},1\right)_{\phi}. && (33.6) \end{aligned}$$

33.2 Equations in momentum space with $\phi = 0$

We are ready to set $\phi = 0$. Once this is done, we can use translational invariance so that $\Sigma\left(1,3\right) = \Sigma\left(1-3\right)$ and $\mathcal{G}\left(1,3\right) = \mathcal{G}\left(1-3\right)$. In addition, spin rotational invariance implies that these objects are diagonal in spin space. We then Fourier transform to take advantage of the translational invariance. In that case, restoring spin indices we can define

$$\mathcal{G}_{\sigma}\left(k\right) = \int d\left(\mathbf{x}_1-\mathbf{x}_2\right)\int_0^{\beta} d\left(\tau_1-\tau_2\right) e^{-i\mathbf{k}\cdot\left(\mathbf{x}_1-\mathbf{x}_2\right)} e^{ik_n\left(\tau_1-\tau_2\right)} \mathcal{G}_{\sigma}\left(1-2\right) \quad (33.7)$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. For clarity then, we have explicitly written a single spin label. For the potential we define

$$V_{\sigma,\sigma'}\left(q\right) = \int d\left(\mathbf{x}_1-\mathbf{x}_2\right)\int_0^{\beta} d\left(\tau_1-\tau_2\right) e^{-i\mathbf{q}\cdot\left(\mathbf{x}_1-\mathbf{x}_2\right)} e^{iq_n\left(\tau_1-\tau_2\right)} V_{\sigma,\sigma'}\left(1-2\right) \quad (33.8)$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_n = 2n\pi T \quad (33.9)$$

with n and integer. Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}\left(1-2\right)$ is independent of spin. 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 114 *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 expressions to evaluate in momentum space, we start from the above position space expressions, and their diagrammatic equivalent, and now write $\mathcal{G}\left(1-2\right)$ and $V\left(1-2\right)$ in terms of their Fourier-Matsubara transforms, namely

$$\mathcal{G}_{\sigma}\left(1-2\right) = \int \frac{d^3\mathbf{k}}{\left(2\pi\right)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot\left(\mathbf{x}_1-\mathbf{x}_2\right)} e^{-ik_n\left(\tau_1-\tau_2\right)} \mathcal{G}_{\sigma}\left(k\right) \quad (33.10)$$

$$V_{\sigma,\sigma'}\left(1-2\right) = \int \frac{d^3\mathbf{q}}{\left(2\pi\right)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot\left(\mathbf{x}_1-\mathbf{x}_2\right)} e^{-iq_n\left(\tau_1-\tau_2\right)} V_{\sigma,\sigma'}\left(q\right) \quad (33.11)$$

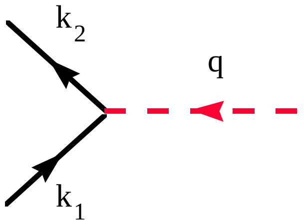


Figure 33-3 A typical interaction vertex and momentum conservation at the vertex.

Then we consider an internal vertex, as illustrated in Fig.(33-3), where one has to do the integral over the space-time position of the vertex, say $1'$. Note that because $V(1-2)=V(2-1)$, we are free to choose the direction of $\mathbf{q}$ on the dotted line at will. Leaving aside the spin coordinates, that behave just as in position space, the integral to perform is

$$\int d\mathbf{x}_1' \int_0^\beta d\tau_1' e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_1'} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_1'} \tag{33.12}$$

$$= (2\pi)^3 \delta(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q}) \beta\delta_{(k_{1,n}-k_{2,n}),q_n} \tag{33.13}$$

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.(34.31) and (34.32) can be done by simply using conservation of momentum and of Matsubara frequencies at each vertex. One must integrate over the momenta and Matsubara frequencies that are not determined by conservation. In general, there are as many integrals to perform as there are closed loops in a diagram.

Writing

$$k=(\mathbf{k},ik_n), \tag{33.14}$$

the Hartree-Fock approximation for the self-energy Eq.(33.1) is

$$\Sigma(k)=-V(q)\mathcal{G}(k+q)+V(q=0)\mathcal{G}\left(\overline{2},\overline{2^+}\right) \tag{33.15}$$

The sign of the wave vector q, or direction of the arrow in the diagram, must be decided once for each diagram but this choice is arbitrary since the potential is invariant under the interchange of coordinates, as mentioned above. This is illustrated in Fig. 33-4

For the four-point function, there are four outside coordinates so we would need three independent outside momenta. However, all that we will need, as we shall see, are the density-density fluctuations. In other words, as we can see from the general expression for the self-energy in Fig. 32-2, we can identify two of the space-time points at the bottom of the graph. We have already written the expression in coordinates in Eq.(33.4). Writing the diagrams for that expression and using our rules for momentum conservation with a four-momentum q flowing top down, the four-point function in Fig. 33-2 becomes as illustrated in Fig. 33-5. You can skp the next chapter is you are satisfied with the functional derivative (source, or Schwinger) approach.

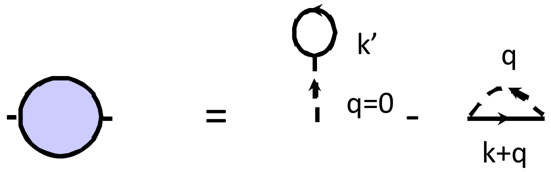


Figure 33-4 Diagram for the self-energy in momentum space in the Hartree-Fock approximation. There is an integral over all momenta and spins not determined by spin and momentum conservation.

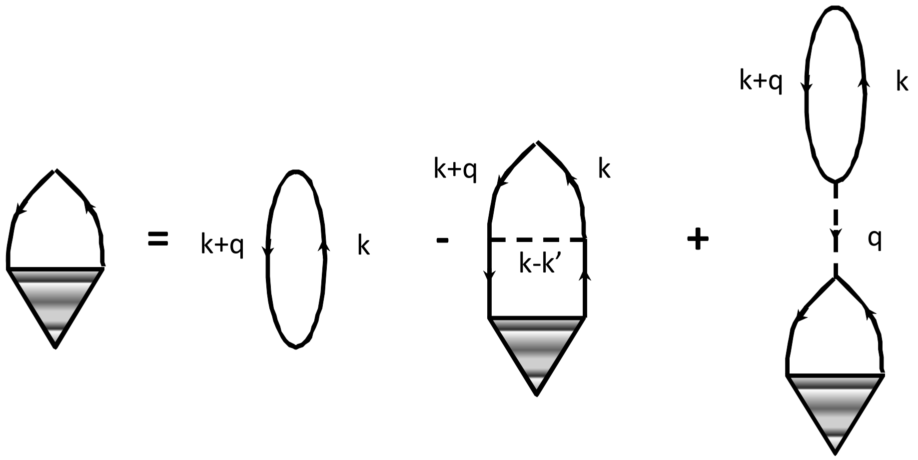


Figure 33-5 Diagrams for the density-density correlation function. We imagine a momentum q flowing from the top of the diagram and conserve momentum at every vertex.

34. 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],[4].

34.1 Hamiltonian and notation

The Hamiltonian we consider is the following. Note that we now introduce spin indices denoted by Greek indices:

$$
\begin{align}
K &= H-\mu N = H_0+V+V_n-\mu N \nonumber\\
H_0 &= \frac{1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \boldsymbol{\nabla}\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\cdot\boldsymbol{\nabla}\psi_{\sigma_1}(\mathbf{x}_1) \tag{34.1}\\
V &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^{\dagger}_{\sigma_1}(\mathbf{x}_1)\,\psi^{\dagger}_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_2}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_1) \nonumber\\
V_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\,\psi^{\dagger}_{\sigma_1}(\mathbf{x}_2)\,\psi_{\sigma_1}(\mathbf{x}_2)\,n_0 \tag{34.2}
\end{align}
$$

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

$$
v(\mathbf{x}_1-\mathbf{x}_2)=\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|} \tag{34.3}
$$

Let us say we want to compute the one-body Green's function in the interaction representation

$$
\begin{align}
\mathcal{G}_{\sigma_1\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) &= -\frac{Tr\left[e^{-\beta K_0}T_\tau\left(\widehat{U}(\beta,\tau_1)\,\widehat{\psi}_{\sigma_1}(\mathbf{x}_1,\tau_1)\,\widehat{U}(\tau_1,\tau_2)\,\widehat{\psi}^{\dagger}_{\sigma_2}(\mathbf{x}_2,\tau_2)\,\widehat{U}(\tau_2,0)\right)\right]}{Tr\left[e^{-\beta K_0}\widehat{U}(\beta,0)\right]} \nonumber\\
&= -\frac{Tr\left[e^{-\beta K_0}T_\tau\left(\widehat{U}(\beta,0)\,\widehat{\psi}_{\sigma_1}(\mathbf{x}_1,\tau_1)\,\widehat{\psi}^{\dagger}_{\sigma_2}(\mathbf{x}_2,\tau_2)\right)\right]}{Tr\left[e^{-\beta K_0}\widehat{U}(\beta,0)\right]} \tag{34.4}
\end{align}
$$

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

$$\widehat{U}\left(\beta,0\right)=T_{\tau}\left[\exp\left(-\int_{0}^{\beta}d\tau_{1}\widehat{V}\left(\tau_{1}\right)\right)\right]$$

Note that by definition of the interaction representation,

$$\widehat{V}\left(\tau_{1}\right)=e^{K_{0}\tau_{1}}\left[\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}}\int d\mathbf{x}_{1}\int d\mathbf{x}_{2}v\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)\psi_{\sigma_{1}}^{\dagger}\left(\mathbf{x}_{1}\right)\psi_{\sigma_{2}}^{\dagger}\left(\mathbf{x}_{2}\right)\psi_{\sigma_{2}}\left(\mathbf{x}_{2}\right)\psi_{\sigma_{1}}\left(\mathbf{x}_{1}\right)\right]e^{-K_{0}\tau_{1}} \tag{34.5}$$

Inserting everywhere the identity operator $e^{-K_0\tau_1}e^{K_0\tau_1}$ this can be made to have a more symmetrical form

$$\begin{aligned}\widehat{U}\left(\beta,0\right) &= T_{\tau}\left[\exp\left(-\frac{1}{2}\sum_{\sigma_{1},\sigma_{2}}\int_{0}^{\beta}d\tau_{1}\int d\mathbf{x}_{1}\int d\mathbf{x}_{2}\right.\right. \quad\times \\ & \left.\left. v\left(\mathbf{x}_{1}-\mathbf{x}_{2}\right)\widehat{\psi}_{\sigma_{1}}^{\dagger}\left(\mathbf{x}_{1},\tau_{1}\right)\widehat{\psi}_{\sigma_{2}}^{\dagger}\left(\mathbf{x}_{2},\tau_{1}\right)\widehat{\psi}_{\sigma_{2}}\left(\mathbf{x}_{2},\tau_{1}\right)\widehat{\psi}_{\sigma_{1}}\left(\mathbf{x}_{1},\tau_{1}\right)\right)\right]\end{aligned} \tag{34.6}$$

This can be made even more symmetrical by defining the potential,

$$\boxed{V_{\sigma_{1},\sigma_{2}}\left(\mathbf{x}_{1},\tau_{1};\mathbf{x}_{2},\tau_{2}\right)=\frac{e^{2}}{\left|\mathbf{x}_{1}-\mathbf{x}_{2}\right|}\delta\left(\tau_{1}-\tau_{2}\right)} \tag{34.7}$$

The right-hand side is independent of spin. In addition to being more symmetrical, this definition has the advantage that we can introduce the short-hand notation

$$V\left(1,2\right) \tag{34.8}$$

where

$$\left(1\right)=\left(\mathbf{x}_{1},\tau_{1};\sigma_{1}\right) \tag{34.9}$$

The evolution operator now systematically involves integrals over time space and a sum over spin indices, so it is possible to further simplify the notation by introducing

$$\int_{1}=\int_{0}^{\beta}d\tau_{1}\int d\mathbf{x}_{1}\sum_{\sigma_{1}=\pm1} \tag{34.10}$$

and

$$\psi\left(1\right)=\widehat{\psi}_{\sigma_{1}}\left(\mathbf{x}_{1},\tau_{1}\right) \tag{34.11}$$

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.(34.4) and the time evolution operator Eq.(34.6) take the simpler looking form

$$\boxed{\mathcal{G}\left(1,2\right)=-\frac{Tr\left[e^{-\beta K_{0}}T_{\tau}\left(U(\beta,0)\psi(1)\psi^{\dagger}(2)\right)\right]}{Tr\left[e^{-\beta K_{0}}U(\beta,0)\right]}} \tag{34.12}$$

$$\boxed{U\left(\beta,0\right)=T_{\tau}\left[\exp\left(-\frac{1}{2}\int_{1}\int_{2}V\left(1,2\right)\psi^{\dagger}\left(1\right)\psi^{\dagger}\left(2\right)\psi\left(2\right)\psi\left(1\right)\right)\right]} \tag{34.13}$$

34.2 In position space

We now proceed to derive Feynman's rules in position space. Multiplying numerator and denominator of the starting expression for the Green's function by $1/Tr\left[e^{-\beta K_0}\right]$ we can use the linked cluster theorem in Subsection (30.2.1) to argue that we can forget about the power series expansion of the evolution operator in the denominator, as long as in the numerator of the starting expression Eq.(34.12) only connected terms are kept. The perturbation expansion for the Green's function thus takes the form

$$\mathcal{G}\left(1,2\right)=-\left\langle T_{\tau}\left(U\left(\beta,0\right)\psi\left(1\right)\psi^{\dagger}\left(2\right)\right)\right\rangle_{0,c} \tag{34.14}$$

The average is over the unperturbed density matrix and only connected terms are kept. A typical term of the power series expansion thus has the form

$$-\frac{1}{n!}\left\langle T_{\tau}\left[\left(-\frac{1}{2}\int_{1'}\int_{2'}V\left(1',2'\right)\psi^{\dagger}\left(1'\right)\psi^{\dagger}\left(2'\right)\psi\left(2'\right)\psi\left(1'\right)\right)^{n}\psi\left(1\right)\psi^{\dagger}\left(2\right)\right]\right\rangle_{0,c} \tag{34.15}$$

To evaluate averages of this sort, it suffices to apply Wick's theorem. Since this process becomes tedious and repetitive, it is advisable to do it once in such a way that simple systematic rules can be extracted that will allow us to write from the outset the simplest expression for a term of any given order. The trick is to write down diagrams and rules both to build them and to associate with them algebraic expressions. These are the Feynman rules.

Wick's theorem tells us that a typical average such as Eq.(34.15) is decomposed into a sum of products of single particle Green's function. Let us represent a Green's function by a straight line, as in Fig.(34-1). Following the convention of Ref. [6] the arrow goes from the left most to the right most label of the corresponding Green's function. Going from the creation to the annihilation operator might have been more natural and would have lead us to the opposite direction of the arrow, as for example in Ref. [7]. Nevertheless it is clear that it suffices to stick to one convention. In any case, contrary to older diagrammatic perturbation techniques, with Feynman diagrams the arrow represents the propagation of either and electron or a hole and the direction is irrelevant. The other building block for diagrams is the interaction potential which is represented by a dotted line. To either end of the dotted line, we have a Green's function that leaves and one that comes in, corresponding to the fact that there is one ψ and one $\psi^{\dagger}$ attached to any given end of a dotted line. The arrow heads in Fig.(34-1) just reminds us of this. They are not really part of the dotted line. Also, it does not matter whether the arrows come in from the top or from the bottom, or from left or right. It is only important that each end of the dotted line is attached to one incoming and one outgoing line.

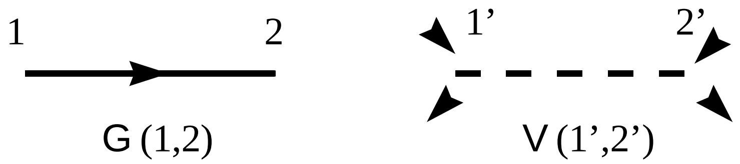


Figure 34-1 Basic building blocks of Feynman diagrams for the electron gas.

Let us give an example of how we can associate contractions and diagrams.

For a term with $n = 1$, a typical term would be

$$-\left\langle T_\tau\left[-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\underset{1}{\psi^\dagger}\left(1'\right)\underset{2}{\psi^\dagger}\left(2'\right)\underset{3}{\psi}\left(2'\right)\underset{2}{\psi}\left(1'\right)\underset{1}{\psi}\left(1\right)\underset{3}{\psi^\dagger}\left(2\right)\right]\right\rangle_{0,c} \tag{34.16}$$

We have marked by a the same number every operator that belongs to the same contraction. The corresponding algebraic expression is

$$-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\mathcal{G}\left(1,1'\right)\mathcal{G}\left(1',2'\right)\mathcal{G}\left(2',2\right) \tag{34.17}$$

and we can represent it by a diagram, as in Fig.(34-2) Clearly, exactly the same contribution is obtained if the roles of the fields at the points $1'$ and $2'$ above are interchanged. More specifically, the set of contractions

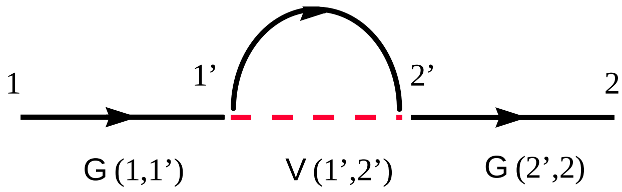


Figure 34-2 A typical contraction for the first-order expansion of the Green's function. THe Fock term.

$$-\left\langle T_\tau\left[-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\underset{2}{\psi^\dagger}\left(1'\right)\underset{1}{\psi^\dagger}\left(2'\right)\underset{2}{\psi}\left(2'\right)\underset{3}{\psi}\left(1'\right)\underset{1}{\psi}\left(1\right)\underset{3}{\psi^\dagger}\left(2\right)\right]\right\rangle_{0,c} \tag{34.18}$$

gives the algebraic expression

$$-\frac{1}{2}\int_{1'}\int_{2'} V\left(1',2'\right)\mathcal{G}\left(2',1'\right)\mathcal{G}\left(1,2'\right)\mathcal{G}\left(1',2\right) \tag{34.19}$$

which, by a change of dummy integration variable, $1' \leftrightarrow 2'$ gives precisely the same contribution as the previous term.

We need to start to be more systematic and do some serious bookkeeping. Let us draw a diagram for each and every one of the possible contractions of this first order term. This is illustrated in Fig.(34-3). 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.(34.17)(34.19). In other words, if we had given the rule that only connected and topologically distinct diagrams contribute and that there is no factor of $1/2$, we would have written down only diagram C and diagram E and obtained correctly all the first order contributions. Two diagrams are topologically distinct if they cannot be transformed one into the other by "elastic" changes that do not cut Green's functions lines.

For a general diagram of order n in the interaction, there are n interaction lines and $2n + 1$ Green's functions. To prove the last statement, it suffices to notice that the four fermion fields attached to each interaction line correspond to four "half lines" and that the creation and annihilation operators corresponding

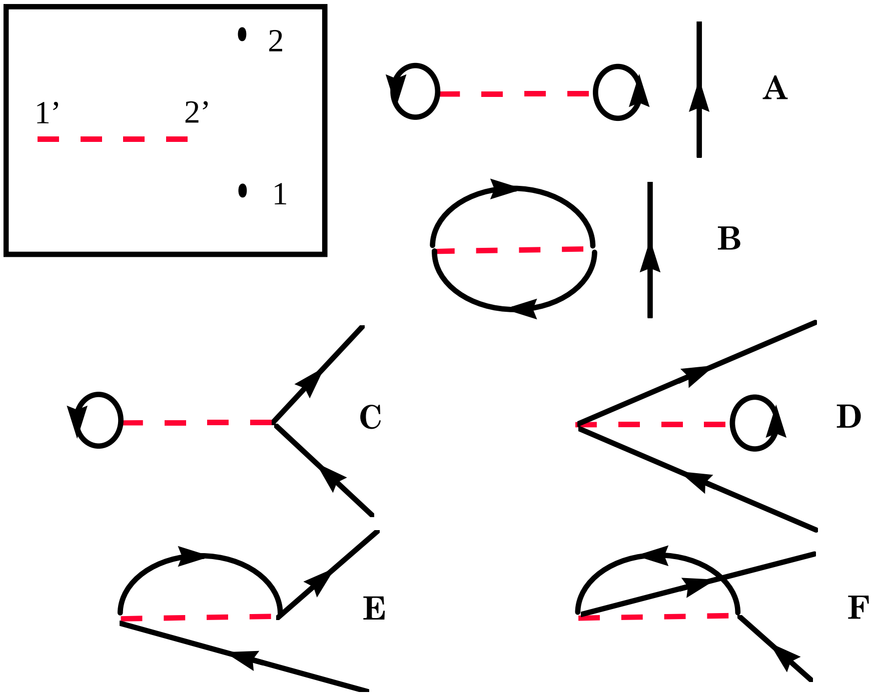


Figure 34-3 All possible contractions for the first-order contribution to the Green’s function. A line must start at point 1 illustrated in the box on the left, and one line must end at 2. Lines must also come in and go out on either side of the dotted line.

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.(34-4). 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 $V(1', 2')$.

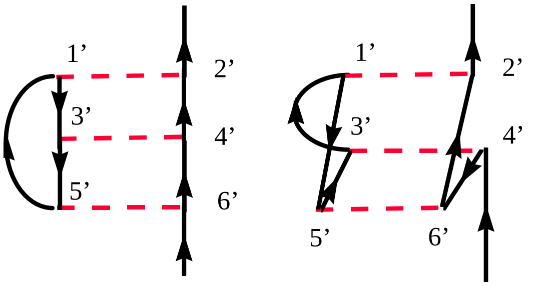


Figure 34-4 Two topologically equaivalent diagrams of order 3.

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.(34.6). (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.(34-5)) the factor

$$\mathcal{G}\left(1,2^+\right) \equiv \lim_{\eta\to 0} \mathcal{G}_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_1+\eta\right) \qquad (34.20)$$

   This last rule must be added because otherwise the rules given before are ambiguous since the Coulomb potential is instantaneous (at equal time) and Green's functions have two possible values at equal time. So it is necessary to specify which of these values it takes. The chosen order is discussed further in the following subsection.

Figure 34-5 Pieces of diagrams for which lead to equal-time Green's functions and for which it is necessary to specify how the $\tau \to 0$ limit is taken.

34.2.1 Proof of the overall sign of a Feynman diagram

To prove the rule concerning the overall sign of a Feynman diagram, consider the expression for a $n'th$ order contribution before the contractions. We leave out the factors of V and other factors to concentrate on field operators, their permutations and the overall sign.

$$-\left(-1\right)^n\left\langle T_\tau\left[\int_{1'}\int_{2'}\dots\int_{2n-1}\int_{2n}\psi^\dagger\left(1'\right)\psi^\dagger\left(2'\right)\psi\left(2'\right)\psi\left(1'\right)\dots\right.\right.\tag{34.21}$$

$$\left.\left.\dots\psi^\dagger\left(2n-1\right)\psi^\dagger\left(2n\right)\psi\left(2n\right)\psi\left(2n-1\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle_{0,c}\tag{34.22}$$

This expression can be rearranged as follows without change of sign by permuting one destruction operator across two fermions in each group of four fermion fields appearing in interactions

$$\begin{aligned}&-\left(-1\right)^n\left\langle T_\tau\left[\int_{1'}\int_{2'}\dots\int_{2n-1}\int_{2n}\left(\psi^\dagger\left(1'^{+}\right)\psi\left(1'\right)\right)\left(\psi^\dagger\left(2'^{+}\right)\psi\left(2'\right)\right)\dots\right.\right.\\&\left.\left.\dots\left(\psi^\dagger\left(\left(2n-1\right)^{+}\right)\psi\left(2n-1\right)\right)\left(\psi^\dagger\left(\left(2n\right)^{+}\right)\psi\left(2n\right)\right)\psi\left(1\right)\psi^\dagger\left(2\right)\right]\right\rangle_{0,c}\end{aligned}\tag{34.23}$$

We have grouped operators with parenthesis to illustrate the appearance of density operators, and we have added plus signs as superscripts to remind ourselves of the original order when we have two fields at equal time. By the way, this already justifies the equal-time rule Eq.(34.20) mentioned above. To clear up the sign question, let us now do contractions, that we will identify as usual by numbers under each creation-annihilation operator pair. We just make contractions in series so that there is a continuous fermion line running from point 1 to point 2 without fermion loops. More specifically, consider the following contractions

$$-\left(-1\right)^n\left\langle T_\tau\left[\int_{1'}\int_{2'}\dots\int_{2n-1}\int_{2n}\underset{2n}{\psi}^\dagger\left(1'^{+}\right)\underset{1}{\psi}\left(1'\right)\underset{1}{\psi}^\dagger\left(2'^{+}\right)\underset{2}{\psi}\left(2'\right)\underset{2}{\dots}\right.\right.\tag{34.24}$$

$$\left.\left.\underset{2n-2}{\dots}\underset{2n-2}{\psi}^\dagger\left(\left(2n-1\right)^{+}\right)\underset{2n-1}{\psi}\left(2n-1\right)\underset{2n-1}{\psi}^\dagger\left(\left(2n\right)^{+}\right)\underset{2n+1}{\psi}\left(2n\right)\underset{2n}{\psi}\left(1\right)\underset{2n+1}{\psi}^\dagger\left(2\right)\right]\right\rangle_{0,c}$$

Not taking into account the $-\left(-1\right)^n$ already in front of the average, the contractions labeled 1 to $2n-1$ give a contribution

$$\left(-1\right)^{2n-1}\mathcal{G}\left(1',2'\right)\mathcal{G}\left(2'3'\right)\dots\mathcal{G}\left(2n-1,2n\right)\tag{34.25}$$

where the overall sign comes from the fact that the definition of $\mathcal{G}$ has the creation and annihilation operators in the same order as they appear in the above contractions, but an overall minus sign in the definition. For the contraction labeled $2n$ one must do an even number of permutations to bring the operators in the order $\psi\left(1\right)\psi^\dagger\left(1'^{+}\right)$ so one obtains a factor $-\mathcal{G}\left(1,1'^{+}\right)$. Similarly, accounting for the new position of $\psi^\dagger\left(1'^{+}\right)$, an even number of permutations is necessary to bring to operators in the order $\psi\left(2n\right)\psi^\dagger\left(2\right)$ so that an overall factor $-\mathcal{G}\left(2n,2\right)$ is generated. The overall sign is thus

$$-\left(-1\right)^n\left(-1\right)^{2n-1}\left(-1\right)^2=\left(-1\right)^n\tag{34.26}$$

In the contractions we have just done there is no closed fermion loop, as illustrated in Fig.(34-6) for the special case where $2n=4$.

Now all we need to show is that whenever we interchange two fermion operators we both introduce a minus sign and either form or destroy a closed fermion loop. The first part of the statement is easy to see. Consider,

$$\left\langle T_\tau\left[\psi^\dagger\left(1'\right)\left(\psi^\dagger\psi\psi\dots\psi\right)\psi^\dagger\left(2\right)\right]\right\rangle_{0,c}\tag{34.27}$$

Suppose we want to compare two sets of contractions that differ only by the fact that two creation operators (or two annihilation operators) interchange their respective role. In the time-ordered product above, bringing $\psi^\dagger\left(1'\right)$ to the left of

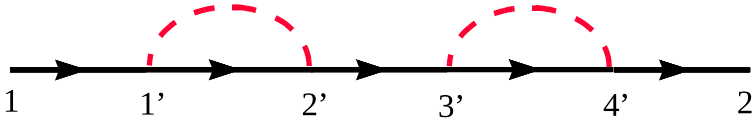


Figure 34-6 Example of a contraction without closed fermion loop.

$\psi^\dagger(2)$ produces a sign $(-1)^p$ where p is the number of necessary permutations. Then, when we take $\psi^\dagger(2)$ where $\psi^\dagger(1')$ was, we create an additional factor of $(-1)^{p+1}$ because $\psi^\dagger(2)$ has to be permuted not only with the operators that were originally there but also with $\psi^\dagger(1')$ that has been brought to its left. The overall sign is thus $(-1)^{2p+1} = -1$, which is independent of the number of operators originally separating the fields. That result was clear from the beginning given that what determines the sign of a permuation is the parity of the number of transpositions (interchange of two objects) necessary to obtain the given permutation. Hence, interchanging *any* pair of fermions gives an extra minus sign. Clearly there would have been something wrong with the formalism if we had not obtained this result.

Diagrammatically, if we start from the situation in Fig.(34-6) and interchange the role of two creation operators, as in Fig.(34-7), then we go from a situation with no fermion loops to one with one fermion loop. Fig.(34-8) illustrates the case where we interchange another pair of creation operators and clearly there also a fermion loop is introduced. In other words, by interchanging two creation operators (or two annihilation operators) we break the single fermion line, and the only way to do this is by creating a loop since internal lines cannot end at an interaction vertex. This completes the proof concerning the overall sign of a diagram.

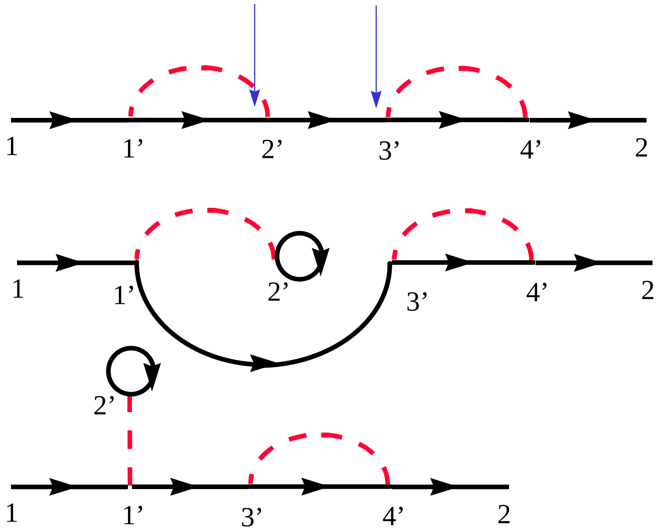


Figure 34-7 Creation of loops in diagrams by interchange of operators: The role of the two creation operators indicated by ligth arrows is interchanged, leading from a diagram with no loop, as on top, to a diagram with one loop. The diagram on the bottom is the same as the one in the middle. It is simply redrawn for clarity.

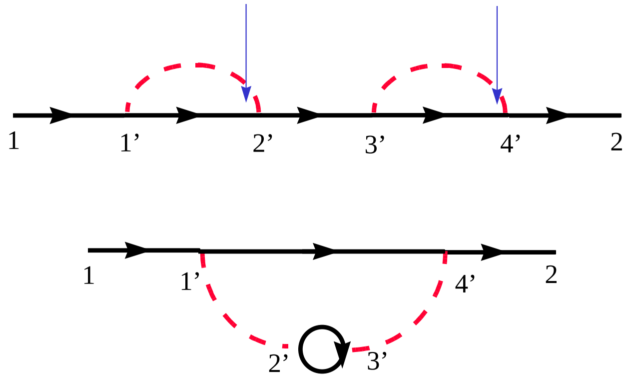


Figure 34-8 Interchange of two fermion operators creating a fermion loop.

Spin sums

A remark is in order concerning spin. In a diagram without loops, as in Fig.(34-6), there is a single spin label running from one end of the diagram to the other. Every time we introduce a loop, there is now a sum over the spin of the fermion in the loop. In the special case where $V(1,2)$ is independent of the spins at the vertices 1 and 2, as is the case for Coulomb interactions, then it is possible to simply disregard spin and add the rule that there is a factor of 2 associated with every fermion loop.

34.3 In momentum space

Starting from our results for Feynman's rule in position space, we can derive the rules in momentum space.[10] First introduce, for a translationally and spin rotationally invariant system, the definition

$$\mathcal{G}_\sigma(k) = \int d(\mathbf{x}_1-\mathbf{x}_2)\int_0^\beta d(\tau_1-\tau_2)\, e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(1-2) \quad (34.28)$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. For clarity then, we have explicitly written a single spin label. For the potential we define

$$V_{\sigma,\sigma'}(q) = \int d(\mathbf{x}_1-\mathbf{x}_2)\int_0^\beta d(\tau_1-\tau_2)\, e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{iq_n(\tau_1-\tau_2)}V_{\sigma,\sigma'}(1-2) \quad (34.29)$$

where q_n is, this time, a bosonic Matsubara frequency, in other words

$$q_n = 2n\pi T \quad (34.30)$$

with n and integer. Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}(1-2)$ is independent of spin. The spin σ is the same as the spin of the two propagators attaching to the vertex 1 while σ' is the same as the spin of the two propagators attaching to the vertex 2.

Remark 115 *General spin-dependent interaction: In more general theories, there are four spin labels attached to interaction vertices. These labels correspond to* *those of the four fermion fields. Here the situation is simpler because the interaction not only conserves spin at each vertex but is also spin independent.*

To find the Feynman rules in momentum space, we start from the above position space diagrams and we now write $\mathcal{G}(1-2)$ and $V(1-2)$ in terms of their Fourier-Matsubara transforms, namely

$$\mathcal{G}_\sigma(1-2)=\int\frac{d^3\mathbf{k}}{(2\pi)^3}T\sum_{n=-\infty}^{\infty}e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(k) \tag{34.31}$$

$$V_{\sigma,\sigma'}(1-2)=\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{n=-\infty}^{\infty}e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-iq_n(\tau_1-\tau_2)}V_{\sigma,\sigma'}(q) \tag{34.32}$$

Then we consider an internal vertex, as illustrated in Fig.(34-9), 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

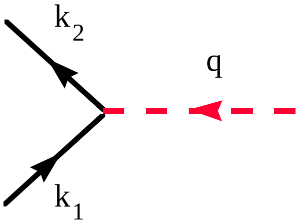


Figure 34-9 A typical interaction vertex and momentum conservation at the vertex.

$$\int d\mathbf{x}_1'\int_0^\beta d\tau_1' e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_1'}e^{i(k_{1,n}-k_{2,n}+q_n)\tau_1'} \tag{34.33}$$

$$=\quad(2\pi)^3\,\delta(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\,\beta\delta_{(k_{1,n}-k_{2,n}),q_n} \tag{34.34}$$

The last delta is a Kronecker delta. Indeed, the sum of two fermionic Matsubara frequencies is a bosonic Matsubara frequency since the sum of two odd numbers is necessarily even. This means that the integral over τ_1' is equal to β if $k_{1,n}-k_{2,n}+q_n=0$ while it is equal to zero otherwise because $\exp\left(i\left(k_{1,n}-k_{2,n}+q_n\right)\tau_1'\right)$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.(34.31) and (34.32) can be done by simply using conservation of momentum and of Matsubara frequencies at each vertex.

The Feynman rules for the perturbation expansion of the Green's function in momentum space thus read as follows.

1. For a term of order n, draw all connected, topologically distinct diagrams with n interaction lines and $2n+1$ oriented propagator lines, taking into account that at every interaction vertex one line comes in and one line comes out.

2. Assign a direction to the interaction lines. Assign also a wave number and a discrete frequency to each propagator and interaction line, conserving momentum and Matsubara frequency at each vertex.

3. To each propagator line, assign

$$\boxed{\mathcal{G}^0_\sigma(k) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)}} \tag{34.35}$$

   (We have to remember that the propagator is independent of spin but still carries a spin label that is summed over.)

4. To each interaction line, associate a factor $V_{\sigma,\sigma'}(q)$, with iq_n a bosonic Matsubara frequency. Note that each of the spin labels is associated with one of the vertices and that it is the same as the spin of the fermion lines attached to it.

5. Perform an integral over wave vector and a sum over Matsubara frequency, namely $\int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty}$ for each momentum and frequency that is not fixed by conservation at the vertex.

6. Sum over all spin indices that are not fixed by conservation of spin.

7. Associate a factor $(-1)^n (-1)^F$ where F is the number of closed Fermion loops to every diagram of order n.

8. For Green's functions whose two ends are on the same interaction line, as in Fig.(34-5), 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.

34.4 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 $\mathcal{G}^0_\sigma(k)$ 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.[9] For example, the first order contribution to the spectral weight $A(k) = -2\,\mathrm{Im}\, G^R$ would be given by a term proportional to

$$\begin{aligned} -2\,\mathrm{Im}\left(\frac{1}{(\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu))^2}\right) &= 2\,\mathrm{Im}\frac{\partial}{\partial\omega}\left(\frac{1}{\omega + i\eta - (\varepsilon_{\mathbf{k}} - \mu)}\right) \\ &= -2\pi \frac{\partial}{\partial\omega}\delta(\omega - (\varepsilon_{\mathbf{k}} - \mu)) \qquad (34.36) \end{aligned}$$

  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

$$\boxed{\mathcal{G}_\sigma(k) = \mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\Sigma_\sigma(k)\mathcal{G}_\sigma(k)} \tag{34.37}$$

or

$$\mathcal{G}_{\sigma}(k)=\frac{1}{\left(\mathcal{G}_{\sigma}^{0}(k)\right)^{-1}-\Sigma_{\sigma}(k)} \tag{34.38}$$

This is the so-called Dyson equation. The iterative solution of this equation

$$\mathcal{G}_{\sigma}(k)=\mathcal{G}_{\sigma}^{0}(k)+\mathcal{G}_{\sigma}^{0}(k)\,\Sigma_{\sigma}(k)\,\mathcal{G}_{\sigma}^{0}(k)+\mathcal{G}_{\sigma}^{0}(k)\,\Sigma_{\sigma}(k)\,\mathcal{G}_{\sigma}^{0}(k)\,\Sigma_{\sigma}(k)\,\mathcal{G}_{\sigma}^{0}(k)+\ldots$$

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.(34-10) is one-particle reducible and hence does not belong to the one-particle irreducible self-energy, but the two diagrams on the right of this figure do.

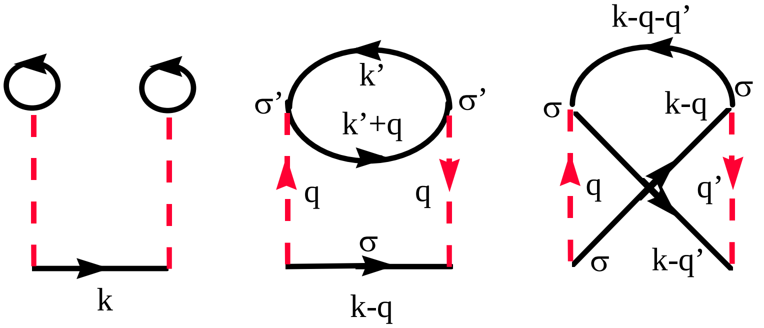


Figure 34-10 Diagram on the left is one-particle reducible, and hence is not an acceptable contribution to the self-energy. The two diagrams on the right however are acceptable contributions to the one-particle irreducible self-energy. In these diagrams, k is the external momentum and Matsubara frequency label while σ is the external spin label. There is a sum over the variables k', q and q' and over the spin σ'.

Remark 116 *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.*

34.5 Feynman diagrams and the Pauli principle

Since operators can be anticommuted at will in a time-ordered product at the price of a simple sign change, it is clear that whenever there are two destruction operators or two creation operators for the same state, the contraction should vanish. This is just the Pauli principle. On the other hand, if we look at a self-energy diagram like the middle one in Fig.(34-10) 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.(34-10). 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.

34.6 Exercices

34.6.1 Théorie des perturbations au deuxième ordre pour la self-énergie

a) En utilisant les règles de Feynman dans l'espace des quantités de mouvement, écrivez les expressions correspondant aux deux diagrammes apparaissant à droite de la figure 34-10 des notes de cours. Ces diagrammes représentent la self-énergie irréductible au deuxième ordre en théorie des perturbations. Effectuez la somme sur les fréquences de Matsubara mais ne faites pas les intégrales.

b) Montrez, avant même de faire la somme sur les fréquences de Matsubara, que lorsque $V_{\mathbf{q}}$ est indépendant de $\mathbf{q}$, le diagramme du milieu est égal à moins deux fois le dernier (troisième sur la figure). Le résultat net est qu'on pourrait considérer seulement le diagramme du milieu en supposant qu'un électron n'interagit qu'avec les autres électrons de spin opposé. Montrez, en remontant à l'Hamiltonien, que ce dernier résultat est général dans le cas où $V_{\mathbf{q}}$ est indépendant de $\mathbf{q}$,(modèle de Hubbard).

c) Écrivez une expression pour la partie imaginaire de la self-énergie obtenue en (a), encore une fois sans faire les intégrales.

34.6.2 Théorie des perturbations au deuxième ordre pour la self-énergie à la Schwinger

a) Utilisez la méthode des dérivées fonctionnelles pour trouver tous les diagrammes au deuxième ordre en interaction $V_{\mathbf{q}}$ pour la self-énergie irréductible. N'oubliez pas que les fonctions de Green dans la méthode décrite en classe sont des fonctions de Green habillées, c'est-à-dire qu'elles contiennent la self-énergie et doivent donc aussi être développées en puissances de l'interaction.

b) Montrez, avant même de faire la somme sur les fréquences de Matsubara, que lorsque $V_{\mathbf{q}}$ est indépendant de $\mathbf{q}$**,** le diagramme du milieu de la figure 34-10 est égal à moins deux fois le dernier (troisième sur la figure). Le résultat net est qu'on pourrait considérer seulement le diagramme du milieu en supposant qu'un électron n'interagit qu'avec les autres électrons de spin opposé. Montrez, en remontant à l'Hamiltonien, que ce dernier résultat est général dans le cas où $V_{\mathbf{q}}$ est indépendant de $\mathbf{q}$,(modèle de Hubbard).

34.6.3 Cas particulier du théorème de Wick avec la méthode de Schwinger

Pour le cas sans interaction, calculez

$$\frac{\delta\mathcal{G}\left(1,2\right)}{\delta\phi\left(3,4\right)\delta\phi\left(5,6\right)} \tag{34.39}$$

et montrez que la fonction de corrélation à six points

$$-\left\langle T_{\tau}\left[\psi^{\dagger}\left(3\right)\psi\left(4\right)\psi^{\dagger}\left(5\right)\psi\left(6\right)\psi\left(1\right)\psi^{\dagger}\left(2\right)\right]\right\rangle_{\phi} \tag{34.40}$$

s'écrit comme une somme de six termes, chacun étant un produit de trois fonctions de Green. Montrez ensuite que le signe de chaque terme peut se déduire des permutations. Ceci est un cas particulier du théorème de Wick qui dit que dans le cas sans interaction les fonction de corrélation d'ordre plus élevé peuvent s'obtenir de toutes les "contractions" posssibles, une contraction correspondant à un appariement d'un $\psi^{\dagger}$ avec un ψ pour en faire une fonction de Green.

35. COLLECTIVE MODES IN NON-INTERACTING LIMIT

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.(14.16) measures

$$S_{\rho\rho}(\mathbf{q},\omega)=\frac{2}{1-e^{-\beta\omega}}\operatorname{Im}\left[\chi^R_{\rho\rho}(\mathbf{q},\omega)\right]=-\frac{2}{1-e^{-\beta\omega}}\frac{q^2}{4\pi}\operatorname{Im}\left[\frac{1}{\epsilon^L(\mathbf{q},\omega)}\right]. \tag{35.1}$$

The longitudinal dielectric constant itself is given by Eq.(14.15)

$$\boxed{\tfrac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)}=1-\tfrac{1}{\varepsilon_0 q^2}\chi^R_{\rho\rho}(\mathbf{q},\omega)}. \tag{35.2}$$

The physical phenomenon of screening will manifest itself in the zero-frequency limit of the longitudinal dielectric constant, $\varepsilon^L\left(\mathbf{q},0\right)$. Interactions between electrons will be screened, hence it is important to know the dielectric constant. Plasma oscillations should come out from the finite frequency zeros of this same function $\varepsilon^L\left(\mathbf{q},\omega\right)=0$, as we expect from our general discussion of collective modes.

We will start this section by a discussion of the Lindhard function, namely $\chi^R_{nn}(\mathbf{q},\omega)=\chi^R_{\rho\rho}(\mathbf{q},\omega)/e^2$ for the free electron gas. We will interpret the poles of this function. Then we introduce interactions with a simple physical discussion of screening and plasma oscillations. A diagrammatic calculation in the so-called Random phase approximation (RPA) will then allow us to recover in the appropriate limiting cases the phenomena of screening and of plasma oscillations.

35.1 Definitions and analytic continuation

We want the Fourier transform of the density-density response function. First note that

$$n_{\mathbf{q}} \equiv \int d^3\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}n\left(\mathbf{r}\right)=\sum_{\sigma=\pm1}\int d^3\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\psi^\dagger_\sigma\left(\mathbf{r}\right)\psi_\sigma\left(\mathbf{r}\right) \tag{35.3}$$

$$= \frac{1}{\left(\sqrt{\mathcal{V}}\right)^2}\sum_\sigma\int d^3\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\mathbf{e}^{i\mathbf{k}'\cdot\mathbf{r}}\mathbf{e}^{-i\mathbf{k}\cdot\mathbf{r}}c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k}',\sigma} \tag{35.4}$$

$$= \sum_\sigma\sum_{\mathbf{k}}c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k}+\mathbf{q},\sigma} \tag{35.5}$$

As before, $\mathcal{V}$ is the quantization volume of the system. We can obtain the retarded density-density response function from

$$\boxed{\chi^R_{nn}(\mathbf{q},\omega) = \lim_{iq_n \to \omega + i\eta} \chi_{nn}(\mathbf{q}, iq_n)} \tag{35.6}$$

with iq_n a bosonic Matsubara frequency, as required by the periodic boundary condition obeyed by the Matsubara density response in imaginary time. The above two functions are defined by

$$\chi_{nn}(\mathbf{q}, iq_n) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_0^\beta d\tau e^{iq_n\tau} \left\langle T_\tau \left[\delta n\left(\mathbf{r},\tau\right) \delta n\left(\mathbf{r}',0\right)\right]\right\rangle \tag{35.7}$$

$$= \frac{1}{\mathcal{V}} \int_0^\beta e^{iq_n\tau} \quad \left\langle T_\tau \left[\delta n_{\mathbf{q}}\left(\tau\right) \delta n_{-\mathbf{q}}\left(0\right)\right]\right\rangle \quad d\tau \tag{35.8}$$

$$\chi^R_{nn}(\mathbf{q},\omega) = \frac{1}{\mathcal{V}} \int_{-\infty}^{\infty} e^{i\omega t} \quad i \left\langle \left[\delta n_{\mathbf{q}}\left(t\right), \delta n_{-\mathbf{q}}\left(0\right)\right]\right\rangle \theta\left(t\right) \quad dt \tag{35.9}$$

Analytic continuation for density response To prove the analytic continuation formula for the density response Eq.(35.6), one can simply use the Lehman representation or deform the integration contour in the Matsubara representation, as we did for propagators in Sec.(27.4). (See Eqs.(27.39) and (27.35) in particular). The fact that we have bosonic Matsubara frequencies means that we will have a commutator in real frequency instead of and anti-commutator because this time $e^{iq_n\beta} = 1$ instead of -1. Furthermore, notice that whether the retarded density response is defined with $n\left(\mathbf{q},t\right)$ or with

$$\delta n\left(\mathbf{q},t\right) = n\left(\mathbf{q},t\right) - \left\langle n\left(\mathbf{q},t\right)\right\rangle = n\left(\mathbf{q},t\right) - n_0\left(2\pi\right)^3 \delta\left(\mathbf{q}\right)$$

is irrelevant since a constant commutes with any operator.

Remark 117 *The density response function is also called charge susceptibility.*

35.2 Density response in the non-interacting limit in terms of $\mathcal{G}^0_\sigma$

The density response can be expressed in terms of Green's function starting either from the Feynman or from the functional derivative approach. In this section we arrive at the same result both ways.

35.2.1 The Feynman way

If you have followed the route of Fenynann, to do the calculation in the non-interacting case, it suffices to use Wick's theorem.

$$\chi^0_{nn}(\mathbf{q}, iq_n) = \frac{1}{\mathcal{V}} \int_0^\beta d\tau e^{iq_n\tau} \sum_\sigma \sum_{\mathbf{k}} \sum_{\sigma'} \sum_{\mathbf{k}'} \tag{35.10}$$

$$\left[\left\langle T_\tau \left[\underset{1}{c^\dagger_{\mathbf{k},\sigma}}\left(\tau\right) \underset{2}{c_{\mathbf{k}+\mathbf{q},\sigma}}\left(\tau\right) \underset{2}{c^\dagger_{\mathbf{k}',\sigma'}} \underset{1}{c_{\mathbf{k}'-\mathbf{q},\sigma'}}\right]\right\rangle_0 - \left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}\right\rangle_0 \left\langle c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma'}\right\rangle_0 \delta_{\mathbf{q},0}\right]$$

Only the contractions indicated survive. The other possible set of contractions is canceled by the disconnected piece $\left\langle c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0 \left\langle c^\dagger_{\mathbf{k}',\sigma'}c_{\mathbf{k}',\sigma'}\right\rangle_0$. Using momentum conservation, all that is left is

$$\chi^0_{nn}(\mathbf{q},iq_n) = -\frac{1}{\mathcal{V}}\int_0^\beta d\tau e^{iq_n\tau}\sum_\sigma\sum_{\mathbf{k}}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},\tau\right)\mathcal{G}^0_\sigma\left(\mathbf{k},-\tau\right) \tag{35.11}$$

Going to the Matsubara frequency representation for the Green's functions, and using again the Kronecker delta that will arise from the τ integration, we are left with something that looks like what could be obtained from the theorem for Fourier transform of convolutions

$$\chi^0_{nn}(\mathbf{q},iq_n) = -\frac{1}{\mathcal{V}}\sum_\sigma\sum_{\mathbf{k}}T\sum_{ik_n}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k},ik_n\right) \tag{35.12}$$

where as usual we will do the replacement in the infinite volume limit

$$\frac{1}{\mathcal{V}}\sum_{\mathbf{k}} \rightarrow \int\frac{d^3\mathbf{k}}{\left(2\pi\right)^3} \tag{35.13}$$

Remark 118 *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.(35-1) if we had followed trivial generalizations of our old rules. There is even an overall minus sign for the closed loop and a sum over wave vectors, Matsubara frequency and spin inside the loop since these are not determined by momentum conservation. However, we needed to perform the contractions explicitly to see this. In particular, it was impossible to guess the overall sign and numerical factors since Feynman's rules that we have developed were for the Green's function, not for the susceptibility. Now that we have obtained the zeroth order term it is clear how to apply Feynman rules for the terms of the perturbation series. But this is the subject of another subsection below.*

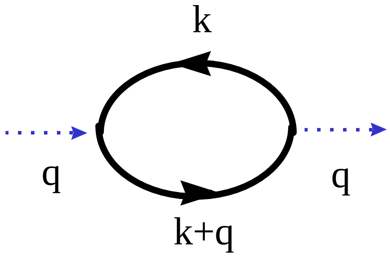


Figure 35-1 Diagram for non-interacting charge susceptibility. Note that the dotted lines just indicate the flow of momentum. No algebraic expression is associated with them.

35.2.2 The Schwinger way (source fields)

Start from the expression for the four-point function Eq.(32.18) for $\phi = 0$ and point $2 = 1^+$ and $3 = 2^+$, and $4 = 2$.Then we find

$$\frac{\delta\mathcal{G}\left(1,1^+\right)}{\delta\phi\left(2^+,2\right)} = -\left\langle T_\tau\psi^\dagger\left(1^+\right)\psi\left(1\right)\psi^\dagger\left(2^+\right)\psi\left(2\right)\right\rangle + \mathcal{G}\left(1,1^+\right)\mathcal{G}\left(2,2^+\right). \tag{35.14}$$

If we sum over the spins associated with point 1 and the spins associated with point 2 and recall that once we sum over spins, we have $\mathcal{G}\left(1,1^{+}\right)=\mathcal{G}\left(2,2^{+}\right)=n$ where n is the average density, then

$$
\begin{aligned}
-\sum_{\sigma_1,\sigma_2}\frac{\delta\mathcal{G}\left(1,1^{+}\right)}{\delta\phi\left(2^{+},2\right)} &= \sum_{\sigma_1,\sigma_2}\left\langle T_\tau\psi^{\dagger}\left(1^{+}\right)\psi\left(1\right)\psi^{\dagger}\left(2^{+}\right)\psi\left(2\right)\right\rangle-n^2 && (35.15)\\
&= \left\langle T_\tau n\left(1\right)n\left(2\right)\right\rangle-n^2 && (35.16)\\
&= \left\langle T_\tau\left(n\left(1\right)-n\right)\left(n\left(2\right)-n\right)\right\rangle\\
&= \chi_{nn}(1-2). && (35.17)
\end{aligned}
$$

The last expression is from the definition of the density-density correlation function in Eq.(35.7). The non-interacting contribution is given by the first term in Fig. 33-5. Alternatively, one can start from the first term in Eq.(33.4) for the functional derivative and take the Fourier transform. One obtains,

$$\chi^0_{nn}(\mathbf{q},iq_n)=-\frac{1}{\mathcal{V}}\sum_{\sigma}\sum_{\mathbf{k}}T\sum_{ik_n}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k},ik_n\right). \tag{35.18}$$

One of the sums over spins has disappeared because we should think of $\mathcal{G}^0_\sigma$ as a matrix that is diagonal in spin indices. This is the so-called Lindhard function.

35.3 Density response in the non-interacting limit: Lindhard function

To compute

$$\chi^0_{nn}(\mathbf{q},iq_n)=-\frac{1}{\mathcal{V}}\sum_{\sigma}\sum_{\mathbf{k}}T\sum_{ik_n}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k},ik_n\right) \tag{35.19}$$

the sums over Matsubara frequency should be performed first and they are easy to do. The technique is standard. First introduce the notation

$$\boxed{\zeta_{\mathbf{k}}\equiv\varepsilon_{\mathbf{k}}-\mu} \tag{35.20}$$

then use partial fractions

$$T\sum_{ik_n}\mathcal{G}^0_\sigma\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0_\sigma\left(\mathbf{k},ik_n\right)=T\sum_{ik_n}\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\frac{1}{ik_n-\zeta_{\mathbf{k}}} \tag{35.21}$$

$$\chi^0_{nn}(\mathbf{q},iq_n)=-2\int\frac{d^3\mathbf{k}}{\left(2\pi\right)^3}T\sum_{ik_n}\left[\frac{1}{ik_n-\zeta_{\mathbf{k}}}-\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right]\frac{1}{iq_n-\zeta_{\mathbf{k}+\mathbf{q}}+\zeta_{\mathbf{k}}}. \tag{35.22}$$

The factor of two comes from the sum over spins. Before the partial fractions, the terms in the ik_n series decreased like $\left(ik_n\right)^{-2}$ 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.(27.81) and (27.82), it is clear that as long as we take the same convergence factor for both terms, the result is

$$\chi^0_{nn}(\mathbf{q},iq_n)=-2\int\frac{d^3\mathbf{k}}{\left(2\pi\right)^3}\frac{f\left(\zeta_{\mathbf{k}}\right)-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)}{iq_n+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{35.23}$$

independently of the choice of convergence factor.

The retarded function is easy to obtain by analytic continuation. It is the so-called Lindhard function

$$\boxed{\chi^{0R}_{nn}(\mathbf{q},\omega) = -2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)}{\omega+i\eta+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}} \tag{35.24}$$

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 119 *Diagrammatic form of particle-hole excitations: If we return to the diagram in Fig.(35-1), we should notice the following general feature. If we cut the diagram in two by a vertical line, we see that it is crossed by lines that go in opposite directions. Hence, we have a particle-hole excitation. In particle-particle or hole-hole excitations, the lines go in the same direction and the two single-particle energies* $\zeta_{\mathbf{k}+\mathbf{q}}$ *and* $\zeta_{\mathbf{k}}$ *add up instead of subtract.*

Remark 120 *Absorptive vs reactive part of the response, real vs virtual excitations: There is a contribution to the imaginary part, in other words absorption, if for a given* $\mathbf{k}$ *and* $\mathbf{q}$ *energy is conserved in the intermediate state, i.e. if the condition* $\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}}$ *is realized. If this condition is not realized, the corresponding contribution is reactive, not dissipative, and it goes to the real part of the response only. The intermediate state then is only virtual. To understand the type of excitations involved in the imaginary part, rewrite* $f(\zeta_{\mathbf{k}}) - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right) = \left(1-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right)f(\zeta_{\mathbf{k}}) - (1-f(\zeta_{\mathbf{k}}))f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)$. *We see that either* $\zeta_{\mathbf{k}}$ *can correspond to a hole and* $\zeta_{\mathbf{k}+\mathbf{q}}$ *to a particle or the other way around. In other words a single Green function line contains both the hole and the particle propagation.*

35.3.1 Zero-temperature value of the Lindhard function: the particle-hole continuum

To evaluate the integral appearing in the Lindhard function, which is what Lindhard did, it is easier to evaluate the imaginary part first and then to obtain the real part using Kramers-Kronig. Let us begin

$$\begin{aligned}\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) &= 2\pi\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left[f(\zeta_{\mathbf{k}}) - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\delta\left(\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}\right) &(35.25)\\ &= 2\pi\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left[\delta\left(\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}\right) - \delta\left(\omega+\zeta_{\mathbf{k}-\mathbf{q}}-\zeta_{\mathbf{k}}\right)\right].\end{aligned}$$

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

$$\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega) = \frac{1}{2\pi}\int_0^{k_F}k^2dk\int_{-1}^{1}d(\cos\theta)\,\frac{m}{kq}\left[\delta\left(\frac{\omega-\varepsilon_{\mathbf{q}}}{kq/m}-\cos\theta\right)-\delta\left(\frac{\omega+\varepsilon_{\mathbf{q}}}{kq/m}-\cos\theta\right)\right] \tag{35.26}$$

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 [12]

$$\varepsilon_{\mathbf{k}} = \sum_{i=1}^{d}\frac{k_i^2}{2m_i} \tag{35.27}$$

$$\operatorname{Im}\chi_{nn}^{0R}(\mathbf{q},\omega) = \frac{\prod_{i=1}^{d}\left(\sqrt{2m_i}\right)}{2^d\pi^{(d-1)/2}\Gamma\left(\frac{d+1}{2}\right)\sqrt{\varepsilon_{\mathbf{q}}}}\times$$

$$\left\{\theta\left(\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}}-\theta\left(\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}}\right\}$$

The real part is also calculable [12] but we do not quote it here.

The functional form of this function in low dimension is quite interesting. Figures (35-2)(35-3) and (35-4) show the imaginary part of the Lindhard function in, respectively, $d = 1, 2, 3$. The small plots on the right show a cut in wave vector at fixed frequency while the plots on the left show $\operatorname{Im}\chi_{nn}^{0R}(\mathbf{q},\omega)$ on the vertical axis, frequency going from left to right and wave vector going from back to front. In all cases, at finite frequency it takes a finite wave vector $\mathbf{q}$ to have absorption. If the wave vector is too large however the delta function cannot be satisfied and there is no absorption either. The one dimensional case is quite special since at low frequency there is absorption only in a narrow wave vector band. This has a profound influence on the interacting case since it will allow room for collective modes to propagate without absorption. In fact, in the interacting one-dimensional case the collective modes become eigenstates. This 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.[12] 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.

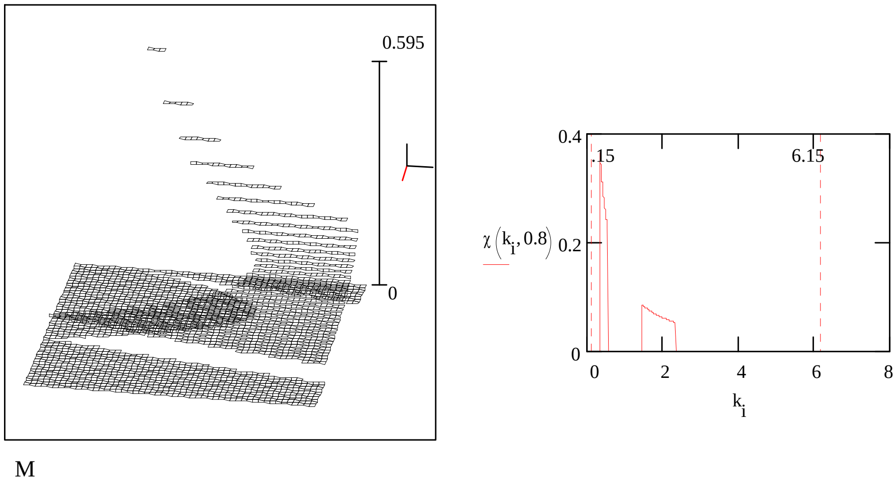


Figure 35-2 Imaginary part of the Lindhard function in $d = 1$ on the vertical axis. Frequency increases from left to right and wave vector from back to front.

To understand the existence of the particle-hole continuum and its shape, it is preferable to return to the original expression Eq.(35.25). In Fig.(35-5) we draw the geometry for the *three-dimensional case.*[13] 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

$$\omega - \frac{q^2}{2m} = \frac{kq}{m}\cos\theta \tag{35.28}$$

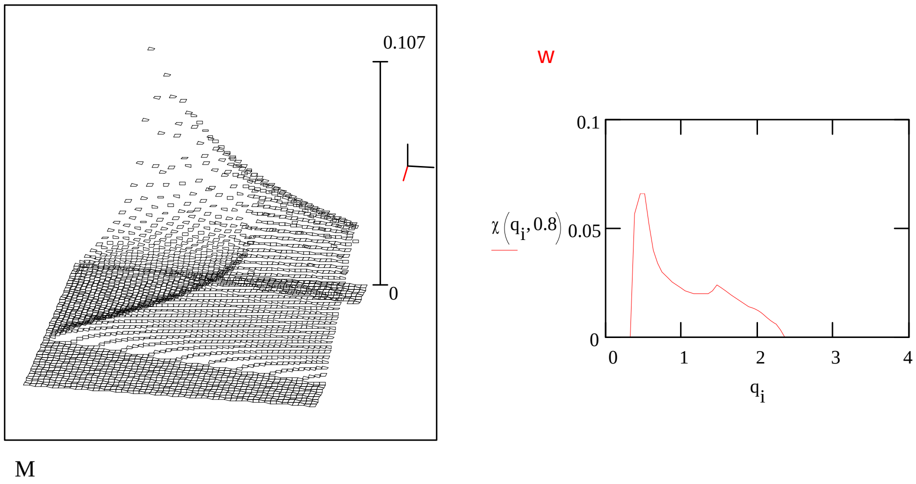


Figure 35-3 Imaginary part of the Lindhard function in $d = 2$. Axes like in the $d = 1$ case.

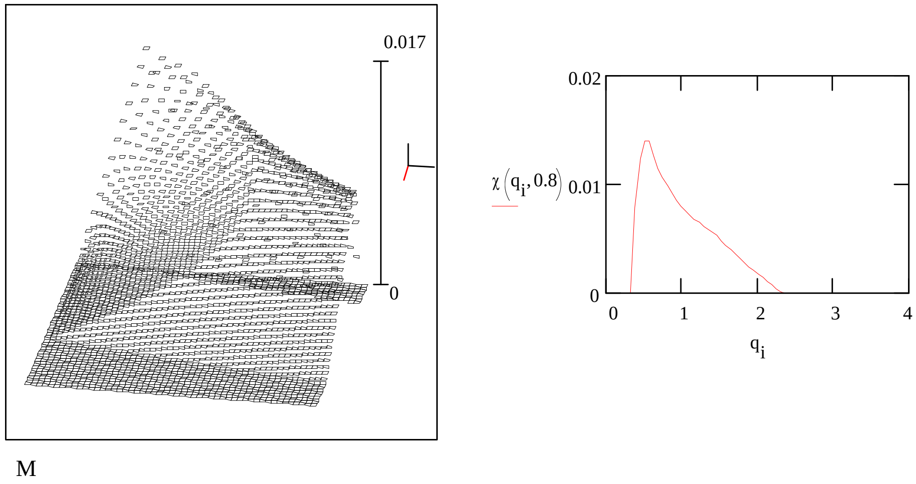


Figure 35-4 Imaginary part of the Lindhard function in $d = 3$. Axes like in the $d = 1$ case.

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 $\mathrm{Im}\,\chi_{nn}^{0R}(\mathbf{q},\omega)$. 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 surface. The corresponding energy is

$$\omega_{change} = \frac{k_F^2}{2m} - \frac{(k_F - q)^2}{2m} = v_F q - \varepsilon_{\mathbf{q}} \tag{35.29}$$

This line, $\omega_{change}(q)$, is shown in Fig.(35-6). Clearly the cases $q < 2k_F$ and $q > 2k_F$ are also different. The figure (35-5) 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

$$\omega_{\max} = \frac{(k_F + q)^2}{2m} - \frac{k_F^2}{2m} \tag{35.30}$$

$$= \varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q < 2k_F \tag{35.31}$$

The minimum allowed value of ω vanishes since both arrows can be right at the Fermi surface in the annulus region.

$$\omega_{\min} = 0 \quad ; \quad q < 2k_F \tag{35.32}$$

For the other case, namely $q > 2k_F$ the two spheres do not overlap anymore. The maximum allowed value of ω is exactly the same as above, but since the two spheres do not overlap 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

$$\omega_{\min} = \frac{(k_F - q)^2}{2m} - \frac{k_F^2}{2m} = \varepsilon_{\mathbf{q}} - v_F q; \quad q > 2k_F \tag{35.33}$$

The region in ω and q space where $\mathrm{Im}\,\chi_{nn}^{0R}(\mathbf{q},\omega)$ is non-vanishing, the particle-hole continuum, is illustrated schematically in Fig.(35-6) for positive frequency. Since $\mathrm{Im}\,\chi_{nn}^{0R}(\mathbf{q},\omega)$ is odd in frequency, there is a symmetrical region at $\omega < 0$.

35.4 Exercices

35.4.1 Fonction de Lindhard et susceptibilité magnétique:

On applique un champ magnétique extérieur $h(\mathbf{x},t)$ produisant sur un système de fermions de spin 1/2 la perturbation

$$H^{ext} = -\mu_0 \int d^3\mathbf{x} \sum_{\sigma=\pm 1} \sigma \psi_\sigma^\dagger(\mathbf{x})\,\psi_\sigma(\mathbf{x})\,h(\mathbf{x},t) \tag{35.34}$$

où μ_0 est le moment magnétique.

a) Utilisez la théorie de la réponse linéaire pour exprimer le coefficient de proportionalité entre le moment magnétique induit

$$M(\mathbf{k},\omega) = \mu_0 \left\langle \int d^3\mathbf{x} \int dt \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}+i\omega t} \sum_{\sigma=\pm 1} \sigma \psi_\sigma^\dagger(\mathbf{x},t)\,\psi_\sigma(\mathbf{x},t) \right\rangle_{hors \quad équilibre} \tag{35.35}$$

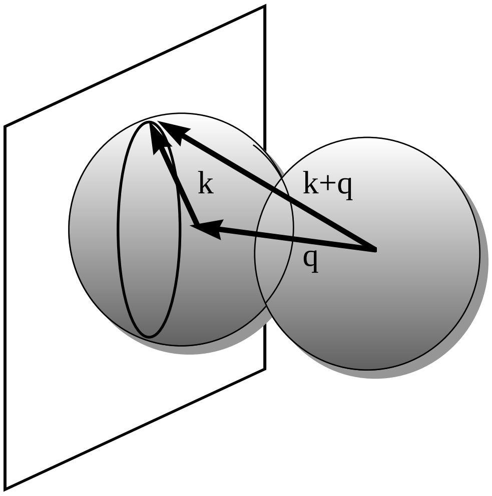


Figure 35-5 Geometry for the integral giving the imaginary part of the $d = 3$ Lindhard function. The wave vectors in the plane satisfy energy conservation as well as the restrictions imposed by the Pauli principle. The plane located symmetrically with respect to the miror plane of the spheres corresponds to energies of opposite sign.

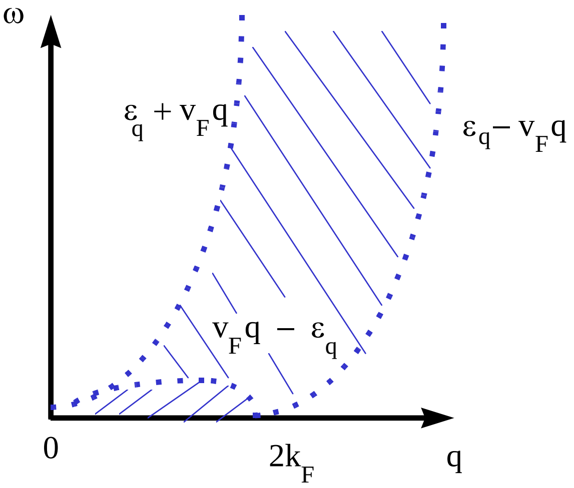


Figure 35-6 Schematic representation of the domain of frequency and wave vector where there is a particle-hole continuum.

et le champ magnétique extérieur comme une fonction de réponse. Ce coefficient de proportionalité est la susceptibilité magnétique

$$\chi\left(\mathbf{k},\omega\right)=M\left(\mathbf{k},\omega\right)/h\left(\mathbf{k},\omega\right) \tag{35.36}$$

b) Supposez qu'il n'y a pas d'interactions dans le système et montrez, en utilisant le théorème de Wick dans le formalisme de Matsubara, que la susceptibilité magnétique est alors proportionnelle à la fonction de Lindhard.

c) Montrez que

$$\lim_{\mathbf{k}\to\mathbf{0}}\chi\left(\mathbf{k},\omega=0\right)=\begin{cases}\frac{3\mu_0^2 n}{2E_F} & T=0\quad\text{(Susceptibilité de Pauli)}\\ \frac{\mu_0^2 n}{T} & T\to\infty\quad\text{(Loi de Curie)}\end{cases} \tag{35.37}$$

36. INTERACTIONS AND COLLECTIVE MODES IN A SIMPLE WAY

Before we start the whole machinery to take into account interactions, it is helpful to recall some of the simple Physics that we should obtain. We begin by identifying the expansion parameter.

36.1 Expansion parameter in the presence of interactions: r_s

In the presence of interactions, it is convenient to define a dimensionless constant that measures the strength of interactions relative to the kinetic energy. If the kinetic energy is very large compared with the interaction strength, perturbative methods may have a chance. Let us begin by recalling some well known results. In the hydrogen atom, potential and kinetic energy are comparable. That defines a natural distance for interacting electrons, namely the Bohr radius. Let us remind ourselves of what this number is. Using the uncertainty principle, we have $\Delta k \sim a_0^{-1}$ so that the kinetic energy can be estimated as $1/\left(ma_o^2\right)$ and the value of a_0 itself is obtained by equating this to the potential energy

$$\frac{1}{ma_o^2} = \frac{e^2}{4\pi\varepsilon_0 a_0} \tag{36.1}$$

giving us for the Bohr radius, in standard units,

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}m \sim 0.5\overset{0}{A} \tag{36.2}$$

It is standard practice to define the dimensionless parameter r_s by setting the density of electrons n_0 equal to 1/(volume of the sphere of radius $r_s a_0$ occupied by a single electron). In other words, we have

$$\boxed{n_0 \equiv \frac{1}{\frac{4\pi}{3}r_s^3 a_0^3}} \tag{36.3}$$

where

$$n_0 = \frac{k_F^3}{3\pi^2} \tag{36.4}$$

is the density of electrons. Another way to write r_s is then

$$\boxed{r_s \equiv \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{k_F a_0}} \tag{36.5}$$

In a way, r_s is the average distance between electrons measured in units of the Bohr radius. Large r_s means that the electrons are far apart, hence that the kinetic energy is small. Using the same uncertainty relation as in the hydrogen atom, this means that interactions are more important than kinetic energy. Conversely, at small r_s kinetic energy is large compared with interactions and the interactions are much less important than the kinetic energy. It is natural then to expect that r_s is a measure of the relative strength of the interactions or, if you want, an expansion parameter. A way to confirm this role of r_s is to show that

$$\frac{Potential}{Kinetic} \sim \frac{\frac{e^2}{4\pi\varepsilon_0}k_F}{k_F^2/2m} \sim \frac{m\frac{e^2}{4\pi\varepsilon_0}}{k_F} \sim \frac{1}{k_F a_0} \sim \left(\frac{1}{n_0 a_0^3}\right)^{1/3} \sim r_s \tag{36.6}$$

These estimates are obtained as follows. The average momentum exchanged in interactions is of order k_F so that $\frac{e^2}{4\pi\varepsilon_0 r} \sim \frac{e^2}{4\pi\varepsilon_0}k_F$ should be a sensible value for the average potential energy while the kinetic energy as usual is estimated from E_F.

It may be counterintuitive at first to think that interactions are less important at large densities but that is a consequence of the uncertainty principle, not a concept of classical mechanics.

36.2 Thomas-Fermi screening

The elementary theory of screening is the Thomas-Fermi theory.[11] 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

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\left[\rho_i(\mathbf{r}) + \delta\rho(\mathbf{r})\right] \tag{36.7}$$

The quantity $\delta\rho(\mathbf{r})$ is the change in charge density of the background produced by the charged impurity

$$\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0 = -e\left[n(\mathbf{r}) - n_0\right] \tag{36.8}$$

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

$$\frac{n(\mathbf{r})}{n_0} = \frac{k_F^3(\mathbf{r})}{k_F^3} \tag{36.9}$$

and electrochemical equilibrium

$$\frac{k_F^2(\mathbf{r})}{2m} + (-e\phi(\mathbf{r})) = E_F = \frac{k_F^2}{2m} \tag{36.10}$$

where E_F is the value of the Fermi energy infinitely far from the impurity potential, lead immediately to the relation between density and electrostatic potential

$$\frac{n(\mathbf{r})}{n_0} = \frac{k_F^3(\mathbf{r})}{k_F^3} = \left[\frac{k_F^2(\mathbf{r})/2m}{k_F^2/2m}\right]^{3/2} = \left[1 - \frac{(-e\phi(\mathbf{r}))}{E_F}\right]^{3/2} \tag{36.11}$$

Substituting this back into Poisson's equation, we have a closed equation for potential

$$\boxed{-\nabla^2\phi\left(\mathbf{r}\right)=4\pi\rho_i\left(\mathbf{r}\right)-\frac{1}{\varepsilon_0}n_0e\left[\left(1-\frac{\left(-e\phi(\mathbf{r})\right)}{E_F}\right)^{3/2}-1\right]} \tag{36.12}$$

In general it is important to solve this full non-linear equation because otherwise at short distances the impurity potential is unscreened $\phi\left(\mathbf{r}\right)\sim 1/r$ which leads to unphysical negative values of the density in the linearized expression for the density,

$$\frac{n\left(\mathbf{r}\right)}{n_0}\approx\left[1-\frac{3}{2}\frac{\left(-e\phi\left(\mathbf{r}\right)\right)}{E_F}\right] \tag{36.13}$$

Nevertheless, if we are interested only in long-distance properties, the linear approximation turns out to be excellent. In this approximation, Poisson's equation Eq.(36.12) becomes

$$-\nabla^2\phi\left(\mathbf{r}\right)=\frac{1}{\varepsilon_0}\rho_i\left(\mathbf{r}\right)+\frac{1}{\varepsilon_0}\frac{3}{2}\frac{n_0e}{E_F}\left(-e\phi\left(\mathbf{r}\right)\right) \tag{36.14}$$

We could have arrived directly at this equation by posing

$$-\nabla^2\phi\left(\mathbf{r}\right)=\frac{1}{\varepsilon_0}\left[\rho_i\left(\mathbf{r}\right)-e\frac{\partial n}{\partial\mu}\left(+e\phi\left(\mathbf{r}\right)\right)\right] \tag{36.15}$$

We now proceed to solve this equation, but first let us define

$$\boxed{q_{TF}^2=\frac{3}{2}\frac{n_0e^2}{\varepsilon_0E_F}=\frac{e^2}{\varepsilon_0}\frac{\partial n}{\partial\mu}} \tag{36.16}$$

Then we can write

$$\left(-\nabla^2+q_{TF}^2\right)\phi\left(\mathbf{r}\right)=\frac{1}{\varepsilon_0}\rho_i\left(\mathbf{r}\right) \tag{36.17}$$

whose solution, by Fourier transforms, is

$$\boxed{\phi\left(\mathbf{q}\right)=\frac{1}{\varepsilon_0}\frac{\rho_i(\mathbf{q})}{q^2+q_{TF}^2}} \tag{36.18}$$

The Thomas-Fermi dielectric constant follows immediately since the definition,

$$\phi\left(\mathbf{q}\right)=\frac{1}{\varepsilon^L\left(\mathbf{q},0\right)}\frac{\rho_i\left(\mathbf{q}\right)}{q^2} \tag{36.19}$$

immediately yields, the value of the zero-frequency dielectric constant

$$\boxed{\varepsilon^L\left(\mathbf{q},0\right)=\varepsilon_0\frac{q^2+q_{TF}^2}{q^2}=\varepsilon_0\left(1+\frac{q_{TF}^2}{q^2}\right).} \tag{36.20}$$

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 sreening is very effective. In real space, one finds an exponential decrease of the potential over a length scale q_{TF}^{-1}, the Thomas-Fermi screening length. Let us write this length in terms of r_s using the definition Eq.(36.3) or (36.5) with $a_0=\frac{4\pi\varepsilon_0\hbar^2}{me^2}$

$$\begin{aligned}\lambda^2 &\equiv q_{TF}^{-2}=\frac{2\varepsilon_0E_F}{3n_0e^2}=\frac{2\varepsilon_0k_F^2/2m}{3n_0e^2}=\frac{k_F^2a_0}{12\pi n_0} &(36.21)\\ &= \frac{k_F^2a_0^4}{12\pi}\left(\frac{4\pi}{3}r_s^3\right)=a_0^2\left(\frac{1}{9}\left(\frac{9\pi}{4}\right)^{2/3}\right)r_s &(36.22)\end{aligned}$$

Roughly speaking then, for $r_s \ll 1$ we have that the screening length

$$\boxed{\lambda \sim \left(a_0 \sqrt{r_s} = \tfrac{a_0 r_s}{\sqrt{r_s}} \right)} \tag{36.23}$$

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 121 *Two dimensional case: As an exercise, note that if the material is two dimensional, then the density is confined to a surface so that* $n_0 \to n_s \delta(z)$ *and* $\rho \to \rho_s \delta(z)$ *where* n_s *and* ρ_s *are surface density and charge surface density. Then, Eq.(36.15) in Fourier space becomes*

$$\left(q_z^2 + q_{||}^2 \right) \phi(\mathbf{q}) = \frac{1}{\varepsilon_0} \left[\rho_s(\mathbf{q}_{||}) - e \frac{\partial n_s}{\partial \mu} \left(+ e\phi(\mathbf{q}_{||}, z=0) \right) \right] \tag{36.24}$$

Dividing by $q_z^2 + q_{||}^2$ *we obtain*

$$\begin{aligned} \int \phi(\mathbf{q}) \frac{dq_z}{2\pi} &= \phi(\mathbf{q}_{||}, z=0) \\ &= \frac{1}{\varepsilon_0} \left[\rho_s(\mathbf{q}_{||}) - e \frac{\partial n_s}{\partial \mu} \left(e\phi(\mathbf{q}_{||}, z=0) \right) \right] \int \frac{1}{q_z^2 + q_{||}^2} \frac{dq_z}{2\pi} \end{aligned} \tag{36.25}$$

The last integral is equal to $(2q_{||})^{-1}$ *so that*

$$\left[1 + \frac{e^2}{2\varepsilon_0 q_{||}} \frac{\partial n_s}{\partial \mu} \right] \phi(\mathbf{q}_{||}, z=0) = \frac{\rho_s(\mathbf{q}_{||})}{2\varepsilon_0 q_{||}} \tag{36.26}$$

and

$$\phi(\mathbf{q}_{||}, z=0) = \frac{\rho_s(\mathbf{q}_{||})}{2\varepsilon_L(\mathbf{q}_{||}) q_{||}} = \frac{1}{2\varepsilon_0} \frac{\rho_s(\mathbf{q}_{||})}{q_{||} + \frac{e^2}{2\varepsilon_0} \frac{\partial n_s}{\partial \mu}} \tag{36.27}$$

$$\frac{\varepsilon_L(\mathbf{q}_{||})}{\varepsilon_0} = 1 + \frac{e^2}{2\varepsilon_0 q_{||}} \frac{\partial n_s}{\partial \mu}. \tag{36.28}$$

This result was obtained by Stern in Phys. Rev. Lett. 1967.

36.3 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

$$\mathbf{j} = -e n_0 \mathbf{v} \tag{36.29}$$

Taking the time derivative and using Newton's equations,

$$\frac{\partial \mathbf{j}}{\partial t} = -en_0 \frac{\partial \mathbf{v}}{\partial t} = -\frac{en_0}{m}\left(-e\mathbf{E}\right) \tag{36.30}$$

Note that in Newton's equation we should use the total time derivative instead of the partial, but since we assume a uniform density ($\mathbf{q} = \mathbf{0}$) the total and partial derivative are identical. We are in a position where one more time derivative

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = \frac{n_0 e^2}{m} \frac{\partial \mathbf{E}}{\partial t} \tag{36.31}$$

and an appeal to the *longitudinal* part of Maxwell's fourth equation

$$0 = \mu_0 \mathbf{j} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{36.32}$$

should give us the desired result, namely

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = -\frac{n_0 e^2}{\varepsilon_0 m} \mathbf{j} \tag{36.33}$$

This equation has an oscillatory solution at a frequency ω_p

$$\boxed{\omega_p^2 \equiv \frac{n_0 e^2}{\varepsilon_0 m}} \tag{36.34}$$

the so-called plasma frequency. Since we know that the longitudinal dielectric constant vanishes at a collective mode, this gives us another expected limit of this function

$$\boxed{\lim_{\omega \to \omega_p} \varepsilon^L \left(\mathbf{q} = \mathbf{0}, \omega\right) = a\left(\omega - \omega_p\right)} \tag{36.35}$$

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.(36.30) and then uses current conservation with Maxwell's first equation to obtain

$$\begin{aligned} \frac{\partial \nabla \cdot \mathbf{j}}{\partial t} &= -\frac{en_0}{m}\left(-e\nabla \cdot \mathbf{E}\right) & (36.36) \\ -\frac{\partial^2 \rho}{\partial t^2} &= \frac{e^2 n_0}{\varepsilon_0 m} \rho & (36.37) \end{aligned}$$

which immediately leads to the desired expression for the plasma frequency. Note that writing $\nabla \cdot \mathbf{E} = -\nabla^2 \phi = \rho/\varepsilon_0$ is equivalent to using the unscreened potential. This is correct at large frequency where screening cannot occur. This will come out automatically from the $\mathbf{q}$ and ω dependence of dielectric constant.

Remark 122 *Two dimensional case: Screening being different in for two dimensional films, as we have just seen, plasma oscillations will be different. In fact, the plasma frequency vanishes at zero wave vector. Indeed, current conservation for the surface quantities reads,*

$$\frac{\partial \rho_s}{\partial t} + \nabla_s \cdot \mathbf{j}_s = 0. \tag{36.38}$$

Taking the two-dimensional divergence of Newton's equation Eq.(36.30) on both sides, we obtain

$$\frac{\partial \nabla_s \cdot \mathbf{j}_s}{\partial t} \delta\left(z\right) = \frac{e^2 n_s}{m} \delta\left(z\right) \nabla_s \cdot \mathbf{E} \tag{36.39}$$

so that Fourier transforming and using charge conservation, we obtain

$$-\frac{\partial^2 \rho_s(q_{||})}{\partial t^2} = \frac{e^2 n_s}{m} i\mathbf{q}_{||} \cdot \mathbf{E}(\mathbf{q}_{||}, z=0). \tag{36.40}$$

We can express the electric field in terms of the surface density to close the system of equations,

$$\mathbf{E}(\mathbf{q}_{||}, z=0) = -\mathbf{i}\mathbf{q}_{||}\phi(\mathbf{q}_{||}, z=0) = -\mathbf{i}\mathbf{q}_{||}\frac{\rho_s}{2\varepsilon_0 q_{||}} \tag{36.41}$$

where we used the unscreened Poisson equation for a film (two-dimensional mateiral). This leads to

$$\frac{\partial^2 \rho_s(q_{||})}{\partial t^2} = -\frac{e^2 n_s}{2\varepsilon_0 m} q_{||}\rho_s \tag{36.42}$$

which means that the plasma frequency is

$$\omega_p^2 = \frac{e^2 n_s}{2\varepsilon_0 m} q_{||} \tag{36.43}$$

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.*

37. DENSITY RESPONSE IN THE PRESENCE OF INTERACTIONS

Since we begin real perturbation theory soon, it is helpful to identify first what is the expansion parameter. Then, we compute the density response and corresponding dielectric function using the RPA.

37.1 Density-density correlations, RPA

As before we derive the relevant equation the Feynman way and the Schwinger way.

37.1.1 The Feynman way

We are now ready to start our diagrammatic analysis. Fig.(37-1) shows all charge susceptibility diagrams to first order in the interaction. The four diagrams on the second line take into account self-energy effects on the single-particle properties. We will worry about this later. Of the two diagrams on the first line, the first one clearly dominates. Indeed, the dotted line leads to a factor $e^2/\left(\varepsilon_0 q^2\right)$ that diverges at small wave vectors. On the other hand, the contribution from the other diagram is proportional to

$$-2\int\frac{d^3k}{(2\pi)^3}T\sum_{ik_n}\int\frac{d^3k'}{(2\pi)^3}T\sum_{ik_n'}\mathcal{G}_\sigma^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}_\sigma^0\left(\mathbf{k},ik_n\right)\times$$

$$\frac{e^2}{\varepsilon_0\left|\mathbf{k}-\mathbf{k}'\right|^2}\mathcal{G}_\sigma^0\left(\mathbf{k}'+\mathbf{q},ik_n'+iq_n\right)\mathcal{G}_\sigma^0\left(\mathbf{k}',ik_n'\right) \tag{37.1}$$

which is a convergent integral with no singularity at $q=0$.

Remark 123 *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

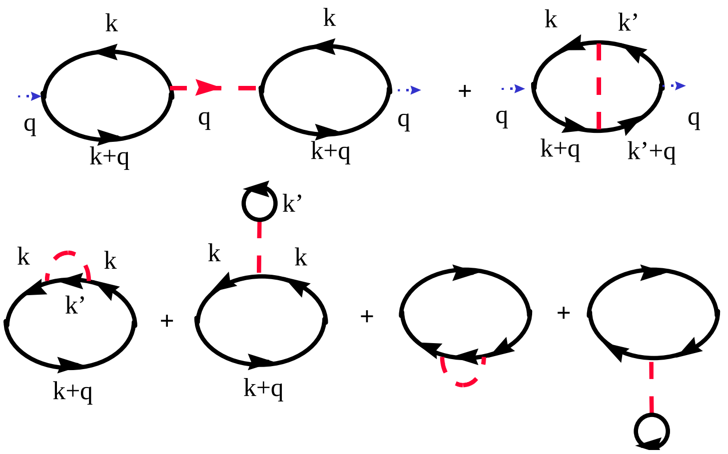


Figure 37-1 Charge susceptibility diagrams to first order in the interaction

illustrated in Fig.(37-2). It is the famous random phase approximation (RPA). One also meets the terminology *ring diagrams* (in the context of free energy calculations) or, more often, one also meets the name bubble diagrams. The full susceptibility is represented by adding a triangle to one of the external vertices. That triangle represents the so-called dressed three point vertex. The reason for this name will come out more clearly later. The full series, represented schematically on the first two lines of the figure, may be summed to infinity by writing down the equation on the last line. This equation looks like a particle-hole version of the Dyson equation. The undressed bubble plays the role of an irreducible susceptibility. It is irreducible with respect to cutting one interaction line.

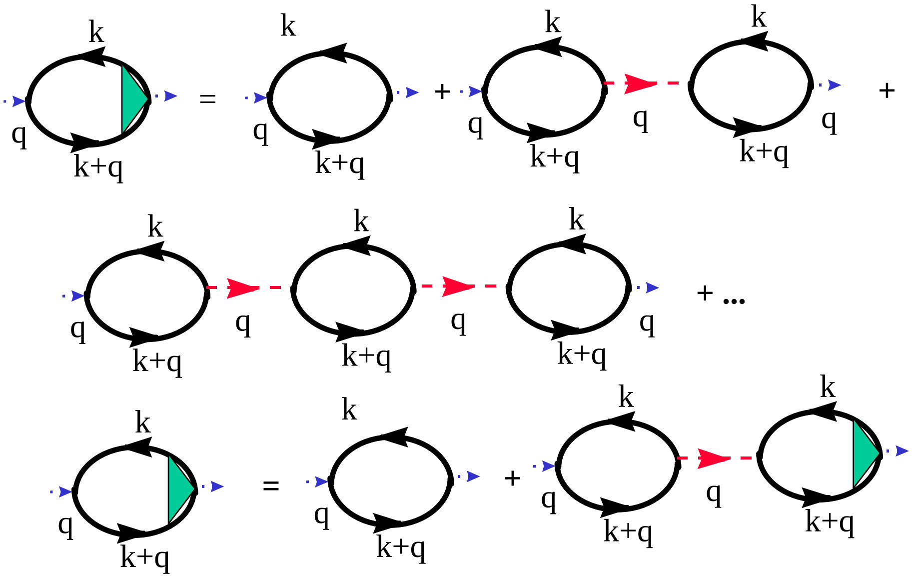


Figure 37-2 Bubble diagrams. Random phase approximation.

From our calculation of the susceptibility for non-interacting electrons we know that Feynman's rules apply for the diagrams on Fig.(37-2). Each bubble is associated with a factor $\chi^0_{nn}(\mathbf{q}, iq_n)$, a quantity defined in such a way that it contains the minus sign associated with the fermion loop. The dashed interaction lines each lead to a factor $-V_{\mathbf{q}}=-e^2/\left(\varepsilon_0 q^2\right)$, the minus sign being associated with the fact that one more $V_{\mathbf{q}}$ means one higher order in perturbation theory (remember the $(-1)^n$ rule). The sum over bubbles, represented by the last line on Fig.(37-2) is easy to do since it is just a geometric series. The result is.

$$\boxed{\chi_{nn}(\mathbf{q},iq_n)=\frac{\chi^0_{nn}(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}}\quad;\quad V_{\mathbf{q}}=\frac{e^2}{\varepsilon_0 q^2}\tag{37.2}$$

The corresponding result for the dielectric constant Eq.(35.2) is

$$\frac{1}{\epsilon^L(\mathbf{q},\omega)}=\frac{1}{\varepsilon_0}\left(1-\frac{e^2}{\varepsilon_0 q^2}\chi^R_{nn}(\mathbf{q},\omega)\right)=\frac{1}{\varepsilon_0\left(1+V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega)\right)}\tag{37.3}$$

or,

$$\boxed{\epsilon^L(\mathbf{q},\omega)=\varepsilon_0\left(1+V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega)\right).}\tag{37.4}$$

Remark 124 *Irreducible polarization: It is customary to call* $-\chi^{0R}_{nn}(\mathbf{q},\omega)$ *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).*

37.1.2 The Schwinger way

We keep following our first step approach that gave us the Hartree-Fock approximation and corresponding susceptibility. Returning to our expression for the susceptibility in terms a functional derivative Eq.(35.15), namely

$$-\sum_{\sigma_1,\sigma_2}\frac{\delta\mathcal{G}\left(1,1^+\right)}{\delta\phi\left(2^+,2\right)}=\chi_{nn}\left(1-2\right)\tag{37.5}$$

and Fourier transforming, we obtain in the case where the irreducible vertex is obtained from functional derivatives of the Hartree-Fock self-energy the set of diagrams in Fig. 33-5. In the middle diagram on the right-hand side of the equality, there is a sum over wave vectors k' because three of the original coordinates of the functional derivative at the bottom of the diagram were different. This means there are two independent momenta, contrary to the last diagram in the figure. One of the independent momenta can be taken as q by momentum conservation while the other one, k', must be integrated over. The contribution from that middle diagram is not singular at small wave vector because the Coulomb potential is integrated over. By contrast, the last diagram has a $1/q^2$ from the interaction potential, which is divergent. We thus keep only that last term. The integral equation, illustrated in Fig., then takes an algebraic form

$$\chi_{nn}(q)=\chi^0_{nn}(q)-\chi^0_{nn}(q)V_{\mathbf{q}}\chi_{nn}(q)\tag{37.6}$$

which is easily solved

$$\chi_{nn}(q)=\frac{\chi^0_{nn}(q)}{1+V_{\mathbf{q}}\chi^0_{nn}(q)}=\frac{1}{\chi^0_{nn}(q)^{-1}+V_{\mathbf{q}}}\tag{37.7}$$

This is the so-called Random Phase Approximation, or RPA. The last form of the equality highlights the fact that the irreducible vertex, here $V_{\mathbf{q}}$, plays the role of an irreducible self-energy in the particle-hole channel. The analytical continuation will be trivial.

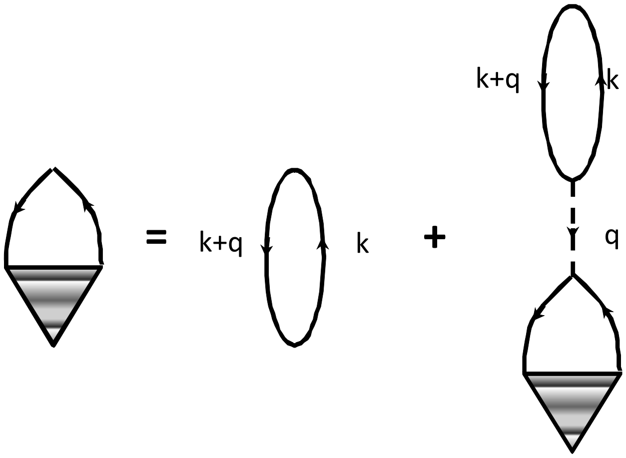


Figure 37-3 Fourier transform of $\frac{\delta\mathcal{G}(1,1^+)}{\delta\phi(2^+,2)}$ with a momentum q flowing top to bottom that is used to compute the density-density correlation function in the RPA approximation.

Note that we have written $\chi^0_{nn}(q)$ for the bubble diagram, i.e. the first term on the right-hand side of the equation in Fig. 33-5 even though everything we have up to now in the Schwinger formalism are dressed Green's functions. The reason is that neglecting the middle diagram on the right-hand side of the equality is like neglecting the contribution from the Fock, or exchange self-energy in Fig. 33-4. The only term left then is is the Hartree term that we argued should vanish because of the neutralizing background. Hence, the Green's functions are bare ones and the corresponding susceptibility is the Linhard function.

Remark 125 *Equivalence to an infinite set of bubble diagrams: The integral equation for the susceptibility has turned into an algebraic equation in 37.6. By recursively replacing $\chi_{nn}(q)$ on the right-hand side of that equation by higher and higher order approximations in powers of $V_{\mathbf{q}}$ we obtain*

$$\begin{aligned}\chi^{(1)}_{nn}(q) &= \chi^0_{nn}(q) - \chi^0_{nn}(q)V_{\mathbf{q}}\chi^0_{nn}(q)\\ \chi^{(2)}_{nn}(q) &= \chi^0_{nn}(q) - \chi^0_{nn}(q)V_{\mathbf{q}}\chi^0_{nn}(q) + \chi^0_{nn}(q)V_{\mathbf{q}}\chi^0_{nn}(q)V_{\mathbf{q}}\chi^0_{nn}(q) \quad (37.8)\end{aligned}$$

etc. By solving the algebraic equation then, it is as if we had summed an infinite series which diagrammatically would look, if we turn it sideways, like Fig. 37-2.The analogy with the self-energy in the case of the Green's function is again clear.

37.2 Explicit form for the dielectric constant and special cases

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

$$\mathrm{Re}\left[\frac{\epsilon^L(\mathbf{q},\omega)}{\varepsilon_0}\right] \equiv \frac{\epsilon^L_1(\mathbf{q},\omega)}{\varepsilon_0} \quad (37.9)$$

$$
\begin{aligned}
&= \quad 1+\frac{q_{TF}^2}{q^2}\left\{\frac{1}{2}+\frac{k_F}{4q}\left[\left(1-\frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right)\ln\left|\frac{\omega-v_Fq-\varepsilon_q}{\omega+v_Fq-\varepsilon_q}\right|\right.\right.\\
&\qquad \left.\left.+\left(1-\frac{(\omega+\varepsilon_q)^2}{q^2v_F^2}\right)\ln\left|\frac{\omega+v_Fq+\varepsilon_q}{\omega-v_Fq+\varepsilon_q}\right|\right]\right\} \qquad (37.10)
\end{aligned}
$$

$$
\operatorname{Im}\left[\epsilon^L(\mathbf{q},\omega)\right]\equiv\epsilon_2^L(\mathbf{q},\omega) \qquad (37.11)
$$

$$
=\left\{\begin{array}{lll}
\left.\begin{array}{ll}
\frac{\pi}{2}\frac{\omega}{v_Fq}\frac{q_{TF}^2}{q^2} \quad ; & \omega\le v_Fq-\varepsilon_q\\
\frac{\pi k_F}{4q}\frac{q_{TF}^2}{q^2}\left(1-\frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right); & v_Fq-\varepsilon_q\le\omega\le\varepsilon_q+v_Fq\\
0 \quad ; & \omega\ge\varepsilon_q+v_Fq
\end{array}\right\} & q<2k_F\\
\left.\begin{array}{ll}
\frac{\pi k_F}{4q}\frac{q_{TF}^2}{q^2}\left(1-\frac{(\omega-\varepsilon_q)^2}{q^2v_F^2}\right); & \varepsilon_q-v_Fq\le\omega\le\varepsilon_q+v_Fq
\end{array}\right\} & q>2k_F
\end{array}\right.
$$

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.

37.2.1 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

$$
\begin{aligned}
\chi^{0R}_{nn}(\mathbf{q},\omega) &= \int\frac{d\omega'}{\pi}\frac{\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')}{\omega'-\omega-i\eta}=\int\frac{d\omega'}{\pi}\frac{\omega'\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')}{(\omega')^2-(\omega+i\eta)^2}\\
&= \sum_{i=1}^{M/2}\frac{A_i}{u_i^2-(\omega+i\eta)^2}=\frac{B\prod_{i=1}^{(M/2)-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M/2}\left(u_i^2-(\omega+i\eta)^2\right)} \qquad (37.12)
\end{aligned}
$$

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.(37.2) for the RPA susceptibility we find,

$$
\chi^R_{nn}(\mathbf{q},\omega)=\frac{B\prod_{i=1}^{(M/2)-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M/2}\left(u_i^2-(\omega+i\eta)^2\right)+V_{\mathbf{q}}B\prod_{i=1}^{(M/2)-1}\left((\omega+i\eta)^2-v_i^2\right)} \qquad (37.13)
$$

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.(37.2) and simple algebra

$$
\operatorname{Im}\left(\frac{x+iy}{1+x+iy}\right)=\frac{y}{(1+x)^2+y^2} \qquad (37.14)
$$

we find the following result for the imaginary part

$$\operatorname{Im}\chi^R_{nn}(\mathbf{q},\omega)=\frac{\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)}{\left(1+V_{\mathbf{q}}\operatorname{Re}\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2+\left(V_{\mathbf{q}}\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2}\tag{37.15}$$

In a discrete system $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ would be proportional to a delta function whenever there is a pole in the non-interacting susceptibility. The square of this delta function that appears in the denominator cancels the corresponding delta function in the numerator, which is another (less clear) way of saying what we have just shown in full generality above, namely that in the interacting system the poles are different from those of the non-interacting system. The new poles are a solution of

$$\frac{1}{V_{\mathbf{q}}}+\operatorname{Re}\chi^{0R}_{nn}(\mathbf{q},\omega)=\frac{1}{V_{\mathbf{q}}}+\sum_{i=1}^{M/2}\frac{A_i}{u_i^2-\omega^2}=0\tag{37.16}$$

The solution of this equation may in principle be found graphically as illustrated in Fig.(37-4). 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 $1/\left(u_i-\omega\right)$ 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 126 *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(37-4), there are six non-interacting poles and six interacting ones.*

Since $\operatorname{Im}\left(\epsilon^L(\mathbf{q},\omega)/\varepsilon_0\right)^{-1}=1+V_{\mathbf{q}}\operatorname{Im}\chi^R_{nn}(\mathbf{q},\omega)$ the zeros of the dielectric constant are at the same location as the poles of $\chi^R_{nn}(\mathbf{q},\omega)$ and, from what we just said, these poles are located basically in the same $(\omega,\mathbf{q})$ domain as the particle-hole continuum of the non-interacting system, except for possibly a pair of poles. This situation is illustrated schematically in Fig.(37-5), that generalizes Fig.(35-6)

37.2.2 Screening

At zero frequency, namely for a static charge perturbation, the imaginary part of the dielectric constant vanishes, as shown by Eq.(37.11), while the real part Eq.(37.9) becomes

$$\frac{\varepsilon_1^L(\mathbf{q},0)}{\varepsilon_0}=1+\frac{q_{TF}^2}{q^2}\left[\frac{1}{2}+\frac{k_F}{2q}\left(1-\frac{q^2}{(2k_F)^2}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right|\right]\tag{37.17}$$

In the long wave length limit, we recover our Thomas Fermi result Eq.(36.20). This limit can also be obtained directly by approximating the integral defining

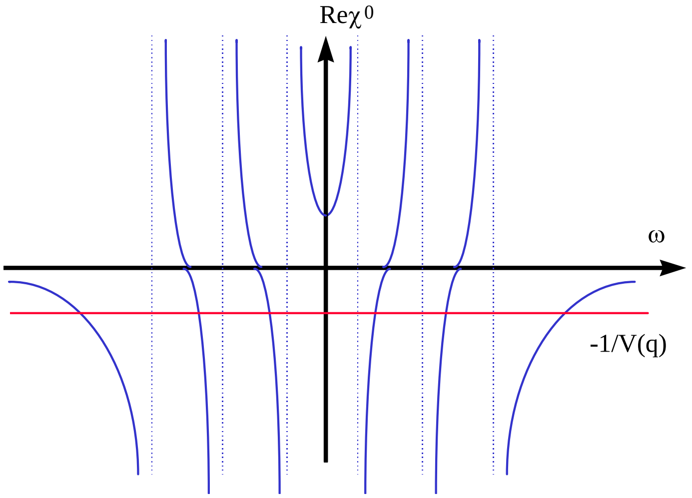


Figure 37-4 Graphical solution for the poles of the charge susceptibility in the interacting system.

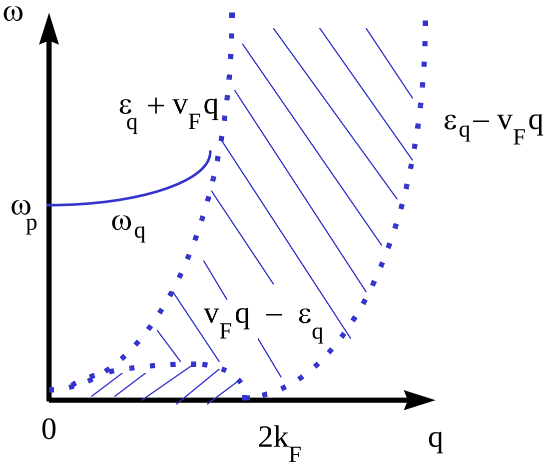


Figure 37-5 Schematic representation of the domain of frequency and wave vector where there are poles in the charge susceptibility, or zeros in the longitudinal dielectric function. In addition to the particle-hole continuum, there is a plasma pole.

Lindhard function Eq.(46.29) that enters the RPA dielectric function Eqs.(37.4)

$$\begin{aligned}
\lim_{\mathbf{q}\to 0}\varepsilon_1^L(\mathbf{q},0) &= \lim_{\mathbf{q}\to 0}\left[1-2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}\right] && (37.18)\\
&= \left[1-2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{\partial f(\zeta_{\mathbf{k}})}{\partial\zeta_{\mathbf{k}}}\right] && (37.19)\\
&= 1+V_{\mathbf{q}}\frac{\partial}{\partial\mu}\left[2\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\right] && (37.20)\\
&= 1+\frac{e^2}{\varepsilon_0 q^2}\frac{\partial n}{\partial\mu} && (37.21)\\
&= 1+\frac{q_{TF}^2}{q^2} && (37.22)
\end{aligned}$$

The definition of q_{TF} is in Eq.(36.16). The corresponding potential

$$V_{eff}(\mathbf{r})=\int\frac{d^3q}{(2\pi)^3}\frac{e^2}{\varepsilon_0}\frac{1}{q^2+q_{TF}^2}e^{i\mathbf{q}\cdot\mathbf{r}}\propto\frac{e^2}{\varepsilon_0 r}e^{-rq_{TF}} \qquad (37.23)$$

is the screened Coulomb interaction.

Remark 127 *The expression* $\varepsilon_1^L(\mathbf{q},0)=\left(1+V_{\mathbf{q}}\chi_{nn}^0(\mathbf{q},0)\right)$ *would be replaced by* $\frac{\varepsilon_1^L(\mathbf{q},0)}{\varepsilon_0}=\left(1-V_{\mathbf{q}}\Pi_{nn}^{R(1)}(\mathbf{q},0)\right)$ *in the general case, with* $-\Pi_{nn}^{R(1)}(\mathbf{q},0)$ *the irreducible polarization. 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.(37.21) would be different from the non-interacting result. This is relevant in effective models such as the Hubbard model.*

37.2.3 Friedel oscillations

If instead of using the limiting Thomas-Fermi form for small wave vectors one does a more careful evaluation[14] of the Fourier transform of $\varepsilon_1(\mathbf{q},0)$ Eq.(37.17), one finds

$$\lim_{r\to\infty}V_{eff}(r)\propto\frac{\cos(2k_F r)}{r^3} \qquad (37.24)$$

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_BT equal to $v_F\hbar\Delta k$ and identifying the spread in wave vector around k_F as $\Delta k\sim\xi_{th}^{-1}$.

37.2.4 Plasmons

We have already suggested in Fig.(37-4) that at small wave numbers, a large frequency pole far from the particle-hole continuum appears. Let us look at this parameter range. Taking $v_F q/\omega$ as a small parameter, the imaginary part of the dielectric constant Eq.(37.11) 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.(37.4) and (46.29). Indeed, when the frequency is large and outside the particle-hole continuum, we can write

$$\lim_{\mathbf{q}\rightarrow 0}\lim_{\omega\rightarrow \mathbf{v}_F q-\varepsilon_q}\frac{\varepsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0}=\lim_{\omega\gg \mathbf{v}_F q-\varepsilon_q}\left[1-2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}\right] \tag{37.25}$$

$$= \lim_{\mathbf{q}\rightarrow 0}\left[1+2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2}\left(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}\right)\right] \tag{37.26}$$

$$= 1+2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2}\left(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}\right) \tag{37.27}$$

$$= 1+\frac{4V_{\mathbf{q}}}{\omega^2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}\right) \tag{37.28}$$

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

$$\lim_{\mathbf{q}\rightarrow 0}\lim_{\omega>>\mathbf{v}_F q-\varepsilon_q}\frac{\varepsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0} = 1-\frac{2V_{\mathbf{q}}n_0}{\omega^2}\frac{q^2}{2m} \tag{37.29}$$

$$= 1-\frac{\omega_p^2}{\omega^2} \tag{37.30}$$

with the value of $\omega_p^2=\frac{n_0e^2}{\varepsilon_0 m}$ defined in Eq.(36.34). One can continue the above approach to higher order or proceed directly with a tedious Taylor series expansion of the real part Eq.(37.9) in powers of $v_F q/\omega$ to obtain

$$\frac{\varepsilon_1^L(\mathbf{q}\rightarrow 0,\omega)}{\varepsilon_0}=1-\frac{\omega_p^2}{\omega^2}-\frac{3}{5}\frac{\omega_p^2}{\omega^2}\frac{(v_F q)^2}{\omega^2}+\ldots \tag{37.31}$$

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,

$$\frac{\varepsilon_1^L(\mathbf{q}\rightarrow 0,\omega\gg\omega_p)}{\varepsilon_0}\rightarrow 1 \tag{37.32}$$

- The collective plasma oscillation that we expected does show up. Indeed, $\varepsilon_1(\mathbf{q}\rightarrow 0,\omega)=0$ when

$$0 = \omega^2-\omega_p^2-\frac{3}{5}\frac{\omega_p^2}{\omega^2}(v_F q)^2+\ldots \tag{37.33}$$

$$\omega^2 \approx \omega_p^2+\frac{3}{5}(v_F q)^2+\ldots \tag{37.34}$$

Letting this solution be called ω_q we have in the vicinity of this solution $\omega \approx \omega_q$

$$\frac{\varepsilon_1^L(\mathbf{q} \to 0, \omega)}{\varepsilon_0} \approx 1 - \frac{\omega_q^2}{\omega^2} \approx \frac{2}{\omega_q}(\omega - \omega_q) \tag{37.35}$$

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.(36.35) has the value $a = 2/\omega_q$.

Fig.(37-6) shows a plot of both the real and the imaginary parts of the dielectric constant for small wave vector $(q \ll q_{TF})$. We see that the dielectric constant is real and very large at zero frequency, representing screening, whereas the vanishing of the real part at large frequency leads to the plasma oscillations, the so-called plasmon. Given the scale of the figure, it is hard to see the limiting behavior $\varepsilon_1(\mathbf{q}, \infty) \to 1$ but the zero crossing is illustrated by the maximum in $\mathrm{Im}(1/\varepsilon)$. There is another zero crossing of ε_1 but it occurs in the region where ε_2 is large. Hence this is an overdamped mode.

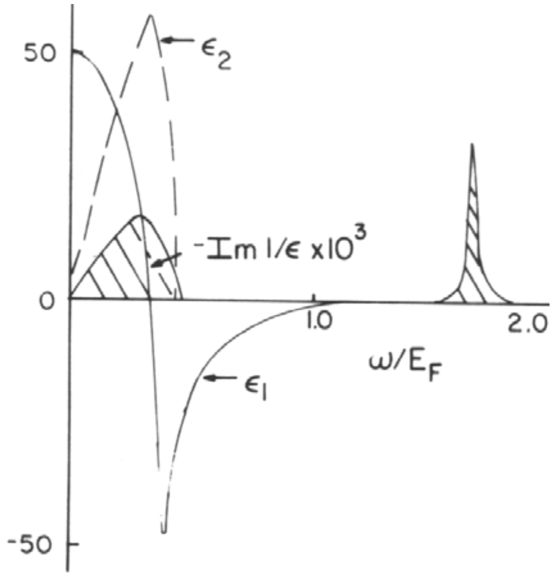


Figure 37-6 Real and imaginary parts of the dielectric constant and $\mathrm{Im}(1/\varepsilon)$ as a function of frequency, calculated for $r_s = 3$ and $q = 0.2k_F$. Shaded plots correspond to $\mathrm{Im}(1/\varepsilon)$. Taken from Mahan *op. cit.* p.430

37.2.5 $f-$sum rule

We have not checked yet whether the $f-$sum rule is satisfied. Let us first recall that it takes the form,

$$2\int_0^\infty \frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{nq^2}{m}. \tag{37.36}$$

Using our relation between dielectric constant and density fluctuations Eq.(35.2) $\varepsilon_0/\epsilon^L(\mathbf{q},\omega) = 1 - V_{\mathbf{q}}\chi^R_{\rho\rho}(\mathbf{q},\omega)$ we obtain the corresponding sum rule for the longitudinal dielectric constant

$$\int_0^\infty \frac{d\omega}{2\pi}\omega\,\mathrm{Im}\left[\frac{\varepsilon_0}{\varepsilon^L(\mathbf{q}\to 0,\omega)}\right] = -V_{\mathbf{q}}\frac{nq^2}{m} \tag{37.37}$$

$$= -\frac{ne^2}{4m\varepsilon_0} = -\frac{\omega_p^2}{4} \tag{37.38}$$

Let us obtain the plasmon contribution to this sum rule by using the approximate form Eq.(37.35)

$$\int_0^\infty \frac{d\omega}{2\pi}\omega\,\mathrm{Im}\left[\frac{1}{\frac{2}{\omega_q}(\omega-\omega_q)+i\eta}\right] = -\pi\int_0^\infty \frac{d\omega}{2\pi}\omega\left|\frac{\omega_q}{2}\right|\delta(\omega-\omega_q) \tag{37.39}$$

$$= -\frac{\omega_q^2}{4} \tag{37.40}$$

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

$$-\frac{\omega_p^2}{4}+\frac{\omega_q^2}{4}=\frac{3}{20}(v_Fq)^2 \tag{37.41}$$

as necessary to satisfy the $f-$sum rule.

Remark 128 *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.*

38. MORE FORMAL MATTERS: CONSISTENCY RELATIONS BETWEEN SINGLE-PARTICLE SELF-ENERGY, COLLECTIVE MODES, POTENTIAL ENERGY AND FREE ENERGY

This Chapter should be read if you followed the Fynman approach. Otherwise part of its main message has already been mentioned in earlier sections and the considerations on the free energy will come later.

We have found an expression for the density fluctuations that appears correct since it has all the correct Physics. It was a non-trivial task since we had to sum an infinite subset of diagrams. We will see that it is also difficult to obtain the correct expression for the self-energy without a bit of physical hindsight. We might have thought that the variational principle would have given us a good starting point but we will see that in this particular case it is a disaster. The following theorems will help us to understand why this is so and will suggest how to go around the difficulty.

We thus go back to some formalism again to show that there is a general relation between self-energy and charge fluctuations. We will have a good approximation for the self-energy only if it is consistent with our good approximation for the density fluctuations. We also take this opportunity to show how to obtain the self-energy since just a few additional lines will suffice.

38.1 Consistency between self-energy and density fluctuations

38.1.1 Equations of motion for the Feynmay way

You do not need to read this section if you have followed the source field approach. You can skip to the next subsection. We start from the equations of motion for the Green's function. We need first those for the field operators.

$$\frac{\partial\psi\left(1\right)}{\partial\tau_1}=-\left[\psi\left(1\right),K\right] \tag{38.1}$$

Using $[A, BC] = \{A, B\} C - B \{A, C\}$ and Eq.(34.1) for K we have

$$\begin{aligned}\frac{\partial \psi_{\sigma_1}(\mathbf{x}_1, \tau_1)}{\partial \tau_1} &= \frac{\nabla_1^2}{2m} \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) + \mu \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \\ &\quad - \sum_{\sigma_{1'}} \int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \psi^\dagger_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_1}(\mathbf{x}_1, \tau_1)\end{aligned} \tag{38.2}$$

Remark 129 *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*

$$+ n_0 \left[\int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \right] \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \tag{38.3}$$

The $\mathbf{q} = \mathbf{0}$ contribution of the potential in the above equation of motion gives on the other hand a contribution

$$- \left[\int d\mathbf{x}_{1'} v(\mathbf{x}_1 - \mathbf{x}_{1'}) \right] \left[\frac{1}{\mathcal{V}} \int d\mathbf{x}_{1'} \sum_{\sigma_{1'}} \psi^\dagger_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \psi_{\sigma_{1'}}(\mathbf{x}_{1'}, \tau_1) \right] \psi_{\sigma_1}(\mathbf{x}_1, \tau_1) \tag{38.4}$$

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.(34.7) the above result can be written in the shorthand notation

$$\frac{\partial \psi(1)}{\partial \tau_1} = \frac{\nabla_1^2}{2m} \psi(1) + \mu \psi(1) - \int_{1'} \psi^\dagger(1') V(1 - 1') \psi(1') \psi(1) \tag{38.5}$$

From this, we can easily find the equation of motion for the Green's function

$$\mathcal{G}(1, 2) = -\left\langle T_\tau \left[\psi(1) \psi^+(2) \right] \right\rangle \tag{38.6}$$

namely,

$$\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu \right) \mathcal{G}(1, 2) = -\delta(1 - 2) + \left\langle T_\tau \left[\int_{1'} \psi^\dagger(1'^+) V(1 - 1') \psi(1') \psi(1) \psi^\dagger(2) \right] \right\rangle \tag{38.7}$$

where as usual the delta function comes from the action of the time derivative on the θ functions implicit in the time ordered product. The right-hand side is not far from what we want. The last term on the right-hand side can be related to the product of the self-energy with the Green's function since, comparing the equation of motion for the Green's function with Dyson's equation

$$\mathcal{G}_0^{-1} \mathcal{G} = 1 + \Sigma \mathcal{G} \tag{38.8}$$

we have that

$$\boxed{\int_{1''} \Sigma(1, 1'') \mathcal{G}(1'', 2) = -\left\langle T_\tau \left[\int_{1'} \psi^\dagger(1'^+) V(1' - 1) \psi(1') \psi(1) \psi^\dagger(2) \right] \right\rangle} \tag{38.9}$$

which, in all generality, can be taken as a *definition* of the self-energy.

The last equation (38.9) has been derived also in Eq.(32.13) in a different notation if you followed the functional derivative approach. In this section we keep the integral on space-time coordinates explicitly. If you have read the first remark in Sec. 32.2 the frist few equations below are nothing new.

In the limit $2 \to 1^+$ where

$$1^+ \equiv \left(\mathbf{x}_1, \tau_1 + 0^+; \sigma_1\right) \tag{38.10}$$

the term on the right-hand side of Eq.(38.9) is

$$\left\langle T_\tau \left[\int_{1'} \psi^\dagger\left(1^+\right) \psi^\dagger\left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle$$

where we have written explicitly the integral. Note that we have placed $\psi^\dagger(2) \to \psi^\dagger(1^+)$ 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

$$2\left\langle V\right\rangle = \sum_{\sigma_1} \int d^3\mathbf{x}_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger\left(1^+\right) \psi^\dagger\left(1'\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle \tag{38.11}$$

we directly get from Eq.(38.9) above a relation between self-energy and potential energy

$$\sum_{\sigma_1} \int d^3\mathbf{x}_1 \int_{1'} \Sigma\left(1,1'\right) \mathcal{G}\left(1',1^+\right) = 2\left\langle V\right\rangle \tag{38.12}$$

We have the freedom to drop the time-ordered product when we recall that the operators are all at the same time and in the indicated order. Using time-translational invariance the last result may also be written

$$\boxed{\int_1 \int_{1'} \Sigma\left(1,1'\right) \mathcal{G}\left(1',1^+\right) = 2\left\langle V\right\rangle \beta = \int_1 \int_{1'} \left\langle T_\tau \left[\psi^\dagger\left(1^+\right) \psi^\dagger\left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right] \right\rangle} \tag{38.13}$$

Remark 130 *The 1^+ on the left-hand side is absolutely necessary for this expression to make sense. Indeed, taken from the point of view of Matsubara frequencies, one knows that the self-energy goes to a constant at infinite frequency while the Green's function does not decay fast enough to converge without ambiguity. On the right-hand side of the above equation, all operators are at the same time, in the order explicitly given.*

The right-hand side of the last equation is in turn related to the density-density correlation function. To see this, it suffices to return to space spin and time indices and to recall that the potential is instantaneous and spin independent so that

$$2\left\langle V\right\rangle \beta = \int_{1'} \int_1 \left\langle \psi^\dagger\left(1^+\right) \psi^\dagger\left(1'^+\right) V\left(1'-1\right) \psi\left(1'\right) \psi\left(1\right) \right\rangle \tag{38.14}$$

$$\begin{aligned}
= \quad & -\beta \sum_{\sigma_1,\sigma_{1'}} \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle \psi^\dagger_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \psi_{\sigma_1}\left(\mathbf{x}_1\right) \right\rangle \delta_{\sigma_1,\sigma_{1'}} \delta\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \\
& +\beta \sum_{\sigma_1,\sigma_{1'}} \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle \psi^\dagger_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) \psi_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) \psi^\dagger_{\sigma_1}\left(\mathbf{x}_1\right) \psi_{\sigma_1}\left(\mathbf{x}_1\right) \right\rangle \\
= \quad & -n_0 \mathcal{V} \beta v\left(0\right) + \beta \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle n\left(\mathbf{x}_{1'}\right) v\left(\mathbf{x}_{1'}-\mathbf{x}_1\right) n\left(\mathbf{x}_1\right) \right\rangle
\end{aligned} \tag{38.15}$$

where in the last equation we have used

$$\int d^3\mathbf{x}_1 \sum_{\sigma_1} \left\langle \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\,\psi_{\sigma_1}(\mathbf{x}_1)\right\rangle = N = n_0\mathcal{V} \tag{38.16}$$

Going to Fourier space, we have

$$\int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 \left\langle n(\mathbf{x}_{1'})\,v(\mathbf{x}_{1'}-\mathbf{x}_1)\,n(\mathbf{x}_1)\right\rangle \tag{38.17}$$

$$= \int d^3\mathbf{x}_{1'} \int d^3\mathbf{x}_1 v(\mathbf{x}_{1'}-\mathbf{x}_1)\,\chi_{nn}(\mathbf{x}_{1'},0;\mathbf{x}_1 0) \tag{38.18}$$

$$= \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[\lim_{\tau\to 0} \mathcal{V}\chi_{nn}(\mathbf{q},\tau)\right] \tag{38.19}$$

We did not have to take into account the disconnected piece that appears in Eq.(38.17) but not in $\chi_{nn}(\mathbf{q},\tau)$ because this disconnected piece contributes only at $\mathbf{q}=0$ and we have argued that $V_{\mathbf{q}=0}=0$. Note that there is no jump in $\chi_{nn}(\mathbf{q},\tau)$ at $\tau=0$ contrary to the case of the single-particle Green's function. Substituting back into Eq.(38.15) we have

$$2\langle V\rangle\beta = \int_{1'}\int_1 \left\langle \psi^\dagger(1^+)\,\psi^\dagger(1'^+)\;V(1'-1)\,\psi(1')\,\psi(1)\right\rangle = \tag{38.20}$$

$$\begin{aligned} &= \quad \beta\mathcal{V}\left[-n_0 v(0) + \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} T \sum_{iq_n} \chi_{nn}(\mathbf{q},iq_n)\right] \\ &= \quad \beta\mathcal{V}\left[\int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) - n_0\right]\right] \end{aligned}$$

Substituting the above Eq.(38.20) into the consistency relation between self-energy and potential energy Eq.(38.13) and then using invariance under time and space translations as well as spin rotation symmetry to replace $\int_1$ by $2\beta\mathcal{V}$, this gives the following relation between self-energy and density fluctuations

$$\int_{1'} \Sigma(1,1')\,\mathcal{G}(1',1^+) = \tag{38.21}$$

$$T\sum_{ik_n}\int \frac{d^3k}{(2\pi)^3} \Sigma(\mathbf{k},ik_n)\,G(\mathbf{k},ik_n)\,e^{ik_n\eta} \tag{38.22}$$

$$= \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) - n_0\right]. \tag{38.23}$$

This plays the role of a sum-rule relating single-particle properties, such as the self-energy and Green function, to a two-particle quantity, the density-density correlation function or potential energy.

Remark 131 *In short range models, we need to restore the* $v_{\mathbf{q}=\mathbf{0}}$ *component and the disconnected piece has to be treated carefully. Also, the spin fluctuations will come in. This subject is for the chapter on the Hubbard model.*

38.2 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 [15]. The proof is simple. First, notice that

$$-\frac{1}{\beta}\frac{\partial \ln Z}{\partial \lambda} = -\frac{1}{\beta}\frac{1}{Z}\frac{\partial Tr\left[e^{-\beta(H_0+\lambda V-\mu N)}\right]}{\partial \lambda} = \frac{1}{Z}Tr\left[e^{-\beta(H_0+\lambda V-\mu N)}V\right] = \frac{1}{\lambda}\left\langle \lambda V\right\rangle_\lambda . \tag{38.24}$$

To differentiate the operator, $e^{-\beta(H_0+\lambda V-\mu N)}$, we have used its definition as a power series and then taken the derivative with respect to λ. Even if the operator V does not commute with H_0, the cyclic property of the trace allows one to always put V on the right-hand side so that in the end, the derivative worked out just as with ordinary number. (Alternatively, one can do the proof in the interaction representation). The subscript λ in $\left\langle \lambda V\right\rangle_\lambda$ is to remind ourselves that the trace is taken for a Hamiltonian with coupling constant λ.

The free energy we are interested in is for $\lambda = 1$, so

$$\boxed{\Omega = -T\ln Z = -T\ln Z_0 + \int_0^1 \frac{d\lambda}{\lambda}\left\langle \lambda V\right\rangle_\lambda .} \tag{38.25}$$

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 132 *Recall that the free energy in this grand-canonical ensemble is related to the pressure.*

$$\Omega = -P\mathcal{V}. \tag{38.26}$$

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.(38.20), how the potential energy may be obtained from density correlations,

$$\begin{aligned}\Omega &= -T\ln Z = -T\ln Z_0 \qquad (38.27)\\ &+\frac{\mathcal{V}}{2}\int_0^1 \frac{d\lambda}{\lambda}\left\langle \lambda \int \frac{d^3q}{(2\pi)^3}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}\left(\mathbf{q},iq_n\right)-n_0\right]\right\rangle_\lambda .\end{aligned}$$

Using our previous relation between self-energy and potential energy, Eq.(38.13) the coupling-constant integration in Eq.(38.25) may also be done with

$$\Omega = -T\ln Z_0 + \frac{T}{2}\int_0^1 \frac{d\lambda}{\lambda}\int d1\int d1\text{"}\,\Sigma_\lambda\left(1,1\text{"}\right)\mathcal{G}_\lambda\left(1\text{"},1^+\right). \tag{38.28}$$

where the subscript λ reminds oneself that the interaction Hamiltonian must be multiplied by a coupling constant λ.

39. SINGLE-PARTICLE PROPERTIES AND HARTREE-FOCK

We have already mentioned several times our strategy. First we will show the failure of Hartree-Fock and try to understand the reason for it by returning to consistency relations between self-energy and density fluctuations. Having cured the problem by using the screened interaction in the calculation, we will discuss the physical interpretation of the result, including a derivation of the Fermi liquid scattering rate that we discussed in the previous Part in the context of photoemission experiments.

It is useful to derive the result from the variational principle as well as directly from a Green's function point of view. Since Hartree-Fock is sometimes actually quite good, it is advisable to develop a deep understanding of this approach.

39.1 Variational approach

In Hartree-Fock theory, we give ourselves a trial one-particle Hamiltonian and use the variational principle to find the parameters. In the electron gas case the true non-interacting part of the Hamiltonian is

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \frac{k^2}{2m} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{39.1}$$

where the spin-sum is represented by a sum over σ. The interacting part, written in Fourier space, takes the form

$$H - H_0 = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \sum_{\mathbf{q}} c^+_{\mathbf{k},\sigma} c^+_{\mathbf{k}',\sigma'} V_{\mathbf{q}} c_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} \tag{39.2}$$

with $V_{\mathbf{q}}$ the Fourier transform of the Coulomb potential

$$V_{\mathbf{q}} = \frac{e^2}{4\pi\varepsilon_0 q^2}. \tag{39.3}$$

Electroneutrality leads to $V_{\mathbf{q}=\mathbf{0}} = 0$ as before. The form of the interaction with all the proper indices is not difficult to understand when we consider the diagrammatic representation in Fig.(39-1). All that is needed is the conservation of momentum coming from integrals over all space and translational invariance. The factor of $1/\mathcal{V}$ in front comes from a factor $\mathcal{V}^{-1/2}$ for each change of variable from real-space to momentum space, $\left(\mathcal{V}^{-1/2}\right)^4$, and one overall factor of volume $\mathcal{V}$ from translational invariance which is used to eliminate one of the momentum sums through momentum conservation. Although there are several ways of labeling the momenta, the above one is convenient. In this notation $\mathbf{q}$ is often referred to as the "transfer variable" while $\mathbf{k}$ and $\mathbf{k}'$ are the band variables.

To apply the variational principle, one takes

$$\boxed{\widetilde{H}_0 = \textstyle\sum_{\mathbf{k},\sigma} \widetilde{\epsilon}_{\mathbf{k}} c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}} \tag{39.4}$$

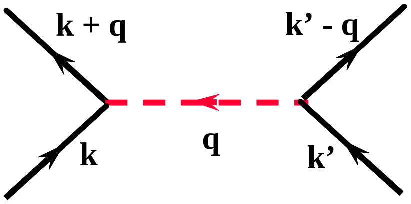


Figure 39-1 Momentum conservation for the Coulomb interaction.

with the variational parameter $\widetilde{\epsilon}_{\mathbf{k}}$. We then minimize

$$-T\ln Z_0+\left\langle H-\widetilde{H}_0\right\rangle_0 \tag{39.5}$$

The partition function for $\widetilde{H}_0-\mu N$ is computed as usual for non-interacting electrons

$$-T\ln Z_0=-T\ln\prod_{\mathbf{k},\sigma}\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right)=-T\sum_{\mathbf{k},\sigma}\ln\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right). \tag{39.6}$$

Then the quantity $\left\langle H-\widetilde{H}_0\right\rangle_0$ is easily evaluated as sums of products of pairs of Greens functions since the average is taken in the case where there are no interactions, i.e. $\widetilde{H}_0$ is quadratic in creation-annihilation operators. This can be derived from the functional derivative approach and is the content of Wick's theorem. Here we use it directly to obtain,

$$\left\langle H-\widetilde{H}_0\right\rangle_0=\sum_{\mathbf{k},\sigma}\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right)\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0 \tag{39.7}$$

$$+\frac{1}{2\mathcal{V}}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'}\sum_{\mathbf{q}}V_{\mathbf{q}}\left[\left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k}'-\mathbf{q},\sigma'}\right\rangle_0\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k}+\mathbf{q},\sigma}\right\rangle_0-\left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k}+\mathbf{q},\sigma}\right\rangle_0\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k}'-\mathbf{q},\sigma'}\right\rangle_0\right]. \tag{39.8}$$

which may be simplified by using

$$\left\langle c^+_{\mathbf{k}',\sigma'}c_{\mathbf{k},\sigma}\right\rangle_0=\delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}\left\langle c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle_0\equiv\delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}f\left(\widetilde{\zeta}_{\mathbf{k}}\right)=\frac{1}{e^{\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}+1} \tag{39.9}$$

to obtain

$$\left\langle H-\widetilde{H}_0\right\rangle_0=\sum_{\mathbf{k},\sigma}\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right)f\left(\widetilde{\zeta}_{\mathbf{k}}\right)-2\frac{1}{2\mathcal{V}}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}V_{\mathbf{k}'-\mathbf{k}}f\left(\widetilde{\zeta}_{\mathbf{k}'}\right)f\left(\widetilde{\zeta}_{\mathbf{k}}\right) \tag{39.10}$$

where the overall factor of 2 comes from what is left of the spin sums. We have dropped the term that leads to $V_{\mathbf{q}=\mathbf{0}}$ as usual because of the neutralizing background.

We can now determine our variational parameter $\widetilde{\epsilon}_{\mathbf{k}}$ by minimizing with respect to it:

$$\frac{\partial}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left[-T\sum_{\mathbf{k},\sigma}\ln\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right)\right]=\frac{2e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}}{\left(1+e^{-\beta(\widetilde{\epsilon}_{\mathbf{k}}-\mu)}\right)}=2f\left(\widetilde{\zeta}_{\mathbf{k}}\right) \tag{39.11}$$

$$\frac{\partial}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left\langle H-\widetilde{H}_0\right\rangle_0=-2f\left(\widetilde{\zeta}_{\mathbf{k}}\right)+\frac{\partial f\left(\widetilde{\zeta}_{\mathbf{k}}\right)}{\partial\widetilde{\epsilon}_{\mathbf{k}}}\left[2\left(\epsilon_{\mathbf{k}}-\widetilde{\epsilon}_{\mathbf{k}}\right)-\frac{2}{\mathcal{V}}\sum_{\mathbf{k}'}V_{\mathbf{k}'-\mathbf{k}}f\left(\widetilde{\zeta}_{\mathbf{k}'}\right)\right]. \tag{39.12}$$

Setting the sum of the last two equations to zero, we see that the coefficient of the square bracket must vanish. Using $V_{\mathbf{q}} = V_{-\mathbf{q}}$ we then have

$$\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} V_{\mathbf{k}'-\mathbf{k}} f\left(\widetilde{\zeta}_{\mathbf{k}'}\right) = \epsilon_{\mathbf{k}} - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} V_{\mathbf{k}-\mathbf{k}'} f\left(\widetilde{\zeta}_{\mathbf{k}'}\right) \tag{39.13}$$

$$\boxed{\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 |\mathbf{k}-\mathbf{k}'|^2} \frac{1}{e^{\beta(\widetilde{\epsilon}_{\mathbf{k}'}-\mu)}+1}} \tag{39.14}$$

As usual the chemical potential is determined by fixing the number of particles. Before we evaluate this integral let us obtain this same result from the Green's function point of view.

In principle we should check that the extremum point that we found by taking the first derivative is a minimum.

39.2 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

$$H = \widetilde{H}_0 + \left(H_0 - \widetilde{H}_0 + V\right) \tag{39.15}$$

The unperturbed Hamiltonian is now $\widetilde{H}_0$ and we assume that it takes the same form as Eq.(39.4) above. In addition to the usual perturbation V, there is now a translationally invariant one-body potential $H_0 - \widetilde{H}_0$. One determines the self-energy in such a way that $\widetilde{H}_0$ becomes the best "effective medium" in the sense that to first order in $\left(H_0 - \widetilde{H}_0 + V\right)$ the self-energy calculated in this effective medium vanishes completely. This is illustrated in Fig.(39-2). This kind of approach is also known as renormalized perturbation theory [24].

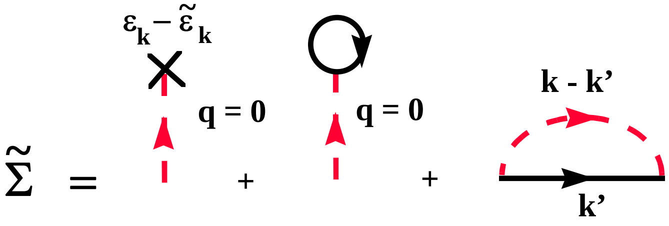


Figure 39-2 Effective medium point of view for the Hartree-Fock approximation. In this figure, the propagators are evaluated with the effective medium $\widetilde{H}_0$.

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.(39-2) gives

$$\widetilde{\Sigma} = \epsilon_{\mathbf{k}} - \widetilde{\epsilon}_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) = 0 \tag{39.16}$$

Using the expression for the exchange, or Fock, diagram $\Sigma^{(1)}(\mathbf{k})$ we get a minus sign when we work directly in the Schwinger approach. In the Feynmann approach, the minus signe is there 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 $\Sigma^{(1)}(\mathbf{k})$

$$\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{e^2}{\varepsilon_0 \left|\mathbf{k}-\mathbf{k}'\right|^2} \widetilde{\mathcal{G}}^0(\mathbf{k}', ik'_n)\, e^{ik'_n\eta} \tag{39.17}$$

that we can evaluate using our formula for Matsubara sums. Substituting back into Eq.(39.16) we get precisely our Hartree-Fock result Eq.(39.14) 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.(39.16) for $\widetilde{\epsilon}_{\mathbf{k}}$ we can remove all reference to $\widetilde{\epsilon}_{\mathbf{k}}$ and write

$$\boxed{\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{e^2}{\varepsilon_0|\mathbf{k}-\mathbf{k}'|^2} \frac{1}{ik'_n-(\epsilon_{\mathbf{k}}-\mu)-\Sigma^{(1)}(\mathbf{k})} e^{ik'_n\eta}} \tag{39.18}$$

Performing the summation over Matsubara frequencies and using Eq.(39.16) to relate $\widetilde{\epsilon}_{\mathbf{k}}$ to $\Sigma^{(1)}(\mathbf{k})$, this expression is found identical to our earlier variational result Eq.(39.14). The above equation Eq.(39.18) looks as if the perturbation expansion for the full Green's function, illustrated by a thick arrow in Fig.(39-3), 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.

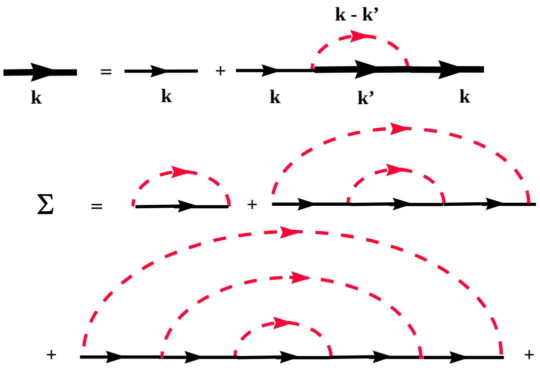


Figure 39-3 Hartree-Fock as a self-consistent approximation for the Green's function. This self-consistent approximation is equivalent to a self-energy that sums all the rainbow diagrams illustrated on the bottom part of the figure. The thick line is the full Green's function.

39.3 The pathologies of the Hartree-Fock approximation for the electron gas.

To evaluate our expression for the Hartree-Fock self-energy $\widetilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k})$ Eq.(39.14) we need the chemical potential. As usual in the grand-canonical ensemble, the chemical potential is determined by requiring that we have the correct density. Let us suppose then that we have a density n. Then

$$\begin{aligned} n &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \widetilde{\mathcal{G}}^0(\mathbf{k}, ik_n)\, e^{ik_n\eta} && (39.19) \\ &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\beta\left(\epsilon_{\mathbf{k}}+\Sigma^{(1)}(\mathbf{k})-\mu\right)}+1} && (39.20) \end{aligned}$$

Let us focus on the zero temperature case. Then the Fermi function is a step function and the last integral reduces to

$$n = 2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\theta\left(k_F - |\mathbf{k}|\right) \qquad (39.21)$$

where the chemical potential is given by

$$\epsilon_{\mathbf{k}_F} + \Sigma^{(1)}(\mathbf{k}_F) - \mu = 0 \qquad (39.22)$$

The equation Eq.(39.21) 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

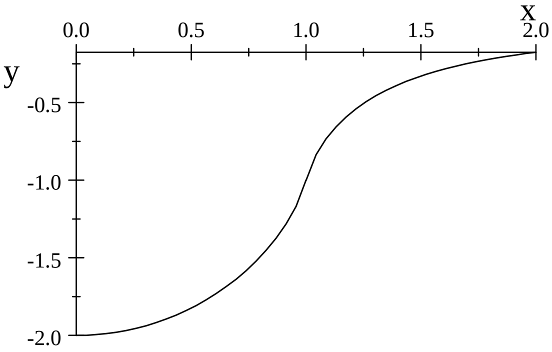
$$\begin{aligned} \Sigma^{(1)}(\mathbf{k}) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 \left|\mathbf{k}-\mathbf{k}'\right|^2}\theta\left(k_F - |\mathbf{k}'|\right) && (39.23) \\ &= -\frac{e^2}{\varepsilon_0 8\pi^3}\int_0^{k_F} (k')^2\, dk' \int_{-1}^{1} \frac{2\pi d(\cos\theta)}{k^2 + (k')^2 - 2kk'\cos\theta} && (39.24) \\ &= -\frac{e^2}{4\pi^2\varepsilon_0}\int_0^{k_F} k'\frac{1}{-2k}\ln\left(\left|\frac{(k'-k)^2}{(k+k')^2}\right|\right) dk' && (39.25) \end{aligned}$$

We evaluated the integral as a principal part integral because we have argued that the potential should have no $q = 0$ component which means $\left|\mathbf{k}-\mathbf{k}'\right|^2 \neq 0$. Pursuing the calculation, we have

$$\Sigma^{(1)}(\mathbf{k}) = -\frac{e^2}{4\pi^2\varepsilon_0}k_F\left[1 + \frac{1-y^2}{2y}\ln\left(\left|\frac{1+y}{1-y}\right|\right)\right] \quad ; \quad y \equiv \frac{k}{k_F} \qquad (39.26)$$

The function $\Sigma^{(1)}(\mathbf{k}) / \left(\frac{e^2}{4\pi^2\varepsilon_0}k_F\right)$ is plotted in Fig.(**??**).

$$\Sigma^{(1)}(k/k_F) / \left(\frac{e^2}{4\pi^2\varepsilon_0}k_F\right)$$



Plot of the Hartree-Fock self-energy at zero temperature.

Since $\lim_{x\to 0} x\ln x = 0$, we have that

$$\Sigma^{(1)}\left(\mathbf{k}_F\right) = -\frac{e^2}{4\pi^2\varepsilon_0}k_F \tag{39.27}$$

The ratio of this term to the zeroth order term, namely the kinetic energy $k_F^2/2m$ is of order r_s

$$\propto \frac{me^2k_F}{k_F^2\varepsilon_0} \propto \frac{1}{k_F a_0} \propto r_s \tag{39.28}$$

as can be seen using the definitions Eqs.(36.2)(36.5).

Up to here everything seems to be consistent, except if we start to ask about the effective mass. The plot of the self-energy suggests that there is an anomaly in the slope at $y = 1$ (or $k = k_F$). This reflects itself in the effective mass. Indeed, using the general formula found in the previous chapter, Eq.(28.37)

$$\frac{m}{m^*} = \lim_{\mathbf{k}\to\mathbf{k}_F} \frac{1 + \frac{\partial}{\partial\zeta_{\mathbf{k}}}\operatorname{Re}\Sigma^R\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right)}{1 - \frac{\partial}{\partial\omega}\operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right)\big|_{\omega=E_{\mathbf{k}}-\mu}} = 1 + \frac{dk}{d\zeta_{\mathbf{k}}}\left.\frac{\partial\Sigma^{(1)}\left(\mathbf{k}\right)}{\partial k}\right|_{k=k_F} \tag{39.29}$$

we have

$$\left.\frac{\partial\Sigma^{(1)}\left(\mathbf{k}\right)}{\partial k}\right|_{k=k_F} \propto k_F\left(\frac{dy}{dk}\right)_{y=1} \left.\frac{d\left[1+\frac{1-y^2}{2y}\ln\left(\left|\frac{1+y}{1-y}\right|\right)\right]}{dy}\right|_{y=1} \tag{39.30}$$

The problem comes from $\ln(1-y)$. Let us concentrate on the contributions proportional to this term

$$\begin{aligned}\frac{d}{dy}\left[\left(\frac{1}{2y}-\frac{y}{2}\right)\ln\left(1-y\right)\right] &= \left(-\frac{1}{2y^2}-\frac{1}{2}\right)\ln\left(1-y\right) \\ &\quad + \left(\frac{1}{2y}-\frac{y}{2}\right)\frac{1}{1-y}\end{aligned} \tag{39.31}$$

As $y \to 1$ we obtain a singularity from $\ln(0) = -\infty$. This corresponds to the unphysical result $m^* = 0$. An effective mass smaller than the bare mass is possible but rather unusual. This is seen for example in three dimension for very small r_s (table 8.7 in Giuliani-Vignale). However, in general, interactions will make quasi-particles look heavier. The result $m^* = 0$ obtained here is as close to ridiculous as one can imagine.

The physical reason for the failure of Hartree-Fock is the following. It is correct to let the electron have exchange interaction of the type included in rainbow diagrams do, but it is incorrect to neglect the fact that the other electrons in the background will also react to screen this interaction. We discuss this in more details below.

40. SECOND STEP OF THE APPROXIMATION: GW CURING HARTREE-FOCK THEORY

In this Section, we present the solution to the failure of Hartree-Fock that was found by Gell-Man and Brueckner[16]. In brief, in the first step of the calculation we obtained collective modes with bare Green's functions. We saw that just trying to do Hartree-Fock at the single-particle level was a disaster. Now we want to improve our calculation of the single-particle properties. The Physics is that the interaction appearing in Hartree-Fock theory should be screened. Or equivalently, the self-energy that we find should be consistent with the density fluctuations found earlier since $\Sigma\mathcal{G}$ is simply related to density fluctuations. The resulting expresssion that we will find is also known as the GW approximation.

The first subsection should be read if you follow the Feynmann way. Otherwise, skip to the next subsection.

40.1 An approximation for $\sum$ that is consistent with the Physics of screening

For Feynmann afficionados, we have seen in a previous Chapter, more specifically Eq.(38.21), that the self-energy is related to density fluctuations. More specifically, if we multiply the self-energy by the Green's function and take the trace, we should have the same thing basically as we would by multiplying the density-density correlation function by the potential and taking the trace. This is illustrated schematically for the Hartree-Fock approximation by the diagram of Fig.(40-1). The diagram on the left is built from the rainbow self-energy of Fig.(39-3) 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.(38.21) is due to the fact that one forces the Green's functions to correspond to a given time order in the self-energy calculation that is different from the one appearing naturally on the right-hand side.

Remark 133 *Equality (38.21) for the Hartree-Fock approximation. Let us check just the sums over Matsubara frequencies on both sides of Eq.(38.21) to see that they are identical. First, the sum on the left hand-side.*

$$T\sum_{ik_n}T\sum_{ik_n'}\frac{e^{ik_n\eta}}{ik_n-\zeta_{\mathbf{k}}}\frac{e^{ik_n'\eta}}{ik_n'-\zeta_{\mathbf{k}'}}=f\left(\zeta_{\mathbf{k}}\right)f\left(\zeta_{\mathbf{k}'}\right) \tag{40.1}$$

While the sum on the right-hand side is

$$T\sum_{ik_n}T\sum_{iq_n}\frac{1}{ik_n-\zeta_{\mathbf{k}}}\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}'}} \tag{40.2}$$

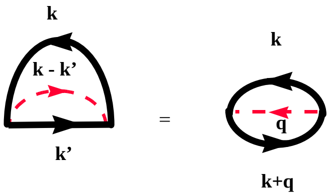


Figure 40-1 Approximation for the density fluctuations that corresponds to the Hartree-Fock self-energy.

$$= T\sum_{ik_n} T\sum_{q_n}\left[\frac{1}{ik_n-\zeta_{\mathbf{k}}}-\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}'}}\right]\frac{1}{iq_n-\zeta_{\mathbf{k}'}+\zeta_{\mathbf{k}}} \tag{40.3}$$

$$= T\sum_{q_n}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}'})}{iq_n-\zeta_{\mathbf{k}'}+\zeta_{\mathbf{k}}} = -\left[f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}'})\right]n_B(\zeta_{\mathbf{k}'}-\zeta_{\mathbf{k}}) \tag{40.4}$$

where we used, with n_B *the Bose function*

$$T\sum_{q_n}\frac{1}{iq_n-a} = -n_B(a) \quad or \quad -n_B(a)-1 \tag{40.5}$$

The result of the sum depends on the convergence factor but the -1 *in the second possibility does not contribute once the sum over wave vectors are done. We are thus left only with*

$$\begin{aligned} -\left[f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}'})\right]n_B(\zeta_{\mathbf{k}'}-\zeta_{\mathbf{k}}) &= -\frac{e^{\beta\zeta_{\mathbf{k}'}}-e^{\beta\zeta_{\mathbf{k}}}}{\left(e^{\beta\zeta_{\mathbf{k}'}}+1\right)\left(e^{\beta\zeta_{\mathbf{k}}}+1\right)}\frac{1}{e^{\beta(\zeta_{\mathbf{k}'}-\zeta_{\mathbf{k}})}-1} \\ &= -\frac{e^{\beta\zeta_{\mathbf{k}}}}{\left(e^{\beta\zeta_{\mathbf{k}'}}+1\right)\left(e^{\beta\zeta_{\mathbf{k}}}+1\right)} \quad (40.6) \\ &= -\left(1-f(\zeta_{\mathbf{k}})\right)f(\zeta_{\mathbf{k}'}) \quad (40.7) \end{aligned}$$

Eq.(40.1) and the last equation are not strictly equal and that is why it is necessary to subtract n_0 *in Eq.(40.1).*

Fig.(40-1) shows that the Hartree-Fock approximation corresponds to a very poor approximation for the density fluctuations, namely one that has no screening, and no plasma oscillation. Knowing that the RPA approximation for the density has all the correct properties, it is clear that we should use for the self-energy the expression appearing in Fig.(40-2). Indeed, in such a case, multiplying Σ by $\mathcal{G}^0$

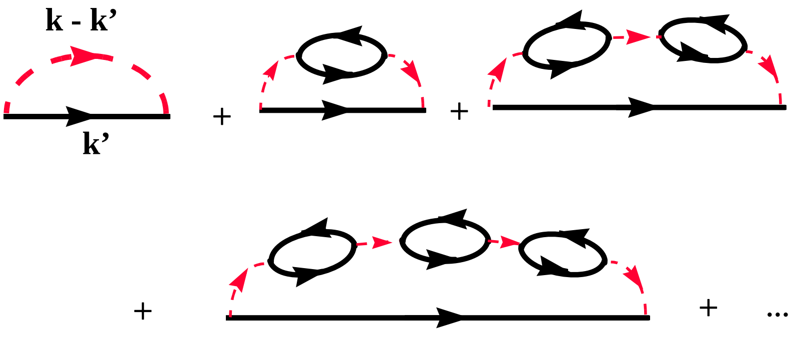


Figure 40-2 Diagrammatic expression for the self-energy in the RPA approximation.

gives a a result, illustrated in Fig.(40-3) that does correspond to multiplying the

RPA expression for the density Fig.(37-2) by $V_{\mathbf{q}}$ and summing over $\mathbf{q}$. These are the ring diagrams.

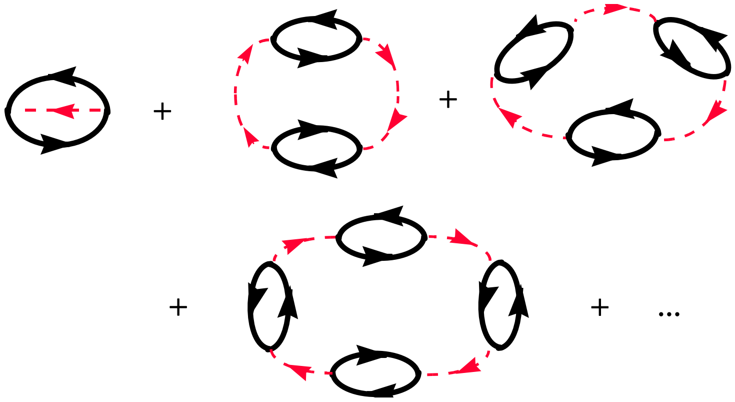


Figure 40-3 Ring diagrams for $\Sigma\mathcal{G}$ in the RPA approximation. The same diagrams are used for the free energy calculation.

Using Feynman's rules, the corresponding analytical expression is

$$\begin{aligned} \Sigma_{RPA}\left(\mathbf{k},ik_n\right) &= \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (40.8)\\ & -\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\\ &= -\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{\varepsilon\left(\mathbf{q},iq_n\right)}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\end{aligned}$$

Comparing with the Hartree-Fock approximation Eq.(39.18) 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.(40-4) which is analogous to the diagram for the Hartree-Fock approximation Fig.(39-3) but with a screened interaction and only the first rainbow diagram, without self-consistency.

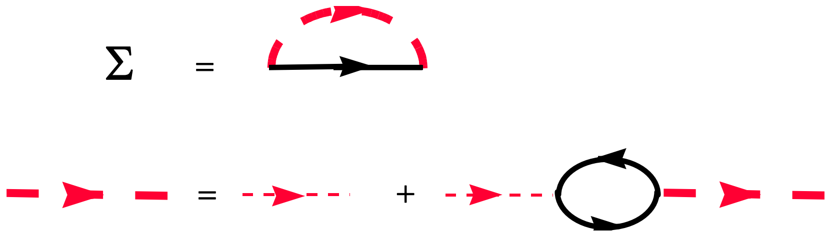


Figure 40-4 RPA self-energy written in terms of the screened interaction.

Remark 134 *If, instead of summing the whole series in Fig.(40-2) we had stopped at any finite order, we would have had to deal with divergent integrals. Indeed, consider expanding the RPA susceptibility to first order in Eq.(40.8). This corresponds to the diagram with one bubble. The corresponding expression is*

$$\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}V^2_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)$$

which is divergent since $V^2_{\mathbf{q}}$ *is proportional to* q^{-4} *while the integral over* q *is in three dimensions only. Higher order bubbles are worse.*

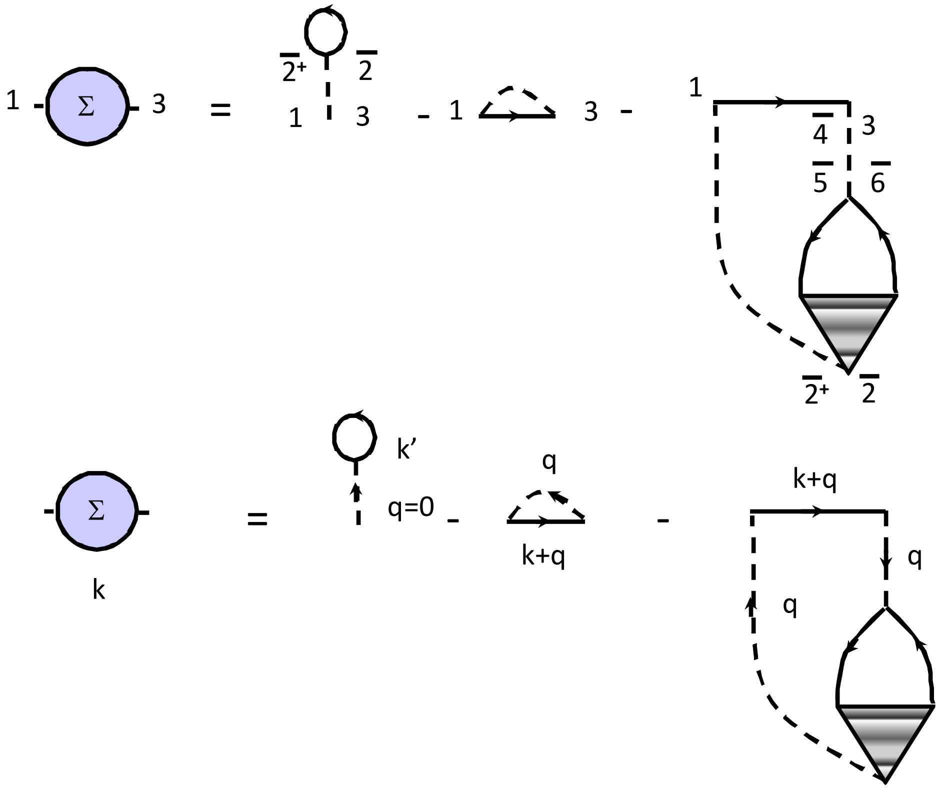


Figure 40-5 Coordinate (top) and momentum space (bottom) expressions for the self-energy at the second step of the approximation. The result, when multiplied by $\mathcal{G}$, is compatible with the density-density correlation function calculated in the RPA approximation.

40.2 Self-energy and screening, the Schwinger way

To obtain an approximation for the self-energy Σ that, when multiplied by $\mathcal{G}$, gives the density-density correlation function that we just evaluated in the RPA approximation, we return to the general expression for the self-energy Eq.(32.29) and the corresponding pictorial representation Eq.(32-2). We replace the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$ by the one shown in Fig. 33-1 that we used to compute the density-density correlation function illustrated in Fig. 33-5. The final result is illustrated in Fig. 40-5. We just need to replace the functional derivative of the Green function appearing at the bottom right by the RPA series illustrated in Fig. 37-3. Recalling that the Hartree term vanishes, the final result is equivalent, when looked at sideways, to the series of bubble diagrams illustrated in Fig. 40-2,

The algebraic expression for this second level of approximation for the self-energy can be read off the figure. It takes the explicit form

$$\begin{aligned}\Sigma_{RPA}(\mathbf{k},ik_n) &= \Sigma^{(2)}(\mathbf{k},ik_n) \qquad (40.9)\\ &= -\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}V_{\mathbf{q}}\left[1-\frac{V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}\right]\mathcal{G}^0(\mathbf{k}+\mathbf{q},ik_n+iq_n)\end{aligned}$$

where the first term comes from the Fock contribution. The two terms can be combined into the single expression

$$\Sigma^{(2)}\left(\mathbf{k},ik_n\right)=-\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right). \tag{40.10}$$

Using our result for the longitudinal dielectric constant that follows from the density fluctuations in the RPA approximation Eq. (37.4), the last result can be written as

$$\Sigma^{(2)}\left(\mathbf{k},ik_n\right)=-\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{\varepsilon_L\left(\mathbf{q},iq_n\right)/\varepsilon_0}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right) \tag{40.11}$$

which has the very interesting interpretation that the effective interaction entering the Fock term should be the screened one instead of the bare one. The two are equal only at very high frequency. The quantity screened potential $\frac{V_{\mathbf{q}}}{\varepsilon_L(\mathbf{q},iq_n)/\varepsilon_0}$ is often denoted W which means that the integrand is $W\mathcal{G}^0$, hence the name GW approximation.

Remark 135 *Diagrammatically, from Fig. 40-5, it is clear that multiplying by $\mathcal{G}^0$ and summing over k, we obtain the series of bubble diagrams for the density fluctuations, multiplied by the potential. That corresponds to the total potential energy. Hence, one recovers the sum-rule relating single and two-particle properties Eq.(38.23). Albegraically, we start from Eq.(40.10) just above and compute*

$$\begin{aligned}\int\frac{d^3\mathbf{k}}{\left(2\pi\right)^3}T\sum_{ik_n}\Sigma^{(2)}\left(\mathbf{k},ik_n\right)\mathcal{G}^0\left(\mathbf{k},ik_n\right)e^{-ik_n0^-} &= -\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\\ &\quad\times\int\frac{d^3\mathbf{k}}{\left(2\pi\right)^3}T\sum_{ik_n}\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0\left(\mathbf{k},ik_n\right)\\ &= \int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}\frac{V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}{1+V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\\ &= \int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}T\sum_{iq_n}V_{\mathbf{q}}\chi_{nn}\left(\mathbf{q},iq_n\right). \qquad (40.12)\end{aligned}$$

The convergence factor $e^{-ik_n0^-}$ is necessary to enforce $\Sigma\left(1,\overline{2}\right)G\left(\overline{2},1^+\right)$ and obtain the potential energy to the right. It is not obvious from the right-hand side that we need the convergence factor until one realizes that there is a sum over k_n and q_n and only two Green's functions $\mathcal{G}^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}^0\left(\mathbf{k},ik_n\right)$ that survive at very large frequency, giving a result that is formally divergent. Hence we should not invert the order of summation over k_n and q_n as we did. That can cost the constant term that appears in Eq.(38.23). ???

41. PHYSICS IN SINGLE-PARTICLE PROPERTIES

In this Chapter, we interpret the results of calculations based on formulas of the previous Chapter, and compare with experiments. In particular, we will recover theoretically the Fermi liquid regime, compute the free energy and compare with experiment.

41.1 Single-particle spectral weight

The real-part and the absolute value of the imaginary part of the RPA self-energy at zero temperature are plotted in Fig.(41-1) as a function of frequency for three different wave vectors. In the Hartree-Fock approximation, the self-energy was completely frequency independent. The result here is quite different. The screened interation contains the plasmons and has a drastic effect on single-particle properties. There are several points worth mentioning.

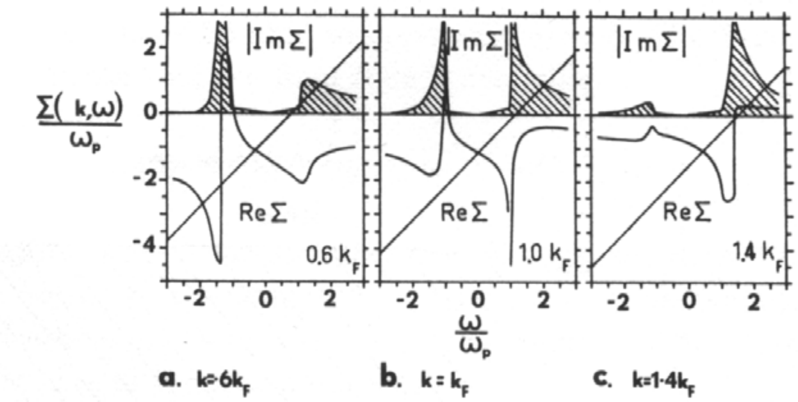


Figure 41-1 Real and imaginary part of the RPA self-energy for three wave vectors, in units of the plasma frequency. The chemical potential is included in ReΣ. The straight line that appears on the plots is $\omega - \varepsilon_{\mathbf{k}}$. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7,** 117 (1968). $r_s = 5$?

- $\operatorname{Im}\Sigma(\mathbf{k},\omega = 0) = 0$ 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 $\omega - \varepsilon_{\mathbf{k}}$. The intersection of this straight line with $\operatorname{Re}\Sigma$, which is defined on the figure to contain the chemical potential, corresponds (in our notation) to the solution of the equation

$$\omega - \varepsilon_{\mathbf{k}} = \operatorname{Re}\Sigma^{R}(\mathbf{k},\omega) - \mu \tag{41.1}$$

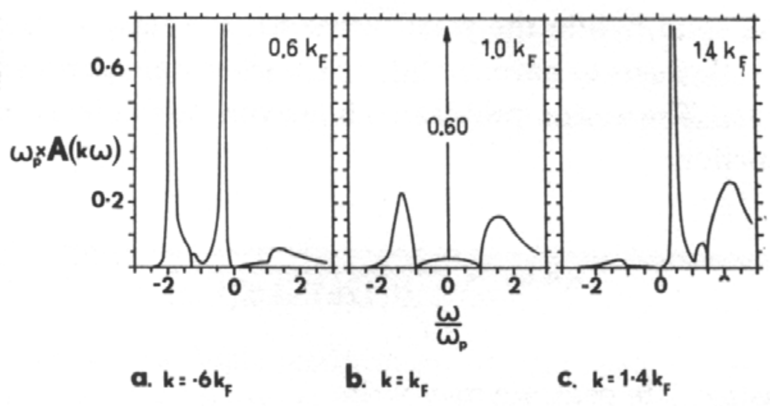


Figure 41-2 RPA spectral weight, in units of the inverse plasma frequency. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7,** 117 (1968).

As we argued in the previous chapter Eq.(28.24), this determines the position of maxima in the spectral weight,

$$A(\mathbf{k},\omega) = -2\,\mathrm{Im}\,G^R(\mathbf{k},\omega) \tag{41.2}$$

$$= \frac{-2\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{\left(\omega-\zeta_{\mathbf{k}}-\mathrm{Re}\sum^R(\mathbf{k},\omega)\right)^2+\left(\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2} \tag{41.3}$$

maxima that we identify as quasiparticles. Let us look at the solutions near $\omega = 0$. These correspond to a peak in the spectral weight Fig.(41-2). At the Fermi wave vector, the peak is located precisely where the imaginary part of the self-energy vanishes, hence the peak is a delta function. On the other hand, away from $\mathbf{k} = \mathbf{k}_F$, the maximum is located in a region where the imaginary part is not too large, hence the quasiparticle has a finite lifetime. Recall that to have the quasiparticle shape described in the previous chapter Eq.(28.29),

$$A(\mathbf{k},\omega) \approx 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{(\omega-E_{\mathbf{k}}+\mu)^2+(\Gamma_{\mathbf{k}}(\omega))^2}\right]+inc \tag{41.4}$$

it is necessary that at the crossing point, the slope of $\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$ be negative because it is necessary that

$$Z_{\mathbf{k}} = \frac{1}{1-\frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}} \geq 0 \tag{41.5}$$

if the previous formula is to make sense. The value of $Z_{\mathbf{k}_F}$, namely 0.6, is indicated on this plot.

- Note that in Fig. 41-1 there is a threshold-like feature at $\omega_p = \pm 1$ where $\mathrm{Im}\,\Sigma^R$ becomes large. This is when the one-particle excitations can emit or absorb real plasmons. This is discussed further below.

- From the previous discussion, we see that the two maxima away from $\omega = 0$ at $k = k_F$ do not correspond to quasiparticle solutions. The weight near the maxima away from $\omega = 0$ come from scattering rates $\mathrm{Im}\,\Sigma^R$ that are large, but not too large compared with the value of $\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\omega)$. At the threshold where $\mathrm{Im}\,\Sigma^R$ is really large, the spectral weight in fact vanishes because of the denominator in the general expression for the spectral weight Eq.(41.2). Note that the maxima away from $\omega = 0$ at $k = k_F$ are near the value of ω where the quasiparticle condition Eq. (41.1) is almost satisfied.

- For the figure on the right, $k = 1.4k_F$, the peak nearest $\omega = 0$ corresponds to a quasiparticle solution. Note however that for wave vectors so far from the Fermi surface, the width of the peak starts to be quite a bit larger. The maxima further away all occur in regions where $\mathrm{Im}\,\Sigma^R$ is large and the quasiparticle condition Eq. (41.1) is almost satisfied.
- For $k = 0.6k_F$, there seems to be an additional quasiparticle solution, namely a solution where $\frac{\partial}{\partial\omega}\,\mathrm{Re}\,\Sigma^R$ is negative and $\mathrm{Im}\,\Sigma^R$ is not too large, located at an energy ω_p below the main quasiparticle energy. Since the free-electron band is bounded from below, $\mathrm{Im}\,\Sigma^R$ vanishes at sufficiently negative frequency, allowing a new solution to develop when interactions are sufficiently strong. This solution looks like a bound state.

41.2 Physical interpretation of $\sum''$

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

$$\Sigma^R\left(\mathbf{k},\omega\right) = \Sigma'\left(\mathbf{k},\omega\right) + i\Sigma''\left(\mathbf{k},\omega\right) \tag{41.6}$$

may be written in the form

$$\boxed{\Sigma''\left(\mathbf{k},\omega\right) = -\tfrac{m}{2|k|}\int \tfrac{d^2q_\perp}{(2\pi)^2}\int \tfrac{d\omega'}{\pi}\left[n_B\left(\omega'\right) + f\left(\omega+\omega'\right)\right] V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp, q_\parallel, \omega'\right)} \tag{41.7}$$

where $q_\parallel$ is the solution of the equation

$$\frac{|k|}{m}q_\parallel + \frac{q_\parallel^2}{2m} = \left[\omega + \omega' - \left(\frac{k^2}{2m} - \mu + \frac{q_\perp^2}{2m}\right)\right] \tag{41.8}$$

Proof: It is preferable to first rewrite the RPA expression Eq.(40.8) in the following form

$$\Sigma_{RPA}\left(\mathbf{k},ik_n\right) = -\int \frac{d^3\mathbf{q}}{\left(2\pi\right)^3} T \sum_{iq_n} V_{\mathbf{q}}\left[1 - \frac{V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}{1 + V_{\mathbf{q}}\chi^0_{nn}\left(\mathbf{q},iq_n\right)}\right]\mathcal{G}^0\left(\mathbf{k}+\mathbf{q}, ik_n + iq_n\right) \tag{41.9}$$

$$= \Sigma_{HF}\left(\mathbf{k}\right) + \int \frac{d^3\mathbf{q}}{\left(2\pi\right)^3} T \sum_{iq_n}\left[V_{\mathbf{q}}\chi^{RPA}_{nn}\left(\mathbf{q},iq_n\right)V_{\mathbf{q}}\right]\mathcal{G}^0\left(\mathbf{k}+\mathbf{q}, ik_n + iq_n\right) \tag{41.10}$$

The first term at $T = 0$ is the Hartree-Fock contribution, as we can see from Eq.(39.23). In other words, wether we use $\mathcal{G}^0$ or the dressed $\widetilde{\mathcal{G}}^0$ 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 $\chi_{nn}^{RPA}\left(\mathbf{q},iq_n\right)$. 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

$$\Sigma_{RPA}\left(\mathbf{k},ik_n\right)-\Sigma_{HF}\left(\mathbf{k}\right)=\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}\int\frac{d\omega'}{\pi}T\sum_{iq_n}\left[V_{\mathbf{q}}\frac{\chi''_{nn}\left(\mathbf{q},\omega'\right)}{\omega'-iq_n}V_{\mathbf{q}}\right]\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{41.11}$$

We cannot perform the analytical continuation $ik_n\to\omega+i\eta$ before we have performed the sum over iq_n because, except for $iq_n=0$, this would necessitate going through the poles at $\omega=-iq_n+\zeta_{\mathbf{k}+\mathbf{q}}$. In addition, recall that we want the high-frequency behavior to be $1/ik_n$ before we do the analytic continuation, but until we have done the sum over iq_n we cannot say that we have that asymptotic behavior since iq_n extends to infinity. To do the sum over bosonic Matsubara frequencies first, we do the partial fraction decomposition as usual

$$-T\sum_{iq_n}\frac{1}{iq_n-\omega'}\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{41.12}$$

$$= -T\sum_{iq_n}\left[\frac{1}{iq_n-\omega'}-\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{41.13}$$

$$= \left[n_B\left(\omega'\right)+f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{41.14}$$

Note that for any ik_n, the sum ik_n+iq_n is a fermionic Matsubara frequency when iq_n is a bosonic one. That is why we obtained a Fermi distribution in the last term. Substituting back into our expression for the self-energy, the analytic continuation $ik_n\to\omega+i\eta$ can be done and we obtain

$$\Sigma^R\left(\mathbf{k},\omega\right)-\Sigma_{HF}\left(\mathbf{k}\right)=\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}\int\frac{d\omega'}{\pi}\left[n_B\left(\omega'\right)+f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)\right]\frac{V_{\mathbf{q}}\chi''_{nn}\left(\mathbf{q},\omega'\right)V_{\mathbf{q}}}{\omega+i\eta+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{41.15}$$

The imaginary part is thus

$$\Sigma''\left(\mathbf{k},\omega\right)=-\pi\int\frac{d^3\mathbf{q}}{\left(2\pi\right)^3}\int\frac{d\omega'}{\pi}\left[n_B\left(\omega'\right)+f\left(\omega+\omega'\right)\right]V_{\mathbf{q}}^2\chi''_{nn}\left(\mathbf{q},\omega'\right)\delta\left(\omega+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}\right) \tag{41.16}$$

Defining $q_{||}$ by the direction parallel to the wave vector $\mathbf{k}$ and calling $q_{\perp}$ the other directions, the integral over $q_{||}$ can be performed, giving the condition in Eq.(41.8). We then obtain, assuming that we are in a region of frequency where the delta function has a solution, the desired result Eq.(41.7)

In the zero temperature limit, $f\left(\omega+\omega'\right)=\theta\left(-\omega-\omega'\right)$ and $n_B\left(\omega'\right)=-\theta\left(-\omega'\right)$ so that if we take $\omega>0$ then the integral over ω' extends over the interval $-\omega<\omega'<0$ where $n_B\left(\omega'\right)+f\left(\omega+\omega'\right)$ takes the value -1. At low temperature, the contributions to Σ'' Eq.(41.7) will come mostly from this same frequency interval since this is where the combination $n_B\left(\omega'\right)+f\left(\omega+\omega'\right)\neq 0$. This immediately allows us to understand why the imaginary part of the self-energy in Fig.(41-1) above starts to be large when the frequency becomes of the order of the plasma frequency. This is only when ω is that large that the contributions from $\omega'\approx\omega_p$ in χ''_{nn} can start to contribute. This is where the quasiparticles can start to absorb or emit plasmons.

Remark 136 *Vanishing of Σ'' at zero temperature: Our general formula for the imaginary part Eq.(41.7) tells us that at zero temperature $\Sigma''(\mathbf{k},\omega=0)=0$ for* ***all*** *wave vectors, as we have seen in Fig.(41-1). Mathematically, this is so because $\lim_{T\to 0}\left[n_B(\omega')+f(\omega')\right]=0$ 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 $\omega'\to-\omega'$. Then the integration window at $T=0$ becomes $-\omega<-\omega'<0$, or $\omega>\omega'>0$. Using

$$n_B(-\omega')=-\left(1+n_B(\omega')\right) \tag{41.17}$$

and $\chi''_{nn}(\mathbf{q},-\omega')=-\chi''_{nn}(-\mathbf{q},\omega')$, the imaginary part of the self-energy becomes

$$\begin{aligned}\Sigma''(\mathbf{k},\omega) &= -\pi\int\frac{d^3\mathbf{q}}{(2\pi)^3}\int\frac{d\omega'}{\pi}\left[(1+n_B(\omega'))-f(\omega-\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}(\mathbf{q},\omega')\,\delta\left(\omega-\omega'-\zeta_{\mathbf{k+q}}\right)\\ &= -\int\frac{d^3\mathbf{q}}{(2\pi)^3}V_{\mathbf{q}}^2\chi''_{nn}\left(-\mathbf{q},\omega-\zeta_{\mathbf{k+q}}\right)\\ &\quad\left[\left(1+n_B\left(\omega-\zeta_{\mathbf{k+q}}\right)\right)\left(1-f\left(\zeta_{\mathbf{k+q}}\right)\right)+n_B\left(\omega-\zeta_{\mathbf{k+q}}\right)f\left(\zeta_{\mathbf{k+q}}\right)\right]\end{aligned}$$

The first term $\left(1+n_B\left(\omega-\zeta_{\mathbf{k+q}}\right)\right)\left(1-f\left(\zeta_{\mathbf{k+q}}\right)\right)$ represents the decay of a particle of energy ω and wave vector $\mathbf{k}$ into an empty particle state of energy $\zeta_{\mathbf{k+q}}$ and momentum $\mathbf{k}+\mathbf{q}$, plus a bosonic excitation (particle-hole continuum or plasmon) of energy $\omega-\zeta_{\mathbf{k+q}}$ and momentum $-\mathbf{q}$. The second term $n_B\left(\omega-\zeta_{\mathbf{k+q}}\right)f\left(\zeta_{\mathbf{k+q}}\right)$ represents the case where the incident state is a hole energy ω and wave vector $\mathbf{k}$ that decays into another hole of energy $\zeta_{\mathbf{k+q}}$ and momentum $\mathbf{k}+\mathbf{q}$ by absorbing a boson of energy $\omega-\zeta_{\mathbf{k+q}}$ 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.

41.3 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.(41.7) for Σ'' but we evaluate it at $\mathbf{k}=\mathbf{k}_F$ and use $v_F\equiv k_F/m$ so that

$$\boxed{\Sigma''(\mathbf{k}_F,\omega)=-\frac{1}{2v_F}\int\frac{d^2q_\perp}{(2\pi)^2}\int\frac{d\omega'}{\pi}\left[n_B(\omega')+f(\omega+\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp,q_\parallel,\omega'\right)} \tag{41.18}$$

where $q_\parallel$ is obtained from the solution of

$$v_Fq_\parallel+\frac{q_\parallel^2}{2m}=\left[\omega+\omega'-\frac{q_\perp^2}{2m}\right] \tag{41.19}$$

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, $\chi''_{nn}(\mathbf{q},\omega')/\omega'$ depends on frequency only on the scale of the Fermi energy. We can assume that it is independent of frequency at low frequency.

Proof: As we can see from the explicit expression for the imaginary part of χ''_{nn} Eq.(37.15), and using the fact that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},0)=0$,

$$\lim_{\omega\to 0}\operatorname{Im}\chi^{R}_{nn}(\mathbf{q},\omega)/\omega=\lim_{\omega\to 0}\frac{\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega}{\left(1+V_{\mathbf{q}}\operatorname{Re}\chi^{0R}_{nn}(\mathbf{q},0)\right)^{2}} \tag{41.20}$$

it suffices that the Lindhard function $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ has the property that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega$ is independent of frequency at low frequency. As expected from the fact that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is odd in frequency, it turns out that $\operatorname{Im}\chi^{0R}_{nn}(\mathbf{q},\omega)$ is indeed linear in frequency at low frequency, which proves our point. The linearity can be explicitly checked from our previous results Eqs.(37.11) and (37.4).

Hence, at low frequency, we can assume that $\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ is independent of frequency in the frequency range over which $n\left(\omega'\right)+f\left(\omega+\omega'\right)$ differs from zero. Also, $V^{2}_{\mathbf{q}}\chi''_{nn}\left(\mathbf{q},\omega'\right)/\omega'$ depends on wave vector over a scale that is of order q_F as we can see from Fig.(37-5). Hence, we can neglect the ω and ω' dependence of the solution for $q_{\parallel}$ in Eq.(41.19) when we substitute it in our expression for Σ''. One then finds

$$\boxed{\Sigma''\left(\mathbf{k}_F,\omega\right)\simeq-\tfrac{A(\mathbf{k}_F)}{2v_F}\int\tfrac{d\omega'}{\pi}\left[n\left(\omega'\right)+f\left(\omega+\omega'\right)\right]\omega'=-\tfrac{A(\mathbf{k}_F)}{4v_F}\left[\omega^{2}+\left(\pi T\right)^{2}\right]} \tag{41.21}$$

where the substitution $x=e^{\beta\omega}$ allowed the integral to be done exactly [17] and where

$$A\left(\mathbf{k}_F\right)\equiv\int\frac{d^{2}q_{\perp}}{\left(2\pi\right)^{2}}\lim_{\omega'\to 0}\frac{V^{2}_{\mathbf{q}}\chi''_{nn}\left(q_{\perp},q_{\parallel}\left(q_{\perp},v_F\right);\omega'\right)}{\omega'} \tag{41.22}$$

The presence of $V^{2}_{\mathbf{q}}$ does not give rise to problems in the integral over $q_{\perp}$ near $q=0$ because in this region the contribution is canceled by $V^{2}_{\mathbf{q}}$ that appears in the denominator of the RPA susceptibility Eq.(41.20). The above result Eq.(41.21) 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 $\chi''_{nn}\left(\mathbf{q},\omega'\right)$ near $\mathbf{q}=\mathbf{0}$. In three dimensions[18] 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.[19][20]

Remark 137 *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.(41.1) gives

$$E_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-0.17r_s\left(\ln r_s+0.2\right)\frac{k_F k}{2m}+cst \tag{41.23}$$

The effective mass appearing in this expression is now obviously finite and given by

$$m^{*}=\frac{m}{1-0.08r_s\left(\ln r_s+0.2\right)} \tag{41.24}$$

If we evaluate the scattering rate for $\omega=E_{\mathbf{k}}-\mu$ we find

$$\Gamma_{\mathbf{k}}\left(E_{\mathbf{k}}-\mu\right)=0.25r_s^{1/2}\frac{\left(k-k_F\right)^{2}}{2m} \tag{41.25}$$

Quinn and Ferrell[21] write the following physically appealing form

$$\Gamma_{\mathbf{k}}\left(\zeta_{\mathbf{k}}\right) Z_{\mathbf{k}}^{-1}=\frac{\sqrt{3}\pi^2}{128}\omega_p\left(\frac{\zeta_{\mathbf{k}}}{E_F}\right)^2 \tag{41.26}$$

The scattering rate is proportional to the plasma frequency, but reduced by an important phase space factor. The more general results, beyons leading order in r_s can be found in Eqs.(8.92-8.93) of Giuliani and Vignale "Quantum theory of the electron liquid".

Fig.(41-3) 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 138 *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.*

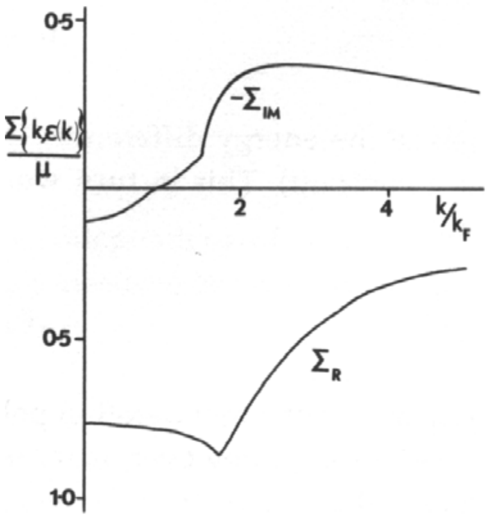


Figure 41-3 Real and imaginary parts of the self-energy of the causal Green's function in the zero-temperature formalism. From L. Hedin and S. Lundqvist, *Solid State Physics* **23,** 1 (1969).

41.4 Free energy

Finally, we use our coupling-constant integration formula Eq.(38.25). In the zero temperature limit, there will be no contribution from entropy and we will obtain the ground state energy in the RPA approximation

$$\begin{aligned} E^{RPA}_{Tot}(T=0)-\mu N &= \lim_{T\to 0}\Omega = \lim_{T\to 0}\left\{ -T\ln\left[\prod_{\mathbf{k},\boldsymbol{\sigma}}\left(1+e^{-\beta\zeta_{\mathbf{k}}}\right)\right]\right. \\ &\quad \left. +\frac{\mathcal{V}}{2}\int_0^1\frac{d\lambda}{\lambda}\lambda\int\frac{d^3q}{(2\pi)^3}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi^{\lambda}_{nn}(\mathbf{q},iq_n)-n_0\right]\right\} \end{aligned} \tag{41.27}$$

We have for the sum over Matsubara frequencies

$$T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) = T\sum_{iq_n}\int\frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-iq_n} \tag{41.28}$$

$$= \int\frac{d\omega'}{\pi}n_B(\omega')\chi''_{nn}(\mathbf{q},\omega') \tag{41.29}$$

In the zero temperature limit,

$$\lim_{T\to 0}\int\frac{d\omega'}{\pi}n_B(\omega')\chi''_{nn}(\mathbf{q},\omega') = -\int_{-\infty}^{0}\frac{d\omega'}{\pi}\chi''_{nn}(\mathbf{q},\omega') \tag{41.30}$$

$$= \int_0^{\infty}\frac{d\omega'}{\pi}\chi''_{nn}(\mathbf{q},-\omega') \tag{41.31}$$

$$= -\int_0^{\infty}\frac{d\omega'}{\pi}\chi''_{nn}(\mathbf{q},\omega') \tag{41.32}$$

so that the expression for the ground state energy becomes

$$\frac{E^{RPA}_{Tot}(T=0)-\mu N}{\mathcal{V}} \tag{41.33}$$

$$\begin{aligned} &= 2\int_{k<k_F}\frac{d^3k}{(2\pi)^3}\left(\frac{k^2}{2m}-\mu\right) \\ &\quad +\frac{\mathcal{V}}{2}\int\frac{d^3q}{(2\pi)^3}\int_0^1\frac{d\lambda}{\lambda}\lambda V_{\mathbf{q}}\left[-\operatorname{Im}\int_0^{\infty}\frac{d\omega'}{\pi}\frac{\chi^{0R}_{nn}(\mathbf{q},\omega')}{1+\lambda V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega')}-n_0\right] \end{aligned} \tag{41.34}$$

Note that we have replaced everywhere $V_{\mathbf{q}}$ by $\lambda V_{\mathbf{q}}$ as prescribed in the coupling constant integration trick.

Remark 139 *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.(40-3) and modified Feynman's rules to add the rule that there is a factor* $1/n$ *for every topologically different diagram of order* n*.*

The coupling constant integration is easy to perform

$$\begin{aligned} &\int_0^1\frac{d\lambda}{\lambda}\lambda V_{\mathbf{q}}\left[-\operatorname{Im}\int_0^{\infty}\frac{d\omega'}{\pi}\frac{\chi^{0R}_{nn}(\mathbf{q},\omega')}{1+\lambda V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega')}-n_0\right] \\ &= -V_{\mathbf{q}}n_0-\int_0^{\infty}\frac{d\omega'}{\pi}\operatorname{Im}\left\{\ln\left[1+V_{\mathbf{q}}\chi^{0R}_{nn}(\mathbf{q},\omega')\right]\right\} \end{aligned} \tag{41.35}$$

The rest of the calculation is tedious. One finds[22]

$$\frac{E_{Tot}^{RPA}(T=0)}{N}=\frac{2.21}{r_s^2}-\frac{0.916}{r_s}+0.0622\ln r_s-0.142+\mathcal{O}\left(r_s,r_s\ln r_s\right) \quad (41.36)$$

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.

41.5 Comparison with experiments

We are finally ready to compare the predictions of this formalism to experiments. The results shown in the present section are taken from Ref.[23].

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.(41-4) illustrates the prediction for sodium at $r_s = 3.97$. The following Table of expected jumps is from Hedin[13].

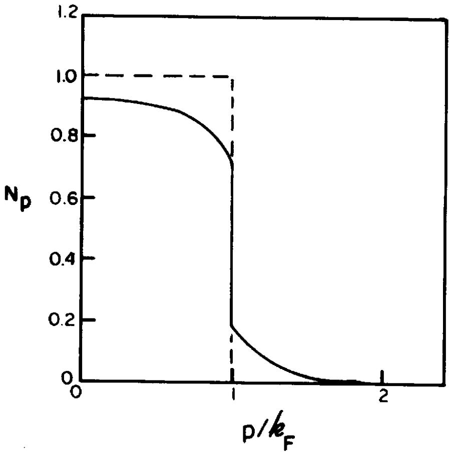


Figure 41-4 Momentum density in the RPA approximation for an electron gas with $r_s = 3.97$. From E. Daniel and S.H. Vosko, Phys. Rev. **120**, 2041 (1960).

r_s	Z_{RPA}
0	1
1	0.859
2	0.768
3	0.700
4	0.646
5	0.602
6	0.568

(41.37)

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

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int d^3\mathbf{k} n_{\mathbf{k}} \delta\left(\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}\right) \tag{41.38}$$

where ω is the energy and $\mathbf{q}$ the wave vector transferred by the photon. Changing to polar coordinates, we see that

$$\begin{aligned} \frac{d^2\sigma}{d\omega d\Omega} &\propto \int k^2 dk d\left(\cos\theta\right) n_{\mathbf{k}} \delta\left(\omega - \varepsilon_{\mathbf{q}} - \frac{kq}{m}\cos\theta\right) && (41.39) \\ &\propto \int kdk\frac{m}{q} n_k \theta\left(k - \left|Q\right|\right) && (41.40) \end{aligned}$$

where

$$Q \equiv \frac{m}{q}\left(\varepsilon_q - \omega\right) \tag{41.41}$$

In terms of Q, we have

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \frac{1}{q}\int_{|Q|}^{\infty} n_k kdk \tag{41.42}$$

For free electrons, this gives

$$\frac{d^2\sigma}{d\omega d\Omega} \propto J\left(Q\right) \propto \frac{1}{2q}\left(k_F^2 - Q^2\right)\theta\left(k_F - Q\right) \tag{41.43}$$

In this case then, the slope is discontinuous at $k_F = Q$ as illustrated on the left of Fig.(41-5). In the interacting case, the change in slope at k_F remains theoretically related to Z. Also, one expects a signal above k_F as illustrated on the left of the figure. Experimental results for sodium, $r_s = 3.96$, are given on the right of the figure along with the theoretical prediction. This metal is the one closest to the free electron model. The experimentalists have verified that Q is a good scaling variable, in other words that the cross section depends mainly on Q. Also, the existence of a tail above k_F is confirmed. However, the agreement with theory is not excellent.

The experimental results for the mean free path are more satisfactory. Let the mean free path $\ell_{\mathbf{k}}$ be defined by

$$\frac{1}{\ell_{\mathbf{k}}} = \frac{\Gamma_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1}{\tau_{\mathbf{k}} v_{\mathbf{k}}} = -\frac{2}{v_{\mathbf{k}}}\operatorname{Im}\Sigma\left(\mathbf{k},\zeta_{\mathbf{k}}\right) \tag{41.44}$$

Remark 140 *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.*

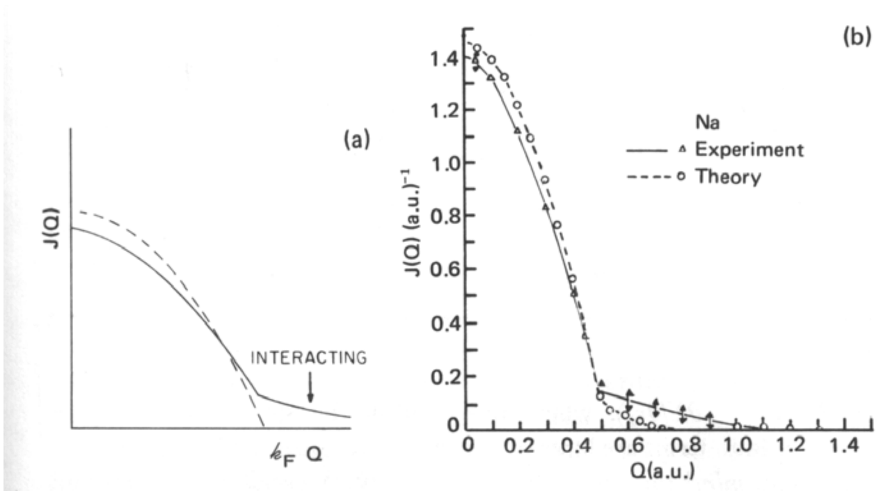


Figure 41-5 a) Dashed line shows the momentum distribution in Compton scattering for the non-interacting case while the solid line is for an interacting system. b) Experimental results in metallic sodium compared with theory, $r_s = 3.96$. Eisenberger *et al.* Phys. Rev. B **6**, 3671 (1972).

Fig.(41-6) 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 $\text{Im}\left(1/\varepsilon^L\right)$, 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.(37-6).

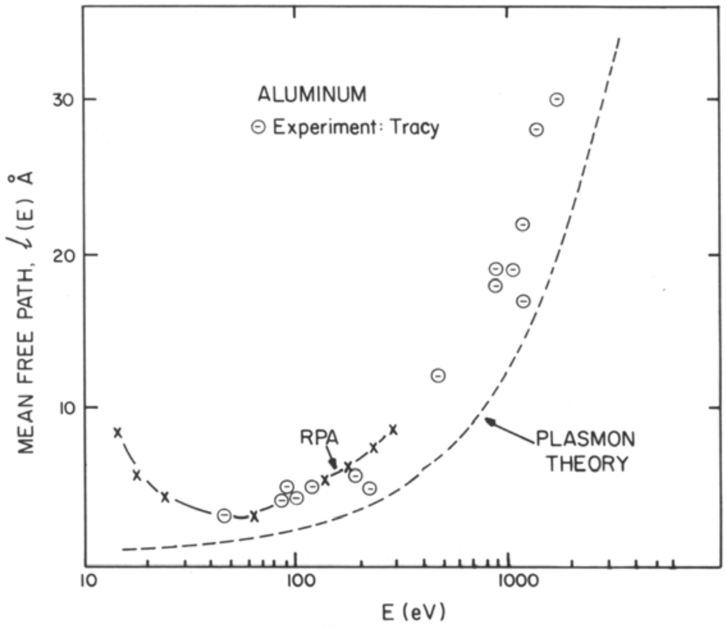


Figure 41-6 Mean free path of electrons in aluminum $(r_s = 2.07)$ as a function of energy above the Fermi surface. Circles are experimental results of J.C. Tracy, J. Vac. Sci. Technol. **11**, 280 (1974). The dashed line with symbols X was obtained with RPA for $r_s = 2$ by B.I. Lundqvist Phys. Status Solidi B **63**, 453 (1974).

42. 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.(41.36), the effective mass Eq.(41.24) or the scattering rate Eq.(41.25) 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.[26] is instructive of the nature of asymptotic expansions.

Suppose we want to evaluate the following integral

$$Z(g) = \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2} - \frac{g}{4}x^4} \tag{42.1}$$

This is an example where the integral does not exist for $g < 0$ but where we will try nevertheless to expand in powers of g around $g = 0$. If we do this then,

$$Z(g) = \sum_{n=0}^{\infty} g^n Z_n \tag{42.2}$$

where

$$\begin{aligned} Z_n &= \frac{(-1)^n}{4^n n!} \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} x^{4n} && (42.3) \\ &= \frac{(-1)^n}{4^n n!} \frac{(4n-1)!!}{2^n} && (42.4) \end{aligned}$$

with

$$\begin{aligned} (4n-1)!! &\equiv (4n-1)(4n-3)(4n-5)\dots 1 && (42.5) \\ &= \frac{(4n)!}{(4n)(4n-2)(4n-4)\dots 2} && (42.6) \\ &= \frac{(4n)!}{2^n (2n)!} && (42.7) \end{aligned}$$

hence,

$$Z_n = \frac{(-1)^n}{16^n n!} \frac{(4n)!}{(2n)!} \tag{42.8}$$

Using Stirling's formula,

$$n! \approx \sqrt{2\pi} n^{n+1/2} e^{-n}$$

we are left with

$$Z_n \propto \frac{1}{\sqrt{n\pi}} \left(\frac{-4n}{e} \right)^n \tag{42.9}$$

The value of each successive term in the power series is illustrated in Fig.(42-1). Clearly, whatever the value of g, if n is sufficiently large, the higher order terms

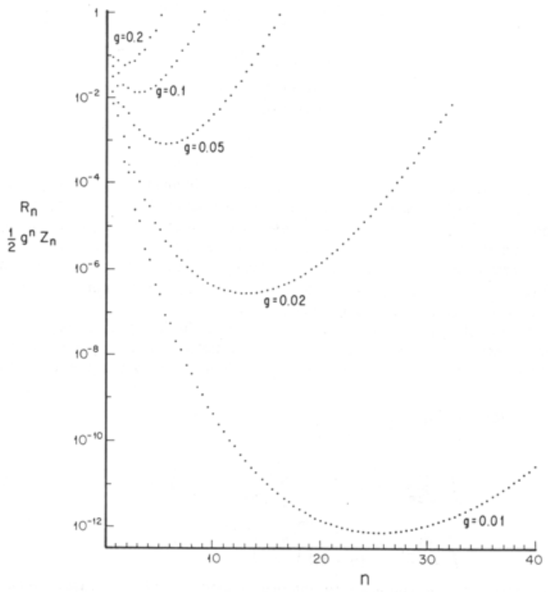


Figure 42-1 Asymptotic expansion of $Z(g)$ for different values of g. The residual error $R_n is$ plotted for the half-integer values. From J.W. Negele and H. Orland, *op. cit.* p.56

start to be larger than the low order ones. This is a characteristic of an asymptotic series.

We can even evaluate the error done when the series is stopped at order n. Let this error be

$$R_n = \left| Z(g) - \sum_{m=0}^{n} g^m Z_m \right| \tag{42.10}$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| e^{-\frac{g}{4}x^4} - \sum_{m=0}^{n} \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \tag{42.11}$$

$$= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \left| \sum_{m=n+1}^{\infty} \frac{(-1)^m}{4^m m!} g^m (x)^{4m} \right| \tag{42.12}$$

The series in the absolute value is an alternating series and it converges. Hence, an upper bound for this series is the value of the first term, as may be seen from the fact that

$$a_{n+1} - (a_{n+2} - a_{n+3}) - (a_{n+4} - a_{n+5}) - \ldots \leq a_{n+1} \tag{42.13}$$

Hence,

$$R_n \leq g^{n+1} |Z_{n+1}| \tag{42.14}$$

We also plot the error in Fig.(42-1). Clearly, the error starts to grow eventually.

Despite this terrible behavior of asymptotic expansions they can be quite useful in practice. For example, for $g = 0.01$, the precision is 10^{-10} after 25 terms. This may be estimated by noting from Eq.(42.9) for the asymptotic value of Z_n that $g^n Z_n$ starts to grow when $4gn$ becomes of order unity. The minimum error is then estimated with our formula for R_n. Even quantum electrodynamics is an asymptotic expansion, but the expansion parameter is $\alpha = 1/137$. It is thus an extremely good expansion parameter. Sometimes the asymptotic series may be resumed, at least partially as in RPA, or mathematical techniques, such as Borel summation, may be used to extract the non-analytic behavior.

43. 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[28]

$$\chi_{nn}\left(\mathbf{q}=\mathbf{0},iq_n\right)=0 \quad ; \quad \text{if} \quad iq_n\neq 0 \tag{43.1}$$

To check that this last equation is a consequence of charge conservation, note that at $\mathbf{q}=\mathbf{0}$ the density operator is the number operator, an operator that commutes with the Hamiltonian. This means that $\chi_{nn}\left(\mathbf{q}=\mathbf{0},\tau\right)$ is independent of imaginary time, which implies that its only non-vanishing Matsubara frequency component is $q_n=0$. Using the spectral representation for the Green's function and inversion symmetry in the Brillouin zone, our single dressed bubble calculation for χ_{nn} on the other hand will give us the following expression

$$\tilde{\chi}_0\left(\mathbf{q},iq_n\right)=\frac{2}{N}\sum_{\mathbf{k}}\int\frac{d\omega}{2\pi}\int\frac{d\omega'}{2\pi}A\left(\mathbf{k},\omega\right)A\left(\mathbf{k}+\mathbf{q},\omega'\right)\frac{\left(\omega-\omega'\right)\left(f\left(\omega'\right)-f\left(\omega\right)\right)}{\left(\omega-\omega'\right)^2+q_n^2}. \tag{43.2}$$

When there are no interactions and $A\left(\mathbf{k},\omega\right)$ is a delta function, it is clear that our exact result Eq.(43.1) 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.(37-1). 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.(43.1),

To see another example of how apparently reasonable improvements over RPA may lead to miserable failures consider the following reasoning. We saw from RPA that there are quasiparticles near the Fermi surface. Also, the low-frequency and small momentum density fluctuations are determined mainly by quantities near the Fermi surface, as one can check from the Lindhard function. It would thus be tempting, in a next iteration, to compute the bubbles entering RPA with a renormalized propagator

$$\frac{Z_{\mathbf{k}}}{ik_n - E_{\mathbf{k}} + \mu} \tag{43.3}$$

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.(43-1). The propagators are fully dressed. The interaction line must also be dressed, as illustrated on the second line. The bubble appearing there is called the polarization propagator since it plays the role of the polarizability in the definition of the dielectric constant. It is defined as the set of all diagrams that cannot be cut in two pieces by cutting a single interaction line. The polarization propagator has a bubble with dressed propagators but this is not enough. We must also include 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.

We will see in a subsequent chapter that the theory for electron-phonon interactions may be written precisely in the form of Fig.(43-1) except for the fact that the interaction line becomes replaced by a phonon propagator. In addition a key theorem, that we shall prove, the so-called Migdal theorem, shows that for electron-phonon interactions vertex corrections may be neglected. The first two lines of Fig.(43-1) 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[27], 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.(43-2). That is our second exact reformulation of perturbation theory[28] (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

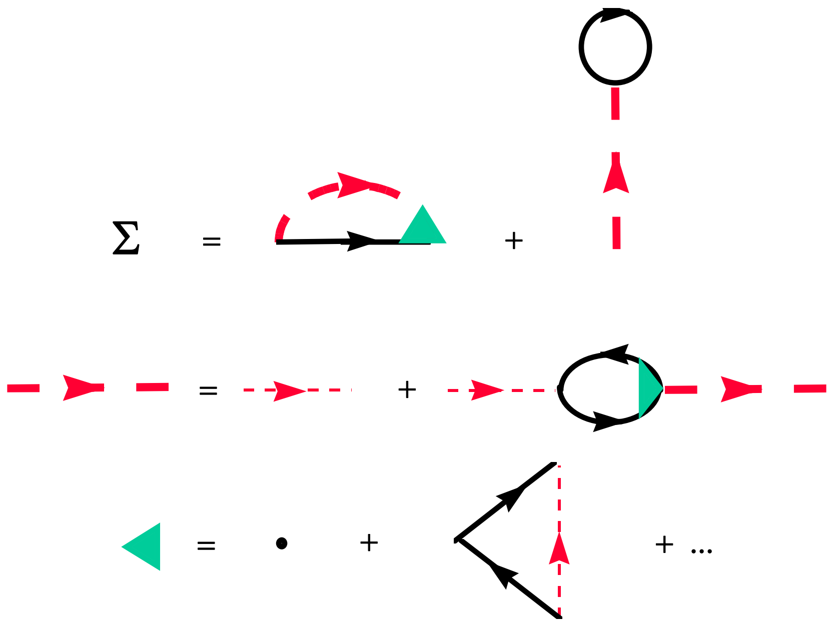


Figure 43-1 Exact resummation of the diagrammatic perturbation expansion. The dressed interaction on the second line involves the one-interaction irreducible polarisation propagator. The last line gives the first terms of the diagrammatic expansion for the vertex corrections.

proceed non-perturbatively, namely to parametrize the box in such a way that it can later be determined by using sum rules and various other exact constraints of many-body theory, such as the Pauli principle and conservation laws. This will be discussed in a later chapter.

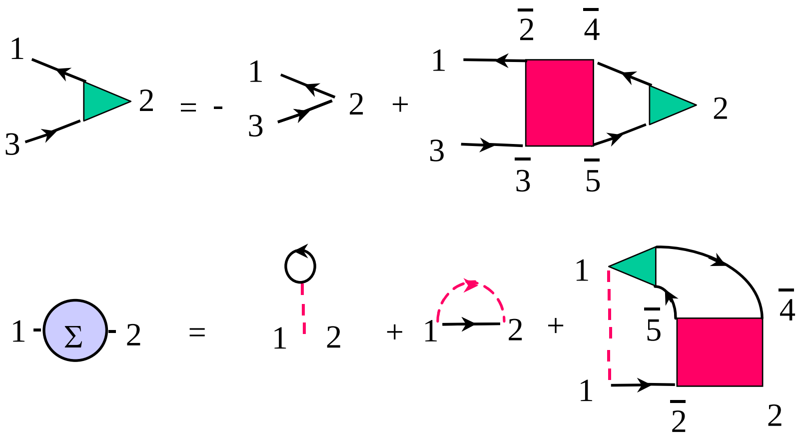


Figure 43-2 Exact representation of the full perturbation series. The triangle now represents the fully reducible vertex whereas the box represents all terms that are irreducible with respect to cutting a particle-hole pair of lines in the indicated channel.

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Part VI

Fermions on a lattice: Hubbard and Mott

The jellium is clearly a gross caricature of real solids. It does a good job nevertheless for simple metals, like sodium or aluminum. But it is important to have more realistic models that take into account the presence of a lattice of ions. The best methods today to find the electronic charge distribution are based on Density Functional Theory (DFT), that we explain very schematically in the first Chapter of this Part. These methods give a band structure that, strictly speaking, should not be interpreted as single-particle excitations. Nevertheless, for elements in the top rows of the periodic table, the band structure found from DFT works well. If we include the long-range Coulomb interaction with the GW approximation described above, then results for band gaps for example can be quite good.

For narrow band materials however, such as transition metal oxides that include d electrons, this is not enough. We will explore the rich Physics contained in a simple model, the Hubbard model, that was proposed to understand narrow band materials. That model adds to the band structure an on-site interaction term U that is supposed to represent the screened Coulomb interaction. We will see that in such a short-range interaction model, spin excitations that had basically disappeared from the electron-gas problem, will now play a prominent role. Even when the interaction is not too strong, we will see why the perturbative methods that we have described in the previous Part are of limited validity. When the interaction is not too strong, we can treat the problem non-perturbatively using the Two-Particle-Self-Consistent approach and others.

The Hubbard model will also allow us to understand why certain materials that are predicted to be good metals by band structure theory are in fact insulators. Insulating behavior can be induced by the interaction U when it is larger than the bandwidth. Such interaction-induced insulators are known as Mott insulators. And the transition between the metallic and the insulating phase that occurs as a function of U is called the Mott transition. The best known method to treat materials that are close to a Mott transition is Dynamical Mean-Field Theory and its cluster generalizations, that we will explain. High-temperature superconductors and layered organic conductors are examples of systems that display Mott insulating phases.

In the next Part we will used the Hubbard model to introduce broken symmetry states with ferromagnetism as an example. In this Part, we restrict ourselves to the “normal” paramagnetic state.

44. DENSITY FUNCTIONAL THEORY

The presence of a static lattice of ions creates bands, as we know from one-electron theory. How do we generalize this to the many-body case with electron-electron interactions. In particular, how do we go beyond Hartree-Fock theory?

Modern versions of band structure calculations are based on Density Functional Theory (DFT). This is a ground state or thermal equilibrium method that is also used for molecules. We begin by describing the general method, then its implementation for band-structure calculations and then finite temperature generalizations.

44.1 The ground state energy is a functional of the local density

The approach is based on a simple theorem of Hohenberg and Kohn [1]. We present the version of Levy [2, 3]. In both cases, we use the variational principle for the ground state: the ground state wave function is that which minimizes the energy,

$$E[\Psi] = \frac{\langle\Psi| H |\Psi\rangle}{\langle\Psi |\Psi\rangle}.$$

Proof: We can expand $|\Psi\rangle$ on a complete basis of energy eigenstates

$$|\Psi\rangle = \sum_i a_i |i\rangle . \tag{44.1}$$

Then the average energy is given by

$$\begin{aligned} \langle\Psi| H |\Psi\rangle &= \sum_{i,j} a_j^* a_i \langle j\ H |i\rangle && (44.2)\\ &= \sum_i a_i^* a_i E_i && (44.3) \end{aligned}$$

where the last line follows because by hypothesis the Hamiltonian is diagonal in that basis. With E_0 the lowest energy state, the inequality follows

$$\sum_i a_i^* a_i E_i \geq \left(\sum_i a_i^* a_i\right) E_0. \tag{44.4}$$

The prefactor on the right-hand side simplifies with the norm of the wave function in the denominator, which proves the theorem.

Let

$$H = \widehat{T}_{kin} + \hat{V}_c + \hat{V}_l \tag{44.5}$$

where $\widehat{T}_{kin}$ is the kinetic energy, $\hat{V}_c$ the Coulomb interaction between electrons and $\hat{V}_l$ the interaction between the electrons and the positive lattice of ions. More specifically, with $n_l(\mathbf{r}')$ the charge density of the lattice we can write

$$\begin{aligned}
\langle\Psi|\hat{V}_l|\Psi\rangle &= \langle\Psi|\int d^3\mathbf{r}\int d^3\mathbf{r}'\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}')|\Psi\rangle && (44.6)\\
&= \int d^3\mathbf{r}\langle\Psi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Psi\rangle\int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') && (44.7)\\
&= \int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r}) && (44.8)
\end{aligned}$$

wher in the last line we have defined the lattice potential

$$V_l(\mathbf{r}) \equiv \int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') \tag{44.9}$$

and the one-body electronic density

$$n(\mathbf{r}) \equiv \int d^3\mathbf{r}\langle\Psi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Psi\rangle.$$

If we take the set of all normalized wave functions, the variational principle can be formulated as

$$E = \min_\Psi\langle\Psi|\widehat{T}_{kin}+\hat{V}_c+\hat{V}_l|\Psi\rangle.$$

We now performe the minimization in two steps. First with respect to all wave functions that have the same one-particle density, then with respect to the one-particle density

$$\begin{aligned}
E &= \min_n\min_{\Psi\to n}\langle\Psi|\widehat{T}_{kin}+\hat{V}_c+\hat{V}_l|\Psi\rangle\\
&= \min_n\left[\left(\min_{\Psi\to n}\langle\Psi|\widehat{T}_{kin}+\hat{V}_c|\Psi\rangle\right)+\int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r})\right] && (44.10)\\
&= \min_n\left[F[n]+\int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r})\right]. && (44.11)
\end{aligned}$$

where we have defined

$$F[n] = \min_{\Psi\to n}\langle\Psi|\widehat{T}_{kin}+\hat{V}_c|\Psi\rangle. \tag{44.12}$$

That functional of n contains kinetic energy and Coulomb interaction between electrons. It is independent of the lattice potential and is thus a universal property of the inhomogeneous electron-gas. We say inhomogeneous because we have to find this function for densities that depend on position.

44.2 The Kohn-Sham approach

How can we transform the general ideas of the previous section into a calculational tool? The Hartree contribution to the potential energy depends only on density. It is less clear how to write the kinetic energy and the rest of the contributions to the Coulomg interaction (exchange for example) in a way that depends only on density. In the Thomas Fermi approach, we wrote the kinetic energy as a function of the local Fermi wave vector, and hence as a function of the density. Nevertheless, that is not very precise when the density changes on short length scales. Kohn and Sham [4] proposed to expand the density in terms of one-body orbitals for N particles in a paramagnetic state of N particles:

$$n\left(\mathbf{r}\right)=\sum_{i=1,\sigma}^{N/2}\left|\phi_{i,\sigma}^{KS}\left(\mathbf{r}\right)\right|^{2}. \tag{44.13}$$

If the wave function was simply obtained by filling these orbitals $\phi_{KS}\left(\mathbf{r}\right)$ up to the Fermi level, the corresponding kinetic energy would be easy to compute

$$T_s=\left\langle\Psi_{KS}\right|\widehat{T}_{kin}\left|\Psi_{KS}\right\rangle=\sum_{i=1,\sigma}\int d^3\mathbf{r}\phi_{i,\sigma}^{KS}\left(\mathbf{r}\right)\left(\frac{-\nabla^2}{2m}\right)\phi_{i,\sigma}^{KS}\left(\mathbf{r}\right). \tag{44.14}$$

The Kohn-Sham method then proposes to write for the universal functional

$$F[n]=\left\langle\Psi_{KS}\right|\widehat{T}_{kin}\left|\Psi_{KS}\right\rangle+\frac{1}{2}\int d^3\mathbf{r}\int d^3\mathbf{r}'\frac{e^2n\left(\mathbf{r}\right)n\left(\mathbf{r}'\right)}{4\pi\varepsilon_0\left|\mathbf{r}-\mathbf{r}'\right|}+E_{xc}[n].$$

The above equation defines the exchange correlation functional $E_{xc}[n]$. Going back to the definition of $F[n]$, we see that

$$\begin{aligned}E_{xc}[n] &= \min_{\Psi\rightarrow n}\left\langle\Psi\right|\widehat{T}_{kin}+\hat{V}_c\left|\Psi\right\rangle-\min_{\Psi_{KS}\rightarrow n}\left\langle\Psi_{KS}\right|\widehat{T}_{kin}\left|\Psi_{KS}\right\rangle\\ &\quad -\frac{1}{2}\int d^3\mathbf{r}\int d^3\mathbf{r}'\frac{e^2n\left(\mathbf{r}\right)n\left(\mathbf{r}'\right)}{4\pi\varepsilon_0\left|\mathbf{r}-\mathbf{r}'\right|}.\end{aligned} \tag{44.15}$$

Note that the Kohn-Sham expression for the kinetic energy is not exact.

Years of experience have yielded good approximations for the universal functional $E_{xc}[n]$. The simplest approximation, the Local Density Approximation (LDA) reads

$$E_{xc}^{LDA}[n]=-\frac{1}{2}\min_{\Psi_{KS}\rightarrow n}\sum_{\sigma,\sigma'}\sum_{i,j}^{N/2}\int d^3\mathbf{r}\int d^3\mathbf{r}'\frac{e^2\phi_{i,\sigma}^{KS}\left(\mathbf{r}\right)\phi_{j,\sigma}^{KS}\left(\mathbf{r}\right)\phi_{i,\sigma'}^{KS}\left(\mathbf{r}'\right)\phi_{j,\sigma'}^{KS}\left(\mathbf{r}'\right)}{4\pi\varepsilon_0\left|\mathbf{r}-\mathbf{r}'\right|}+\int d^3\mathbf{r}C^Xn^{4/3}\left(\mathbf{r}\right)$$

Instead of minizing with respect to the Kohn-Sham orbitals restricted to a given density and then with respect to the density, one minimizes with respect to the Kohn-Sham orbitals, obtaining equations that have the structure of the integro-differential Hartree-Fock equation.

It is important to realize that the Kohn-Sham orbitals serve to compute the ground-state single-particle density. The eigenstates are Bloch states with a band index. The corresponding eigenenergies cannot be interpreted as exact single-particle excitations. They may however serve as a starting point for further calculations using many-body theory, as we explain in the next Chapter on the Hubbard model.

44.3 Finite temperature

Mermin [5] has used the Feynmann variational principle to show that in the presence of an external potential, the grand potential is a functional of the density and that there is a universal part to it.

We have already shown, with ϱ the density matrix, that

$$\Omega\left[\varrho\right] < \Omega\left[\varrho'\right] + \left\langle H - H'\right\rangle_{\varrho'} . \tag{44.16}$$

We assume that the difference between ϱ and ϱ' is only the lattice potential but that suffices to state that there is really an inequality and that the two sides cannot be equal. Writing explicitly the difference between the two Hamiltonians,

$$\Omega\left[\varrho\right] < \Omega\left[\varrho'\right] + \int d^3\mathbf{r} n'\left(\mathbf{r}\right)\left(V_l\left(\mathbf{r}\right) - V_l'\left(\mathbf{r}\right)\right). \tag{44.17}$$

We could also use the inequality by interchanging the role of ϱ and ϱ' so that the following inequality is also valid

$$\Omega\left[\varrho'\right] < \Omega\left[\varrho\right] + \int d^3\mathbf{r} n\left(\mathbf{r}\right)\left(V_l'\left(\mathbf{r}\right) - V_l\left(\mathbf{r}\right)\right). \tag{44.18}$$

If the densities are identical for the two different lattice potentials, then $n'\left(\mathbf{r}\right) = n\left(\mathbf{r}\right)$ and adding the two inequalities together we find the absurd result

$$\Omega\left[\varrho\right] + \Omega\left[\varrho'\right] < \Omega\left[\varrho'\right] + \Omega\left[\varrho\right]. \tag{44.19}$$

Hence, if the two lattice potentials are different, the densities have to differ. In other words the local density is uniquely determined by the external lattice potential.

If we know the external lattice potential, we can write down the density matrix ϱ in the usual way. Since there is a one-to-one correspondance between $V_l\left(\mathbf{r}\right)$ and $n\left(\mathbf{r}\right)$, the density matrix ϱ is a functional of $n\left(\mathbf{r}\right)$ and

$$\Omega\left[n\right] = \int d^3\mathbf{r} n\left(\mathbf{r}\right) V_l\left(\mathbf{r}\right) + \mathcal{F}\left[n\right] \tag{44.20}$$

where

$$\mathcal{F}\left[n\right] = \left\langle \widehat{T}_{kin} + \hat{V}_c\right\rangle_n - TS\left[n\right] \tag{44.21}$$

with S the entropy $-\mathrm{Tr}[\varrho \ln \varrho]$ determined from the density matrix that is uniquely determined by the density.

One thus obtains a minimization problem with respect to the density $n\left(\mathbf{r}\right)$ that is very similar to what we had at zero temperature.

Remark 141 *The original Hohenberg-Kohn theorem is along the lines of the arguments in this section. We could also formulate the Mermin result in a manner similar to that of Levy for the ground state. The density matrix would replace the wave function.*

45. THE HUBBARD MODEL

Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. The Kohn-Sham orbitals give highly accurate electronic density and energy for the ground state. If the problem has been solved for a translationally invariant lattice, the one-particle states will be Bloch states indexed by crystal momentum $\mathbf{k}$ and band index n. Nevertheless, these one-particle states cannot be used to build single-particle states that diagonalize the many-body Hamiltonian. More specifically, if we expand the creation-annihilation operators in that basis using the general formulas for one-particle and two-particle parts of the Hamiltonian, it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

After providing a "derivation" of the model, we will solve limiting cases that will illustrate one limit where states are extended, and one limit where they are localized, giving a preview of the Mott transition.

45.1 Assumptions behind the Hubbard model

A qualitative derivation of the model is as follows. We restrict ourselves to a single band and expand in the Wannier basis associated with the Bloch states. The Hamiltonian in the presence of the Coulomb interaction then takes the form

$$H=\sum_{\sigma}\sum_{i,j}c_{i\sigma}^{\dagger}\left\langle i\right|\widehat{T}_{kin}+\hat{V}_{l}\left|j\right\rangle c_{j\sigma}+\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\left\langle i\right|\left\langle j\right|\hat{V}_{c}\left|k\right\rangle\left|l\right\rangle c_{i\sigma}^{\dagger}c_{j\sigma'}^{\dagger}c_{l\sigma'}c_{k\sigma} \quad (45.1)$$

where $\widehat{T}$ contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. Here, $c_{i\sigma}^{\dagger}$ $(c_{i\sigma})$ are creation and annihilation operators for electrons of spin σ in the Wannier orbital centered around site i. A single many-particle state formed by filling orbitals, leading to a Slater determinant as wave function, cannot diagonalize this Hamiltonian because of the interaction part that empties orbitals and fills other ones. The true eigenstates are linear combinations of Slater determinants.

The one-body part by itself is essentially the DFT band structure. In 1964, Hubbard, Kanamori and Gutzwiller did the most dramatic of approximations, hoping to have a model simple enough to solve. They assumed that $\left\langle i\right|\left\langle j\right|\hat{V}_{c}\left|k\right\rangle\left|l\right\rangle$ would be much larger than all other interaction matrix elements when all lattice sites are equal. Defining $t_{ij}\equiv\left\langle i\right|\widehat{T}\left|j\right\rangle$ and $U\equiv\left\langle i\right|\left\langle i\right|\hat{V}_{c}\left|i\right\rangle\left|i\right\rangle$, and using $c_{i\sigma}c_{i\sigma}=0$

they were left with

$$
\begin{aligned}
H &= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{i} U c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} \\
&= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \qquad (45.2) \\
&= \sum_{\sigma}\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow}. \qquad (45.3)
\end{aligned}
$$

In this expression, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the density of spin σ electrons, $t_{ij} = t^{*}_{ji}$ is the hopping amplitude, and U is the screened Coulomb repulsion that acts only on electrons on the same site. Most of the time, one considers hopping only to nearest neighbors. In general, we write $-t, -t', -t''$ respectively for the first-, second- and third-nearest neighbor hopping amplitudes. To go from the first to the second line we used the Pauli principle $c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma} = 0$.

Remark 142 *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.*

The model can be solved exactly only in one dimension using the Bethe ansatz, and in infinite dimension. The latter solution is the basis for Dynamical Mean Field Theory (DMFT) that we will discuss below. Despite that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable. A laser interference pattern can be used to create an optical lattice potential using the AC Stark effect. One can control tunneling between potential minima as well as the interation of atoms between them and basically build a physical system that will be described by the Hubbard Hamiltonian that we will study further. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of cold atoms, one can find conditions where the Hubbard model description is very accurate. By the way, in optical lattices, interesting physics occurs mostly in the nano Kelvin range. Discussing how such low temperatures are achieved would distract us to much.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a Mott insulator. The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe high-temperature superconductivity, depending on lattice and range of interaction parameters.

To gain a feeling of the Physics contained in the Hubbard model, let us first discuss two limiting cases where it can be solved exactly.

45.2 The non-interacting limit $U = 0$

As a simple exemple 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

$$H_0 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \tag{45.4}$$

where t_{ij} is a Hermitian matrix. When there is no magnetic field the one-body states can all be taken real and t_{ij} is symmetric. To take advantage of translational invariance we use our Fourier transforms

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma} \tag{45.5}$$

$$c^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c^\dagger_{\mathbf{k}\sigma} \tag{45.6}$$

with $\mathbf{r}_i$ the position of site i, and

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = N\delta_{\mathbf{k},0}. \tag{45.7}$$

Here N is the nmber of atoms and we take the lattice spacing a to be unity. Defining $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}$ and noting that the hopping matrix depends only on the distance to the neighbors $\boldsymbol{\delta}$, we find

$$\begin{aligned} H_0 &= \frac{1}{N} \sum_{\mathbf{r}_i,\boldsymbol{\delta},\sigma} \sum_{\mathbf{k}'} t_{\boldsymbol{\delta}} e^{i\mathbf{k}'\cdot(\mathbf{r}_i+\boldsymbol{\delta})} c^\dagger_{\mathbf{k}'\sigma} \sum_{\mathbf{k}'} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma} \\ &= \sum_{\boldsymbol{\delta},\sigma} t_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \qquad (45.8) \\ &= \sum_{\mathbf{k},\boldsymbol{\sigma}} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \qquad (45.9) \end{aligned}$$

In the case of nearest-neighbor hopping only, on a two-dimensional square lattice for example where $t_{ij} = -t$ for nearest-neighbor hopping, we have the dispersion relation

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y).$$

Clearly, if the Fermi wave vector is sufficiently small, we can define $t^{-1} = 2m_b$ and approximate the dispersion relation by its quadratic expansion, as in the free electron limit

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) \sim C + \frac{k_x^2 + k_y^2}{2m_b}. \tag{45.10}$$

45.3 The strongly interacting, atomic, limit $t = 0$

If there are no hoppings and only disconnected atomic sites,

$$K = U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \tag{45.11}$$

there are two energy levels, correspondig to empty, singly (zero energy) and doubly occupied site (energy U). It is apparently much simpler than the previous problem. But not quite. A simple thing to compute is the partition function. Since each site is independent, $Z = Z_1^N$ where Z_1 is the partition function for one site. We find, since there are four possible states on a site, empty, spin up, spin down and doubly occupied,

$$Z_1 = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta(U-2\mu)}. \tag{45.12}$$

Already at this level we see that there are "correlations". $Z_{\ 1}$can be factored into $\left(1+e^{\beta\mu}\right)^2$ only if there are no interactions.

Things become more subtle when we consider the "dynamics", as embodied for example in the Green function

$$\mathcal{G}_\sigma\left(\tau\right) = -\left\langle T_\tau\left[c_\sigma\left(\tau\right)c_\sigma^\dagger\right]\right\rangle. \tag{45.13}$$

We can consider only one site at a time since the Hamiltonian is diagonal in site indicies. Imagine using Lehman representation. It is clear that when the time evolution operator acts on the intermediate state, we will need to know if in this intermediate state the system is singly or doubly occupied. We cannot trace only on up electrons without worrying about down electrons. The Lehman representation gives a staightforward way of obtaining the Green function. We can also proceed with the equation of motion approach, a procedure we will adopt to introduce the concept of hierarchy of equations (the analog of the BBGKY hierarchy in classical systems). All that we need is

$$\frac{\partial c_\sigma}{\partial\tau} = [K, c_\sigma] = [Un_\sigma n_{-\sigma} - \mu n_\sigma, c_\sigma] = -Uc_\sigma n_{-\sigma} + \mu c_\sigma.$$

From this, the equation of motion for the Green function is

$$\begin{aligned} \frac{\partial\mathcal{G}_\sigma\left(\tau\right)}{\partial\tau} &= -\delta\left(\tau\right) - \left\langle T_\tau\left[\left[K, c_\sigma\left(\tau\right)\right]c_\sigma^\dagger\right]\right\rangle & (45.14)\\ &= -\delta\left(\tau\right) + \mu\mathcal{G}_\sigma\left(\tau\right) + U\left\langle T_\tau\left[c_\sigma\left(\tau\right)n_{-\sigma}\left(\tau\right)c_\sigma^\dagger\right]\right\rangle & (45.15)\end{aligned}$$

The structure of the equation of motion is very general result. One-body Green functions are coupling to higher order correlation functions. Let us write down the equation of motion for that higher order correlation function that we define as follows

$$\mathcal{G}_{2,\sigma}\left(\tau\right) = -\left\langle T_\tau\left[c_\sigma\left(\tau\right)n_{-\sigma}\left(\tau\right)c_\sigma^\dagger\right]\right\rangle = -\left\langle T_\tau\left[c_\sigma n_{-\sigma}c_\sigma^\dagger\left(-\tau\right)\right]\right\rangle. \tag{45.16}$$

Following the usual approach, and recalling that here $\partial n_{-\sigma}\left(\tau\right)/\partial\tau = \left[K, n_{-\sigma}\left(\tau\right)\right] = 0$ because the Hamiltonian preserves the number of particles, we find

$$\frac{\partial\mathcal{G}_{2,\sigma}\left(\tau\right)}{\partial\tau} = -\delta\left(\tau\right)\left\langle n_{-\sigma}\right\rangle + \mu\mathcal{G}_{2,\sigma}\left(\tau\right) - U\mathcal{G}_{2,\sigma}\left(\tau\right). \tag{45.17}$$

Instead of generating a higher order correlation function in the term coming from $\left[K, c_\sigma\left(\tau\right)\right]$, 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 (45.15) and (45.17) form a closed set of equations that is easy to solve in Matsubara frequencies where they become

$$\begin{aligned} \left(i\omega_n + \mu\right)\mathcal{G}_\sigma\left(i\omega_n\right) &= 1 + U\mathcal{G}_{2,\sigma}\left(i\omega_n\right) & (45.18)\\ \left(i\omega_n + \mu\right)\mathcal{G}_{2,\sigma}\left(i\omega_n\right) &= \left\langle n_{-\sigma}\right\rangle + U\mathcal{G}_{2,\sigma}\left(i\omega_n\right). & (45.19)\end{aligned}$$

Substituting the second equation in the first

$$\left(i\omega_n + \mu\right)\mathcal{G}_\sigma\left(i\omega_n\right) = 1 + \frac{U\left\langle n_{-\sigma}\right\rangle}{\left(i\omega_n + \mu - U\right)}. \tag{45.20}$$

Since

$$\frac{U\left\langle n_{-\sigma}\right\rangle}{\left(i\omega_n+\mu\right)\left(i\omega_n+\mu-U\right)}=\frac{U\left\langle n_{-\sigma}\right\rangle}{U}\left[\frac{1}{\left(i\omega_n+\mu-U\right)}-\frac{1}{\left(i\omega_n+\mu\right)}\right] \tag{45.21}$$

we are left with

$$\mathcal{G}_\sigma\left(i\omega_n\right)=\frac{1-\left\langle n_{-\sigma}\right\rangle}{i\omega_n+\mu}+\frac{\left\langle n_{-\sigma}\right\rangle}{i\omega_n+\mu-U} \tag{45.22}$$

$$\mathcal{G}_\sigma^R\left(\omega\right)=\frac{1-\left\langle n_{-\sigma}\right\rangle}{\omega+i\eta+\mu}+\frac{\left\langle n_{-\sigma}\right\rangle}{\omega+i\eta+\mu-U}.$$

The imaginary part gives us the single-particle spectral weight. Instead of a single delta function located at a $\mathbf{k}$ dependent position, we have two delta functions that are completely independent of $\mathbf{k}$, as we must expect for a localized state. The two levels correspond respectively to the electron afinity and ionization potential of the atom. Physically speaking, if there the fraction of sites occuied by down electrons is $\left\langle n_{-\sigma}\right\rangle$, then a spin up electron will have an energy $-\mu+U$ a fraction $\left\langle n_{-\sigma}\right\rangle$ of the time, and an energy $-\mu$ for a fraction $1-\left\langle n_{-\sigma}\right\rangle$ of the time. And that is independent of the momentum. That is very different from a quasiparticle. There is no pole à $\omega=0$ unless $\mu=0$.

The non-interacting limit is not a good starting point for this problem clearly. One expects perturbation theory to breakdown. This is simple to see for example at half filling when $\left\langle n_{-\sigma}\right\rangle=-1/2$ and $\mu=U/2$. Then,

$$\begin{aligned}\mathcal{G}_\sigma^R\left(\omega\right) &= \frac{1}{2}\left(\frac{1}{\omega+i\eta+U/2}+\frac{1}{\omega+i\eta-U/2}\right)=\frac{\left(\omega+i\eta\right)}{\left(\omega+i\eta\right)^2-\left(\frac{U^2}{4}\right)} && (45.23)\\ &= \frac{1}{\left(\omega+i\eta\right)-\frac{U^2}{4\left(\omega+i\eta\right)}} && (45.24)\end{aligned}$$

so that clearly, the retarded self-energy $\Sigma^R\left(\omega\right)=\frac{U^2}{4\left(\omega+i\eta\right)}$ is singular at low frequency. It gets rid of the pole that is at $\omega=0$ when there is no interaction.

If t is not zero but $U/t\gg 1$, then we have a Mott insulator. In a Mott insulator, the two peaks that we just found in the single-particle spectral weight are somewhat broadened, but there is a gap at zero frequency. We will leave this concept aside for the moment and discuss the weak coupling case.

45.4 Exercices

45.4.1 Symétrie particule-trou pour Hubbard

Soit le modèle de Hubbard sur un réseau carré bi-dimensionnel. On pose une intégrale de saut t pour les premiers voisins et t' pour les seconds voisins.

a) Montrez que la relation de dispersion prend la forme suivante lorsque le pas du réseau est pris égal à l'unité:

$$\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-2t'\left(\cos\left(k_x+k_y\right)+\cos\left(k_x-k_y\right)\right). \tag{45.25}$$

b) Montrez que la transformation canonique suivante

$$\begin{aligned}d_{\mathbf{k}\sigma} &= c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger\\ d_{\mathbf{k}\sigma}^\dagger &= c_{\mathbf{k}+\mathbf{Q}\sigma} && (45.26)\end{aligned}$$

où $\mathbf{Q} = (\pi, \pi)$, transforme $H - \mu N$ en un Hamiltonien ayant la même forme mais avec des paramètres différents. Sachant ce résultat, montrez que la solution obtenue avec $t' > 0$ pour le modèle original est reliée à la solution qu'on obtiendrait pour ce modèle avec $t' < 0$ à un potentiel chimique différent. Quelle est la relation entre la densité évaluée à ces deux potentiels chimiques? Finalement, lorsque $t' = 0$, montrez que $\mu = U/2$ correspond au demi-remplissage.

45.4.2 Règle de somme f

En utilisant la définition exacte de χ_{ch} et de χ_{sp} et l'expression pour leurs parties imaginaires comme des commutateurs, montrez que pour le modèle de Hubbard, la règle de somme f devient

$$\int \frac{d\omega}{\pi}\omega\chi''_{ch,sp}(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}} - 2\epsilon_{\mathbf{k}}\right)n_{\mathbf{k}\sigma} \tag{45.27}$$

où $n_{\mathbf{k}\sigma} = \left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle$.

46. THE HUBBARD MODEL IN THE FOOTSTEPS OF THE ELECTRON GAS

In this Chapter, we follow the same steps as the electron gas and derive RPA equations for the response functions. While spin fluctuations did not play a prominent role in the electron gas, they will be dominant in the Hubbard model and we will see why. RPA for the Hubbard model however has a major deficiency: It does not satisfy the Pauli principle, as we will see. This had no major consequence for the eletron gas, but in the case of the Hubbard model this is crucial. We will see how to cure this problem and others using the Two-Particle Self-Consistent Approach in the next Chapter.

46.1 Single-particle properties

Following functional methods of the Schwinger school[**?**, **?**, **?**], we begin, as we have done earlier, with the generating function with source fields ϕ_σ and field destruction operators ψ in the grand canonical ensemble

$$\ln Z\left[\phi\right] = \ln \mathrm{Tr} \quad [e^{-\beta\left(\widehat{H}-\mu\widehat{N}\right)} \mathrm{T}_\tau \left(e^{-\psi^\dagger_{\overline{\sigma}}\left(\overline{1}\right)\phi_{\overline{\sigma}}\left(\overline{1},\overline{2}\right)\psi_{\overline{\sigma}}\left(\overline{2}\right)}\right)] \tag{46.1}$$

We adopt the convention that 1 stands for the position and imaginary time indices $(\mathbf{r}_1, \tau_1)$. The over-bar means summation over every lattice site and integration over imaginary-time from 0 to β, and $\overline{\sigma}$ summation over spins. T_τ is the time-ordering operator. Before, the spin index was included in the labels.

The propagator in the presence of the source field is obtained from functional differentiation

$$\mathcal{G}_\sigma\left(1,2\right)_\phi = -\left\langle \psi_\sigma\left(1\right)\psi^\dagger_\sigma\left(2\right)\right\rangle_\phi = -\frac{\delta \ln Z\left[\phi\right]}{\delta\phi_\sigma\left(2,1\right)}. \tag{46.2}$$

Physically, relevant correlation functions are obtained for $\phi = 0$ but it is extremely convenient to keep finite ϕ in intermediate steps of the calculation.

Using the equation of motion for the field ψ and the definition of the self-energy, one obtains the Dyson equation in the presence of the source field [**?**]

$$\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 + \Sigma\mathcal{G} \quad ; \quad \mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma \tag{46.3}$$

where, from the commutator of the interacting part of the Hubbard Hamiltonian H, one obtains

$$\begin{aligned} \Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},2\right)_\phi &= -U\left\langle T_\tau \psi^\dagger_{-\sigma}\left(1^+\right)\psi_{-\sigma}\left(1\right)\psi_\sigma\left(1\right)\psi^\dagger_\sigma\left(2\right)\right\rangle_\phi && (46.4) \\ &\quad -U\left[\frac{\delta\mathcal{G}_\sigma\left(1,2\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)} - \mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi \mathcal{G}_\sigma\left(1,2\right)_\phi\right]. && (46.5) \end{aligned}$$

The imaginary time in 1^+ is infinitesimally larger than in 1. This formula can be deduced from our previous one with the Coulomb interaction by specializing to a local interaction only between opposite spins. That removes one integral and one spin sum.

As in the electron gas, we need to know response functions, more specifically $\delta\mathcal{G}_\sigma\left(1,2\right)_\phi/\delta\phi_{-\sigma}\left(1^+,1\right)$.

46.2 Response functions

Response (four-point) functions for spin and charge excitations can be obtained from functional derivatives $(\delta\mathcal{G}/\delta\phi)$ of the source-dependent propagator. We will see that a linear combination of these response functions is related to $\delta\mathcal{G}_\sigma\left(1,2\right)_\phi/\delta\phi_{-\sigma}\left(1^+,1\right)$ above. Following the standard approach and using matrix notation to abbreviate the summations and integrations we have,

$$\mathcal{G}\mathcal{G}^{-1}=1 \tag{46.6}$$

$$\frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1}+\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}=0. \tag{46.7}$$

Using the Dyson equation (46.3) $\mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\phi-\Sigma$ this may be rewritten

$$\frac{\delta\mathcal{G}}{\delta\phi}=-\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}=\mathcal{G}\,\hat{}\,\mathcal{G}+\mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}, \tag{46.8}$$

where the symbol $\hat{}$ reminds us that the neighboring labels of the propagators have to be the same as those of the ϕ in the functional derivative. If perturbation theory converges, we may write the self-energy as a functional of the propagator. From the chain rule, one then obtains an integral equation for the response function in the particle-hole channel that is the analog of the Bethe-Salpeter equation in the particle-particle channel

$$\frac{\delta\mathcal{G}}{\delta\phi}=\mathcal{G}\,\hat{}\,\mathcal{G}+\mathcal{G}\left[\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right]\mathcal{G}. \tag{46.9}$$

The labels of the propagators in the last term are attached to the self energy, as in Eq.(46.8) [1].

To obtain spin and charge fluctuations from the above formula, we restore spin indices explicitly and represent coordinates with numbers (in our previous convention, numbers included spin labels, but not here). When the external field is diagonal in spin indices we need only one spin label on $\mathcal{G}$ and ϕ. The response function that can be used then to build both spin and charge fluctuations is

$$\begin{aligned}-\frac{\delta\mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} &= \left\langle T_\tau\psi_\sigma^\dagger\left(1^+\right)\psi_\sigma\left(1\right)\psi_{\sigma'}^\dagger\left(2^+\right)\psi_{\sigma'}\left(2\right)\right\rangle_\phi-\mathcal{G}_\sigma\left(1,1^+\right)_\phi\mathcal{G}_{\sigma'}\left(2,2^+\right)_\phi\\ &= \left\langle T_\tau n_\sigma\left(1\right)n_{\sigma'}\left(2\right)\right\rangle_\phi-\left\langle n_\sigma\left(1\right)\right\rangle_\phi\left\langle n_{\sigma'}\left(2\right)\right\rangle_\phi.\end{aligned} \tag{46.10}$$

The charge and spin given by

$$n_i\equiv n_{i\uparrow}+n_{i\downarrow} \tag{46.11}$$

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[1] To remind ourselves of this, we may also adopt an additional "vertical matrix notation" convention and write Eq.(7) as $\frac{\delta G}{\delta\phi}=G\,\hat{}\,G+G\left[\begin{array}{c}\frac{\delta\Sigma}{\delta G}\\ \frac{\delta G}{\delta\phi}\end{array}\right]G$.

$$S_i^z \equiv n_{i\uparrow}(\tau) - n_{i\downarrow}(\tau) . \tag{46.12}$$

Hence, the charge fluctuations are obtained from

$$\chi_{ch}(1,2) = -\sum_{\sigma,\sigma'} \frac{\delta\mathcal{G}_\sigma(1,1^+)}{\delta\phi_{\sigma'}(2^+,2)} \tag{46.13}$$

and the spin fluctuations from

$$\chi_{sp}(1,2) = -\sum_{\sigma,\sigma'} \sigma \frac{\delta\mathcal{G}_\sigma(1,1^+)}{\delta\phi_{\sigma'}(2^+,2)} \sigma' . \tag{46.14}$$

Restoring spin indices, the integral equation for the spin resolved fluctuations is

$$\frac{\delta\mathcal{G}_\sigma}{\delta\phi_{\sigma'}} = \mathcal{G}\hat{}\mathcal{G}\delta_{\sigma,\sigma'} + \mathcal{G}\left[\frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\overline{\sigma}}}\frac{\delta\mathcal{G}_{\overline{\sigma}}}{\delta\phi_{\sigma,}}\right]\mathcal{G}. \tag{46.15}$$

There is a sum over $\overline{\sigma}$. The spin indices on the Green's function are unncessary when there is rotational invariance, hence we dropped them. Similarly the following quantities

$$\sum_\sigma \frac{\delta\mathcal{G}_\sigma}{\delta\phi_{\sigma'}} \; ; \; \sum_\sigma \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\sigma'}} \tag{46.16}$$

are independent of σ' and

$$\sum_{\sigma'} \frac{\delta\mathcal{G}_\sigma}{\delta\phi_{\sigma'}} \tag{46.17}$$

is independent of σ. From this, we easily deduce by summing the general spin resolved response function Eq.(46.15) that

$$\chi_{ch} = -\sum_{\sigma,\sigma'} \frac{\delta\mathcal{G}_\sigma}{\delta\phi_{\sigma'}} = -2\mathcal{G}\hat{}\mathcal{G} - \mathcal{G}\left[\sum_\sigma \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\sigma'''}} \sum_{\sigma''}\sum_{\sigma'} \frac{\delta\mathcal{G}_{\sigma''}}{\delta\phi_{\sigma,}}\right]\mathcal{G}. \tag{46.18}$$

where the value of σ''' does ne influence the result. The irreducible charge vertex is given by $U_{ch} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} + \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}$.

For the spin response function, we notice that

$$\begin{aligned}
\sum_\sigma \sigma \frac{\delta\Sigma_\sigma}{\delta\phi_{\sigma'}}\sigma' &= \left(\frac{\delta\Sigma_\uparrow}{\delta\phi_{\sigma'}} - \frac{\delta\Sigma_\downarrow}{\delta\phi_{\sigma'}}\right)\sigma' & (46.19)\\
&= \left(\frac{\delta\Sigma_\uparrow}{\delta\phi_\uparrow} - \frac{\delta\Sigma_\downarrow}{\delta\phi_\uparrow}\right) & (46.20)
\end{aligned}$$

It suffices to take σ' up $(+1)$ and then down (-1) and use rotational invariance to see that the result is independent of σ'.This means that the general spin resolved response function Eq.(46.15) yieds for the spin susceptibility, given $(\sigma'')^2 = 1$

$$\begin{aligned}
\chi_{sp} &= -\sum_{\sigma,\sigma'} \sigma \frac{\delta\mathcal{G}_\sigma}{\delta\phi_{\sigma'}}\sigma' = -2\mathcal{G}\hat{}\mathcal{G} \\
&\quad -\mathcal{G}\left[\sum_{\sigma''}\sum_{\sigma'}\left(\sum_\sigma \sigma \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\sigma''}}\sigma''\right)\sigma''\frac{\delta\mathcal{G}_{\sigma''}}{\delta\phi_{\sigma,}}\sigma'\right]\mathcal{G}. \\
&= -2\mathcal{G}\hat{}\mathcal{G} + \mathcal{G}\left[\left(\frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}\right)\sum_{\sigma''}\sum_{\sigma'}\sigma''\frac{\delta\mathcal{G}_{\sigma''}}{\delta\phi_{\sigma,}}\sigma'\right]\mathcal{G}. \qquad (46.21)
\end{aligned}$$

In summary, we define irreducible vertices appropriate for spin and charge responses as follows,

$$U_{sp} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow} \quad ; \quad U_{ch} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} + \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}. \tag{46.22}$$

46.3 Hartree-Fock and RPA

As an example of calculation of response functions, consider the Hartree-Fock approximation which corresponds to factoring the four-point function in the definition of the self-energy Eq.(46.4) as if there were no interactions, in which case it is easy to see that $\frac{\delta\mathcal{G}_\sigma(1,2)_\phi}{\delta\phi_{-\sigma}(1^+,1)}=0$. To be more specific, starting from

$$\begin{aligned}
\Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},2\right)_\phi &= -U\left\langle T_\tau \psi^\dagger_{-\sigma}\left(1^+\right)\psi_{-\sigma}\left(1\right)\psi_\sigma\left(1\right)\psi^\dagger_\sigma\left(2\right)\right\rangle_\phi && (46.23)\\
&= -U\left[\frac{\delta\mathcal{G}_\sigma\left(1,2\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)}-\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi\mathcal{G}_\sigma\left(1,2\right)_\phi\right] && (46.24)
\end{aligned}$$

the Hartree-Fock approximation is

$$\Sigma^H_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}^H_\sigma\left(\overline{1},2\right)_\phi = U\mathcal{G}^H_{-\sigma}\left(1,1^+\right)_\phi\mathcal{G}^H_\sigma\left(1,2\right)_\phi .$$

Multiplying the above equation by $\left(G^H_\sigma\right)^{-1}$, we are left with

$$\Sigma^H_\sigma\left(1,2\right)_\phi = U\mathcal{G}^H_{-\sigma}\left(1,1^+\right)_\phi\delta\left(1-2\right), \tag{46.25}$$

so that

$$\left.\frac{\delta\Sigma^H_\uparrow\left(1,2\right)_\phi}{\delta\mathcal{G}^H_\downarrow\left(3,4\right)_\phi}\right|_{\phi=0} = U\delta\left(1-2\right)\delta\left(3-1\right)\delta\left(4-2\right), \tag{46.26}$$

and

$$\left.\frac{\delta\Sigma^H_\uparrow\left(1,2\right)_\phi}{\delta\mathcal{G}^H_\uparrow\left(3,4\right)_\phi}\right|_{\phi=0} = 0.$$

which, when substituted in the integral equation (46.9) for the response function, tells us that we have generated the random phase approximation (RPA) with, from Eq.(46.22), $U_{sp}=U_{ch}=U$. Indeed, when the irreducible vertex comes from the Hartree term, the same structure as the one found before for the electron gas results. The charge susceptibility that follows from the result of the previous section Eq.(46.18) is

$$\chi_{ch}\left(1,2\right) = \chi^{(0)}\left(1,2\right)-\frac{1}{2}\chi^{(0)}\left(1,\overline{3}\right)U_{ch}\chi_{ch}\left(\overline{3},2\right) \tag{46.27}$$

with $\chi^{(0)}\left(1,2\right)=-2\mathcal{G}\left(1,2\right)\mathcal{G}\left(2,1\right)$. The Fourier transform is

$$\chi_{ch}\left(q\right) = \chi^{(0)}\left(q\right)-\frac{U_{ch}}{2}\chi^{(0)}\left(q\right)\chi_{ch}\left(q\right). \tag{46.28}$$

Since at this point the self-energy is a constant, we take for $\mathcal{G}$ the non-interacting Green's function. In Fourier-Matsubara space, $\chi_0(q)$ then is the Lindhard function that, in analytically continued retarded form is, for a discrete lattice of N sites,

$$\chi^{0R}(\mathbf{q},\omega) = -\frac{2}{N}\sum_{\mathbf{k}}\frac{f\left(\zeta_{\mathbf{k}}\right)-f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)}{\omega+i\eta+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}. \tag{46.29}$$

Similarly, for the spin susceptibility

$$\chi_{sp}\left(q\right) = \chi^{(0)}\left(q\right)+\frac{U_{sp}}{2}\chi^{(0)}\left(q\right)\chi_{sp}\left(q\right). \tag{46.30}$$

The equations for the spin and charge fluctuations can easily be solved and yield, respectively

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} \tag{46.31}$$

$$\chi_{ch}(q) = \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)} \tag{46.32}$$

It is known on general grounds [**?**] that RPA satisfies conservation laws. We will describe the general methods that lead to approximations that are consistent with conservation laws in a later chapter. But it is easy to check that for a special case. Since spin and charge are conserved, then the equalities $\chi_{sp}^R(\mathbf{q}=\mathbf{0},\omega)=0$ and $\chi_{ch}^R(\mathbf{q}=\mathbf{0},\omega)=0$ for $\omega\neq 0$ follow from the corresponding equality for the non-interacting Lindhard function $\chi^{0R}(\mathbf{q}=\mathbf{0},\omega)=0$.

Remark 143 *If we had used dressed Green's function to compute the Lindhard susceptibility, the conservation law* $\chi_{sp,ch}(\mathbf{q}=\mathbf{0},i\omega_n)=0$ *for* $i\omega_n\neq 0$ *would have been violated, as shown in Appendix A of Ref.[20]. In general,irreducible vertices and self-energy (and corresponding Green's functions) must be taken at the same level of approximation.*

46.4 RPA and violation of the Pauli principle

RPA has a drawback that is particularly important for the Hubbard model. It violates the Pauli principle that is assumed to be satisfied exactly in its definition where up spins interact only with down spins. To see this requires a bit more thinking. We derive a sum rule that rests on the use of the Pauli principle and check that it is violated by RPA to second order in U. First note that if we sum the spin and charge susceptibilities over all wave vectors $\mathbf{q}$ and all Matsubara frequencies iq_n, we obtain local, equal-time correlation functions, namely

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_{sp}(\mathbf{q},iq_n)=\left\langle (n_\uparrow-n_\downarrow)^2\right\rangle=\langle n_\uparrow\rangle+\langle n_\downarrow\rangle-2\langle n_\uparrow n_\downarrow\rangle \tag{46.33}$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_{ch}(\mathbf{q},iq_n)=\left\langle (n_\uparrow+n_\downarrow)^2\right\rangle-\langle n_\uparrow+n_\downarrow\rangle^2=\langle n_\uparrow\rangle+\langle n_\downarrow\rangle+2\langle n_\uparrow n_\downarrow\rangle-n^2 \tag{46.34}$$

where on the right-hand side, we used the Pauli principle $n_\sigma^2=\left(c_\sigma^\dagger c_\sigma\right)\left(c_\sigma^\dagger c_\sigma\right)=c_\sigma^\dagger c_\sigma-c_\sigma^\dagger c_\sigma^\dagger c_\sigma c_\sigma=c_\sigma^\dagger c_\sigma=n_\sigma$ that follows from $c_\sigma^\dagger c_\sigma^\dagger=c_\sigma c_\sigma=0$. This is the simplest version of the Pauli principle. Full antisymmetry is another matter [**?**, **?**]. We call the first of the above displayed equations the local spin sum-rule and the second one the local charge sum-rule. For RPA, adding the two sum rules yields

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\left(\chi_{sp}(\mathbf{q},iq_n)+\chi_{ch}(\mathbf{q},iq_n)\right) = \tag{46.35}$$

$$\frac{T}{N}\sum_{q}\left(\frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)}+\frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)}\right) = 2n-n^2. \tag{46.36}$$

Since the non-interacting susceptibility $\chi_0(q)$ satisfies the sum rule, we see by expanding the denominators that in the interacting case it is violated already to second order in U because $\chi_0(q)$ being real and positive, (See Eq.(48.12)), the quantity $\sum_q \chi_0(q)^3$ cannot vanish.

46.5 RPA, phase transitions and the Mermin-Wagner theorem

The RPA predicts that the normal state is sometimes unstable, namely that if we decrease the temperature, spin fluctuations at zero frequency start, in certain cases, to diverge. Below the temperature where that occurs, the spin susceptibility is negative, which is prohibited by thermodynamic stability, which indicates that a paramagnetic ground state is an unstable state. Let us illustrate this with a specific example. Let us evaluate the Lindhard function Eq.(46.29) at zero frequency in the case where we have only nearest neighbor hopping on a cubic lattice, in other words, $\zeta_{\mathbf{k}} = \varepsilon_{\mathbf{k}} = -2t\left(\cos k_x + \cos k_y + \cos k_z\right)$.Then, if we take $\mu = 0$, which in this case corresponds to half-filling, and choose the wave vector corresponding to an antiferromagnetic fluctuation, namely $Q = (\pi, \pi, \pi)$ that leads to a phase $+1$ or -1 on alternating sites, we find

$$\chi^{0R}(\mathbf{Q}, 0) = -\frac{2}{N}\sum_{\mathbf{k}} \frac{2f\left(\varepsilon_{\mathbf{k}}\right) - 1}{2\varepsilon_{\mathbf{k}}} \tag{46.37}$$

because of the equality $f(-\varepsilon) = 1 - f(\varepsilon)$ and the co-called nesting property $\varepsilon_{\mathbf{k}} = -\varepsilon_{\mathbf{k}+\mathbf{Q}}$. But $2f\left(\varepsilon_{\mathbf{k}}\right) - 1 = -\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)$ which allows one to write by using the definition of the density of states $N(\varepsilon)$

$$\begin{aligned}
\chi^{0R}(\mathbf{Q}, 0) &= \frac{2}{N}\sum_{\mathbf{k}} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} && (46.38)\\
&\sim 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} && (46.39)\\
&\sim \int d\varepsilon N(\varepsilon) \frac{\tanh\left(\beta\varepsilon/2\right)}{2\varepsilon}. && (46.40)
\end{aligned}$$

The last integral diverges when $T \to 0$ or $\beta \to \infty$. Indeed, take $N(\varepsilon)$ constant near the Fermi level, up to a cutoff energy $\pm E_F$. Near the Fermi level, $\varepsilon = 0$, when $\varepsilon > T$ we can approximate $\tanh\left(\beta\varepsilon/2\right)/2\varepsilon \sim 1/4T$. So we can extract the logarithmically divergent part of the integral as follows:

$$\begin{aligned}
\int d\varepsilon N(\varepsilon) \frac{\tanh\left(\beta\varepsilon/2\right)}{2\varepsilon} &\sim \int_T^{E_F} d\varepsilon N(0) \frac{1}{\varepsilon} \\
&\sim N(0) \ln\left(\frac{E_F}{T}\right). && (46.41)
\end{aligned}$$

For T sufficiently small, $\chi^{0R}(\mathbf{Q}, 0)$ diverges, which means that at a certain temperature, the denominator of the spin susceptibility Eq.(46.31) goes through zero. At that temperature, the spin susceptibility diverges. Below that it is negative. If we look at the thermodynamic sum rule in Sec. 11.10.1

$$\chi_{sp}(\mathbf{Q}, 0) = \int \frac{d\omega}{\pi} \frac{\chi''_{sp}(\mathbf{Q}, \omega)}{\omega} \tag{46.42}$$

this means that the imaginary part of the spin susceptibility for positive frequencies has to be negative. It is positive at negative frequencies since it must be odd. This violates the positivity criterion imposed by stability, Sec. 11.7, namely $\chi''_{sp}(\mathbf{Q},\omega)\omega > 0$. Hence, the system is unstable.

This instability signals a second-order phase transition that it physical. However, in two-dimensions, one cannot have a phase transition that breaks a continuous symmetry in two dimensions. That is the content of the Mermin Wagner theorem.[**?**, **?**] Hence, RPA fails miserably on many grounds in two dimensions: It violates the Pauli principle and the Mermin-Wagner theorem. The approach in the next section fixes these two problems and more.

47. THE TWO-PARTICLE-SELF-CONSISTENT APPROACH

The two-particle-self-consistent approach (TPSC) is designed to remedy the deficiencies found above in the study of the the one-band Hubbard model. It is also possible to generalize to cases where near-neighbor interactions are included.

TPSC is valid from weak to intermediate coupling. Hence, on the negative side, it does not describe the Mott transition. Nevertheless, there is a large number of physical phenomena that it allows to study. An important one is antiferromagnetic fluctuations. It is extremely important physically that in two dimensions there is a wide range of temperatures where there are huge antiferromagnetic fluctuations in the paramagnetic state, without long-range order, as imposed by the Mermin-Wagner theorem. The standard way to treat fluctuations in many-body theory, the Random Phase Approximation (RPA) misses this and also, as we saw, the RPA also violates the Pauli principle in an important way. The composite operator method (COM), by F. Mancini, is another approach that satisfies the Mermin-Wagner theorem and the Pauli principle. [**?**, **?**, **?**] The Fluctuation Exchange Approximation (FLEX) [**?**, **?**], and the self-consistent renormalized theory of Moriya-Lonzarich [**?**, **?**, **?**] are other approaches that satisfy the Mermin-Wagner theorem at weak coupling? Each has its strengths and weaknesses, as discussed in Refs. [20, **?**]. Weak coupling renormalization group approaches become uncontrolled when the antiferromagnetic fluctuations begin to diverge [**?**, **?**, **?**, **?**]. Other approaches include the effective spin-Hamiltonian approach [**?**].

In summary, the advantages and disadvantages of TPSC are as follows. Advantages:

- There are no adjustable parameters.
- Several exact results are satisfied: Conservation laws for spin and charge, the Mermin-Wagner theorem, the Pauli principle in the form $\left\langle n_{\uparrow}^{2}\right\rangle = \langle n_{\uparrow}\rangle$, the local moment and local-charge sum rules and the f sum-rule.
- Consistency between one and two-particle properties serves as a guide to the domain of validity of the approach. (Double occupancy obtained from sum rules on spin and charge equals that obtained from the self-energy and the Green function).
- Up to intermediate coupling, TPSC agrees within a few percent with Quantum Monte Carlo (QMC) calculations. Note that QMC calculations can serve as benchmarks since they are exact within statistical accuracy, but they are limited in the range of physical parameter accessible.
- We do not need to assume that Migdal's theorem applies to be able to obtain the self-energy.

The main successes of TPSC include

- Understanding the physics of the pseudogap induced by precursors of a long-range ordered phase in two dimensions. For this understanding, one needs a method that satisfies the Mermin-Wagner theorem to create a broad temperature range where the antiferromagnetic correlation length is larger than the thermal de Broglie wavelength. That method must also allow one to compute the self-energy reliably. Only TPSC does both.

- Explaining the pseudogap in electron-doped cuprate superconductors over a wide range of dopings.
- Finding estimates of the transition temperature for d-wave superconductivity that were found later in agreement with quantum cluster approaches such as the Dynamical Cluster Approximation.
- Giving quantitative estimates of the range of temperature where quantum critical behavior can affect the physics.

The drawbacks of this approach, that I explain as we go along, are that

- It works well in two or more dimensions, not in one dimension [1] [?].
- It is not valid at strong coupling, except at very high temperature and large U where it recovers the atomic limit [?].
- It is not valid deep in the renormalized classical regime [?].
- For models other than the one-band Hubbard model, one usually runs out of sum rules and it is in general not possible to find all parameters self-consistently. With nearest-neighbor repulsion, it has been possible to find a way out.

For detailed comparisons with QMC calculations, discussions of the physics and detailed comparisons with other approaches, you can refer to Ref.[20, ?]. You can read Ref.[?] for a review of the work related to the pseudogap and superconductivity up to 2005 including detailed comparisons with Quantum Cluster approaches in the regime of validity that overlaps with TPSC (intermediate coupling).

47.1 TPSC First step: two-particle self-consistency for $\mathcal{G}^{(1)}, \Sigma^{(1)}$, $\Gamma_{sp}^{(1)} = U_{sp}$ and $\Gamma_{ch}^{(1)} = U_{ch}$

Details of the more formal derivation may be also be found in Ref. [?]. In conserving approximations, the self-energy is obtained from a functional derivative $\Sigma\left[\mathcal{G}\right] = \delta\Phi\left[\mathcal{G}\right]/\delta\mathcal{G}$ of Φ the Luttinger-Ward functional, which is itself computed from a set of diagrams. We will see this approach later in the course. To liberate ourselves from diagrams and find results that are valid beyond perturbation theoty, we start instead from the exact expression for the self-energy, Eq.(46.4)

$$\Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},2\right)_\phi = -U\left\langle T_\tau \psi^\dagger_{-\sigma}\left(1^+\right)\psi_{-\sigma}\left(1\right)\psi_\sigma\left(1\right)\psi^\dagger_\sigma\left(2\right)\right\rangle_\phi$$

and notice that when label 2 equals 1^+, the right-hand side of this equation is equal to double-occupancy $\langle n_\uparrow n_\downarrow\rangle$. Factoring as in Hartree-Fock amounts to assuming no correlations. Instead, we should insist that $\langle n_\uparrow n_\downarrow\rangle$ should be obtained self-consistently. After all, in the Hubbard model, there are only two local four point functions: $\langle n_\uparrow n_\downarrow\rangle$ and $\left\langle n_\uparrow^2\right\rangle = \left\langle n_\downarrow^2\right\rangle$. The latter is given exactly, through the

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[1] Modifications have been proposed in zero dimension to use as impurity solver for DMFT [?]

Pauli principle, by $\left\langle n_\uparrow^2 \right\rangle = \left\langle n_\downarrow^2 \right\rangle = \langle n_\uparrow \rangle = \langle n_\downarrow \rangle = n/2$, when the filling n is known. In a way, $\langle n_\uparrow n_\downarrow \rangle$ in the self-energy equation (46.4), can be considered as an initial condition for the four point function when one of the points, 2, separates from all the others which are at 1. When that label 2 does not coincide with 1, it becomes more reasonable to factor *à la* Hartree-Fock. These physical ideas are implemented by postulating

$$\Sigma_\sigma^{(1)}\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma^{(1)}\left(\overline{1},2\right)_\phi = A_\phi \mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)_\phi \mathcal{G}_\sigma^{(1)}\left(1,2\right)_\phi \tag{47.1a}$$

where A_ϕ depends on external field and is chosen such that the exact result [2]

$$\Sigma_\sigma\left(1,\overline{1}\right)_\phi \mathcal{G}_\sigma\left(\overline{1},1^+\right)_\phi = U\left\langle n_\uparrow(1)\, n_\downarrow(1)\right\rangle_\phi \tag{47.2}$$

is satisfied. It is easy to see that the solution is

$$A_\phi = U\frac{\left\langle n_\uparrow(1)\, n_\downarrow(1)\right\rangle_\phi}{\left\langle n_\uparrow(1)\right\rangle_\phi \left\langle n_\downarrow(1)\right\rangle_\phi}. \tag{47.3}$$

Substituting A_ϕ back into our *ansatz* Eq.(48.3) we obtain our first approximation for the self-energy by right-multiplying by $\left(\mathcal{G}_\sigma^{(1)}\right)^{-1}$:

$$\Sigma_\sigma^{(1)}\left(1,2\right)_\phi = A_\phi \mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)_\phi \delta\left(1-2\right). \tag{47.4}$$

We are now ready to obtain irreducible vertices using the prescription of section 46.2, Eq.(46.22), namely through functional derivatives of Σ with respect to $\mathcal{G}$. In the calculation of U_{sp}, the functional derivative of $\langle n_\uparrow n_\downarrow \rangle / \left(\langle n_\uparrow \rangle \langle n_\downarrow \rangle\right)$ drops out, so we are left with [3],

$$\begin{aligned}
\left.\frac{\delta\Sigma_\uparrow^{(1)}\left(1,2\right)_\phi}{\delta\mathcal{G}_\downarrow^{(1)}\left(3,4\right)_\phi}\right|_{\phi=0} - \left.\frac{\delta\Sigma_\uparrow^{(1)}\left(1,2\right)_\phi}{\delta\mathcal{G}_\uparrow^{(1)}\left(3,4\right)_\phi}\right|_{\phi=0} &= U_{sp}\delta\left(1-2\right)\delta\left(3-1\right)\delta\left(4-2\right) \\
U_{sp} &= A_{\phi=0} = U\frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}. \qquad (47.5)
\end{aligned}$$

The renormalization of this irreducible vertex may be physically understood as coming from the physics described by Kanamori and Brueckner [20] (in the latter case in the context of nuclear physics): The value of the bare interaction is renormalized down by the fact that the two-particle wave function will want to be smaller where U is larger. In the language of perturbation theory, one must sum the Born series to compute how two particles scatter off each other and not work in the first Born approximation. This completes the derivation of the *ansatz* that is central to TPSC.

The functional-derivative procedure generates an expression for the charge vertex U_{ch} which involves the functional derivative of $\langle n_\uparrow n_\downarrow \rangle / \left(\langle n_\uparrow \rangle \langle n_\downarrow \rangle\right)$ which contains six point functions that one does not really know how to evaluate. But, if we again assume that the vertex U_{ch} is a constant, it is simply determined by the requirement that charge fluctuations also satisfy the fluctuation-dissipation theorem and the Pauli principle, as in Eq.(46.34). In summary, spin and charge fluctuations are obtained from

$$\chi_{sp}(q) = \frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} \tag{47.6}$$

$$\chi_{ch}(q) = \frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}. \tag{47.7}$$

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[2] See footnote (14) of Ref. [?] for a discussion of the choice of limit 1^+ vs 1^-.

[3] For $n > 1$, all particle occupation numbers must be replaced by hole occupation numbers.

with the irreducible vertices determined from the sum rules

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)}=n-2\left\langle n_{\uparrow}n_{\downarrow}\right\rangle \tag{47.8}$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}=n+2\left\langle n_{\uparrow}n_{\downarrow}\right\rangle -n^2. \tag{47.9}$$

along with the relations that relates U_{sp} to double occupancy, Eq.(47.5).

Remark 144 *Note that, in principle,* $\Sigma^{(1)}$ *also depends on double-occupancy, but since* $\Sigma^{(1)}$ *is a constant, it is absorbed in the definition of the chemical potential and we do not need to worry about it in this case. That is why the non-interacting irreducible susceptibility* $\chi^{(1)}(q)=\chi_0(q)$ *appears in the expressions for the susceptibility, even though it should be evaluated with* $\mathcal{G}^{(1)}$ *that contains* $\Sigma^{(1)}$*. A rough estimate of the renormalized chemical potential (or equivalently of* $\Sigma^{(1)}$*), is given in the appendix of Ref. ([**?**]). One can check that spin and charge conservation are satisfied by the TPSC susceptibilities.*

Remark 145 $U_{sp}\left\langle n_{\uparrow}\right\rangle\left\langle n_{\downarrow}\right\rangle=U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle$ *can be understood as correcting the Hatree-Fock factorization so that the correct double occupancy be obtained. Expressing the irreducible vertex in terms of an equal-time correlation function is inspired by the approach of Singwi [**?**] to the electron gas. But TPSC is different since it also enforces the Pauli principle and connects to a local correlation function, namely* $\left\langle n_{\uparrow}n_{\downarrow}\right\rangle$ *.*

47.2 TPSC Second step: an improved self-energy $\Sigma^{(2)}$

Collective charge and spin excitations can be obtained accurately from Green's functions that contain a simple self-energy, as we have just seen. Such modes are emergent objects that are less influenced by details of the single-particle properties than the other way around, especially at finite temperature where the lowest fermionic Matsubara frequency is not zero. The self-energy on the other hand is much more sensitive to collective modes since these are important at low frequency. The second step of TPSC is thus to find a better approximation for the self-energy. This is similar in spirit to what is done in the electron gas [3] where plasmons are found with non-interacting particles and then used to compute an improved approximation for the self-energy. This two step process is also analogous to renormalization group calculations where renormalized interactions are evaluated to one-loop order and quasiparticle renormalization appears only to two-loop order [**?**, **?**, **?**].

The procedure will be the same as for the electron gas. But before we move to the algebra, we can understand physically the result by looking at Fig. 47-1 that shows the exact diagrammatic expressions for the three-point vertex (green triangle) and self-energy (blue circle) in terms of Green's functions (solid black lines) and irreducible vertices (red boxes). The bare interaction U is the dashed line. One should keep in mind that we are not using perturbation theory despite the fact that we draw diagrams. Even within an exact approach, the quantities defined in the figure have well defined meanings. The numbers on the figure refer

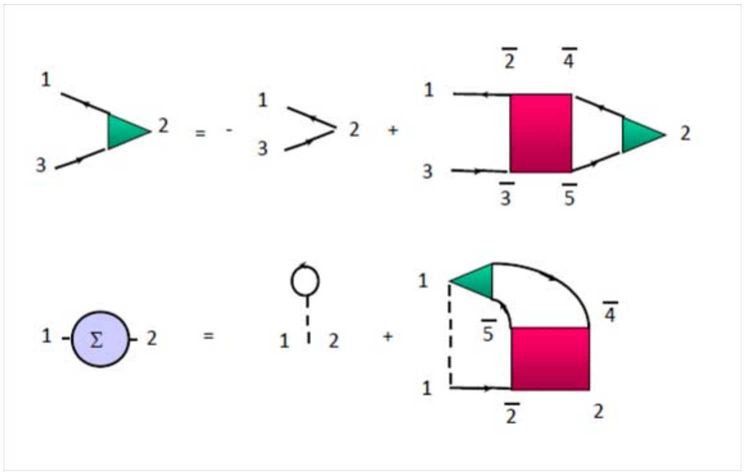

Figure 47-1 Exact expression for the three point vertex (green triangle) in the first line and for the self-energy in the second line. Irreducible vertices are the red boxes and Green's functions solid black lines. The numbers refer to spin, space and imaginary time coordinates. Symbols with an over-bard are summed/integrated over. The self-energy is the blue circle and the bare interaction U the dashed line.

to spin, space and imaginary time coordinates. When there is an over-bar, there is a sum over spin and spatial indices and an integral over imaginary time.

In TPSC, the irreducible vertices in the first line of Fig. 47-1 are local, i.e. completely momentum and frequency independent. They are given by U_{sp} and U_{ch}. If we set point 3 to be the same as point 1, then we can obtain directly the TPSC spin and charge susceptibilities from that first line. In the second line of the figure, the exact expression for the self-energy is displayed[4]. The first term on the right-hand side is the Hartree-Fock contribution. In the second term, one recognizes the bare interaction U at one vertex that excites a collective mode represented by the green triangle and the two Green's functions. The other vertex is dressed, as expected. In the electron gas, the collective mode would be the plasmon. If we replace the irreducible vertex using U_{sp} and U_{ch} found for the collective modes, we find that here, both types of modes, spin and charge, contribute to the self-energy [**?**].

Moving now to the algebra, let us repeat our procedure for the electron gas to show how to obtain an improved approximation for the self-energy that takes advantage of the fact that we have found accurate approximations for the low-frequency spin and charge fluctuations. We begin from the general definition of the self-energy Eq.(46.4) obtained from Dyson's equation. The right-hand side of that equation can be obtained either from a functional derivative with respect to an external field that is diagonal in spin, as in our generating function Eq.(46.1), or by a functional derivative of $\left\langle \psi_{-\sigma}(1)\,\psi_{\sigma}^{\dagger}(2)\right\rangle_{\phi_t}$ with respect to a transverse external field ϕ_t, namely an external field that is not diagonal in spin indices.

Working first in the longitudinal channel, the right-hand side of the general definition of the self-energy Eq.(46.4) may be written as

$$\Sigma_{\sigma}\left(1,\bar{1}\right)\mathcal{G}_{\sigma}\left(\bar{1},2\right)=-U\left[\left.\frac{\delta\mathcal{G}_{\sigma}\left(1,2\right)_{\phi}}{\delta\phi_{-\sigma}\left(1^{+},1\right)}\right|_{\phi=0}-\mathcal{G}_{-\sigma}\left(1,1^{+}\right)_{\phi}\mathcal{G}_{\sigma}\left(1,2\right)_{\phi}\right]. \quad (47.10)$$

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[4] In the Hubbard model the Fock term cancels with the same-spin Hartree term

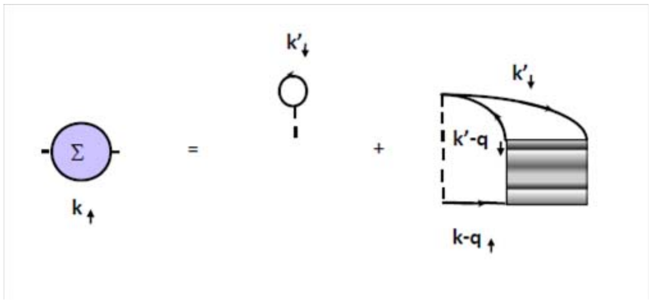

Figure 47-2 Exact self-energy in terms of the Hartree-Fock contribution and of the fully reducible vertex Γ represented by a textured box.

The last term is the Hartree-Fock contribution. It gives the exact result for the self-energy in the limit $\omega \rightarrow \infty$.[20] The $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ term is thus a contribution to lower frequencies and it comes from the spin and charge fluctuations. Right-multiplying the last equation by $\mathcal{G}^{-1}$ and replacing the lower energy part $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ by its general expression in terms of irreducible vertices, Eq.(46.9) (recalling that for $\delta\mathcal{G}_\sigma/\delta\phi_{-\sigma}$ the first term vanishes) we find

$$\begin{aligned} \Sigma_\sigma^{(2)}\left(1,2\right) &= U\mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)\delta\left(1-2\right) \\ &\quad -U\mathcal{G}_\sigma^{(1)}\left(1,\overline{3}\right)\left[\left.\frac{\delta\Sigma_\sigma^{(1)}\left(\overline{3},2\right)_\phi}{\delta\mathcal{G}_{\overline{\sigma}}^{(1)}\left(\overline{4},\overline{5}\right)_\phi}\right|_{\phi=0}\left.\frac{\delta\mathcal{G}_{\overline{\sigma}}^{(1)}\left(\overline{4},\overline{5}\right)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)_\phi}\right|_{\phi=0}\right]. \end{aligned} \tag{47.11}$$

Every quantity appearing on the right-hand side of that equation has to be taken from the TPSC results. This means in particular that the irreducible vertices $\delta\Sigma_\sigma^{(1)}/\delta\mathcal{G}_{\sigma'}^{(1)}$ are at the same level of approximation as the Green functions $\mathcal{G}_\sigma^{(1)}$ and self-energies $\Sigma_\sigma^{(1)}$. In other approaches one often sees renormalized Green functions $\mathcal{G}^{(2)}$ appearing on the right-hand side along with unrenormalized vertices, $\delta\Sigma_\sigma/\delta\mathcal{G}_{\sigma'} \rightarrow U$. We will see later in the context of electron-phonon interactions that this is equivalent to assuming, without justification, that the so-called Migdal's theorem applies to spin and charge fluctuations.

In terms of U_{sp} and U_{ch} in Fourier space, the above formula[?] reads,

$$\Sigma_\sigma^{(2)}(k)_{long} = Un_{-\sigma} + \frac{U}{4}\frac{T}{N}\sum_q\left[U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q)\right]\mathcal{G}_\sigma^{(1)}(k+q). \tag{47.12}$$

The approach to obtain a self-energy formula that takes into account both longitudinal and transverse fluctuations is detailed in Ref.([?]). Crossing symmetry, rotational symmetry and sum rules and comparisons with QMC dictate the final formula for the improved self-energy $\Sigma^{(2)}$ as we now sketch.

There is an ambiguity in obtaining the self-energy formula [?]. Within the assumption that only U_{sp} and U_{ch} enter as irreducible particle-hole vertices, the self-energy expression in the transverse spin fluctuation channel is different. What do we mean by that? Consider the exact formula for the self-energy represented symbolically by the diagram of Fig. 47-2. In this figure, the textured box is the fully reducible vertex $\Gamma\left(q, k-k', k+k'-q\right)$ that depends in general on three momentum-frequency indices. The longitudinal version of the self-energy corresponds to expanding the fully reducible vertex in terms of diagrams that are irreducible in the longitudinal (parallel spins) channel illustrated in Fig. 47-1. This takes good care of the singularity of Γ when its first argument q is near (π,π).

The transverse version [**?**, **?**] does the same for the dependence on the second argument $k-k'$, which corresponds to the other (antiparallel spins) particle-hole channel. But the fully reducible vertex obeys crossing symmetry. In other words, interchanging two fermions just leads to a minus sign. One then expects that averaging the two possibilities gives a better approximation for Γ since it preserves crossing symmetry in the two particle-hole channels [**?**]. By considering both particle-hole channels only, we neglect the dependence of Γ on $k+k'-q$ because the particle-particle channel is not singular. The final formula that we obtain is [**?**]

$$\Sigma_{\sigma}^{(2)}(k)=Un_{-\sigma}+\frac{U}{8}\frac{T}{N}\sum_{q}\left[3U_{sp}\chi_{sp}(q)+U_{ch}\chi_{ch}(q)\right]\mathcal{G}_{\sigma}^{(1)}(k+q). \tag{47.13}$$

The superscript (2) reminds us that we are at the second level of approximation. $\mathcal{G}_{\sigma}^{(1)}$ is the same Green's function as that used to compute the susceptibilities $\chi^{(1)}(q)$. Since the self-energy is constant at that first level of approximation, this means that $\mathcal{G}_{\sigma}^{(1)}$ is the non-interacting Green's function with the chemical potential that gives the correct filling. That chemical potential $\mu^{(1)}$ is slightly different from the one that we must use in $\left(\mathcal{G}^{(2)}\right)^{-1}=iq_n+\mu^{(2)}-\varepsilon_{\mathbf{k}}-\Sigma^{(2)}$ to obtain the same density [**?**]. Estimates of $\mu^{(1)}$ may be found in Ref. [**?**, **?**]). Further justifications for the above formula are given below in Sect.47.3.

47.3 TPSC, internal accuracy checks

How can we make sure that TPSC is accurate? We will show sample comparisons with benchmark Quantum Monte Carlo calculations, but we can check the accuracy in other ways. For example, we have already mentioned that the f-sum rule Eq.(48.5) is exactly satisfied at the first level of approximation (i.e. with $n_{\mathbf{k}}^{(1)}$ on the right-hand side). Suppose that on the right-hand side of that equation, one uses $n_{\mathbf{k}}$ obtained from $\mathcal{G}^{(2)}$ instead of the Fermi function. One should find that the result does not change by more than a few percent. This is what happens when agreement with QMC is good.

When we are in the Fermi liquid regime, another way to verify the accuracy of the approach is to verify if the Fermi surface obtained from $\mathcal{G}^{(2)}$ satisfies Luttinger's theorem very closely. Luttinger's theorem says that even an interacting system, when there is a jump in $n_{\mathbf{k}}$ at the Fermi surface at $T=0$ (as we have seen in the electron gas) then the particle density is determined by the number of $\mathbf{k}$ points inside the Fermi surface, as in the non-interacting case.

Finally, there is a consistency relation between one- and two-particle quantities (Σ and $\langle n_{\uparrow}n_{\downarrow}\rangle$). The relation

$$\Sigma_{\sigma}\left(1,\overline{1}\right)\mathcal{G}_{\sigma}\left(\overline{1},1^{+}\right)\equiv\frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{G}\right)=\frac{T}{N}\sum_{\mathbf{k}}\sum_{n}\Sigma(\mathbf{k},iq_n)\mathcal{G}(\mathbf{k},iq_n)e^{-iq_n0^{-}}=U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle \tag{47.14}$$

should be satisfied exactly for the Hubbard model. In standard many-body books [**?**], it is encountered in the calculation of the free energy through a coupling-constant integration. We have seen this in the previous Chapter 38. In TPSC, it is not difficult to show [5] that the following equation

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right)=U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle \tag{47.15}$$

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[5] Appendix B or Ref. [20]

is satisfied exactly with the self-consistent $U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle$ obtained with the susceptibilities[6]. An internal accuracy check consists in verifying by how much $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(2)}\right)$ differs from $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right)$. Again, in regimes where we have agreement with Quantum Monte Carlo calculations, the difference is only a few percent.

The above relation between Σ and $\left\langle n_{\uparrow}n_{\downarrow}\right\rangle$ gives us another way to justify our expression for $\Sigma^{(2)}$. Suppose one starts from Fig. 47-1 to obtain a self-energy expression that contains only the longitudinal spin fluctuations and the charge fluctuations, as was done in the first papers on TPSC [**?**]. One finds that each of these separately contributes an amount $U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle/2$ to the consistency relation Eq.(47.15). Similarly, if we work only in the transverse spin channel [**?**, **?**] we find that each of the two transverse spin components also contributes $U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle/2$ to $\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right)$. Hence, averaging the two expressions also preserves rotational invariance. In addition, one verifies numerically that the exact sum rule (Ref. [20] Appendix A)

$$-\int\frac{d\omega'}{\pi}\Sigma_{\sigma}^{\prime\prime R}\left(\mathbf{k},\omega'\right)=U^{2}n_{-\sigma}\left(1-n_{-\sigma}\right)\tag{47.16}$$

determining the high-frequency behavior is satisfied to a higher degree of accuracy with the symmetrized self-energy expression Eq. (47.13).

Eq. (47.13) for $\Sigma^{(2)}$ is different from so-called Berk-Schrieffer type expressions [**?**] that do not satisfy [7] the consistency condition between one- and two-particle properties, $\frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{G}\right)=U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle$.

Remark 146 *Schemes, such as the fluctuation exchange approximation (FLEX), that we will discuss later, use on the right-hand side* $G^{(2)}$*, are thermodynamically consistent (Sect.* **??***) and might look better. However, as we just saw, in Fig. 48-2, FLEX misses some important physics. The reason [20] is that the vertex entering the self-energy in FLEX is not at the same level of approximation as the Green's functions. Indeed, since the latter contain self-energies that are strongly momentum and frequency dependent, the irreducible vertices that can be derived from these self-energies should also be frequency and momentum dependent, but they are not. In fact they are the bare vertices. It is as if the quasi-particles had a lifetime while at the same time interacting with each other with the bare interaction. Using dressed Green's functions in the susceptibilities with momentum and frequency independent vertices leads to problems as well. For example, the conservation law* $\chi_{sp,ch}\left(\mathbf{q}=\mathbf{0},iq_{n}\right)=0$ *is violated in that case, as shown in Appendix A of Ref.[20]. Further criticism of conserving approaches appears in Appendix E of Ref.[20] and in Ref.[***?***].*

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[6] FLEX does not satisfy this consistency requirement. See Appendix E of [20]. In fact double-occupancy obtained from ΣG can even become negative [**?**].

[7] [20] Appendix E)

48. TPSC, BENCHMARKING AND PHYSICAL ASPECTS

In this chapter, we present a physically motivated approach to TPSC and benchmark the theory by comparing with Quantum Monte Carlo simulations. We also discuss physical consequences of the approach, in particular the appearance of a pseudogap that is the precursor of long-range order that occurs only at zero temperature. We show that this physics seems to be realized in electron-doped cuprates.

48.1 Physically motivated approach, spin and charge fluctuations

As basic physical requirements, we would like our approach to satisfy a) conservation laws, b) the Pauli principle and c) the Mermin Wagner theorem. The standard RPA approach satisfies the first requirement but not the other two as we saw in Sec. 46.4.

How can we go about curing this violation of the Pauli principle while not damaging the fact that RPA satisfies conservation laws? The simplest way is to proceed in the spirit of Fermi liquid theory and assume that the effective interaction (irreducible vertex in the jargon) is renormalized. This renormalization has to be different for spin and charge so that

$$\chi_{sp}(q) = \frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} \tag{48.1}$$

$$\chi_{ch}(q) = \frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}. \tag{48.2}$$

In practice $\chi^{(1)}(q)$ is the same[1] as the Lindhard function $\chi_0(q)$ for $U=0$ but, strictly speaking, there is a constant self-energy term that is absorbed in the definition of μ [**?**]. We are almost done with the collective modes. Substituting the above expressions for $\chi_{sp}(q)$ and $\chi_{ch}(q)$ in the two sum-rules, local-spin and local-charge appearing in Eqs.(46.33,46.34), we could determine both U_{sp} and U_{ch} if we knew $\langle n_\uparrow n_\downarrow\rangle$. The following *ansatz*

$$U_{sp}\langle n_\uparrow\rangle\langle n_\downarrow\rangle = U\langle n_\uparrow n_\downarrow\rangle \tag{48.3}$$

gives us the missing equation. Now notice that U_{sp}, or equivalently $\langle n_\uparrow n_\downarrow\rangle$ depending on which of these variables you want to treat as independent, is determined self-consistently. That explains the name of the approach, "Two-Particle-Self-Consistent". Since the the sum-rules are satisfied exactly, when we add them up the resulting equation, and hence the Pauli principle, will also be satisfied exactly.

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[1] The meaning of the superscripts differs from that in Ref. [20]. Superscripts (2) (1) here correspond respectively to (1) (0) in Ref. [20]

In other words, in Eq.(46.36) that follows from the Pauli principle, we now have U_{sp} and U_{ch} on the left-hand side that arrange each other in such a way that there is no violation of the principle. In standard many-body theory, two-particle self-consistency is achieved in a much more complicated by solving parquet equations. [?, ?]

The ansatz Eq.(48.3) is inspired from the work of Singwi [?, ?] and was also found independently by M. R. Hedeyati and G. Vignale [?]. The whole procedure was justified in the previous Chapter. For now, let us just add a few physical considerations.

Since U_{sp} and U_{ch} are renormalized with respect to the bare value, one might have expected that one should use the dressed Green's functions in the calculation of $\chi_0\left(q\right)$. It is explained in appendix A of Ref.[20] that this would lead to a violation of the results $\chi_{sp}^R(\mathbf{q}=\mathbf{0},\omega)=0$ and $\chi_{ch}^R(\mathbf{q}=\mathbf{0},\omega)=0$. In the present approach, the f-sum rule

$$\begin{aligned}\int\frac{d\omega}{\pi}\omega\chi_{ch,sp}''\left(\mathbf{q},\omega\right) &= \lim_{\eta\rightarrow 0}T\sum_{iq_n}\left(e^{-iq_n\eta}-e^{iq_n\eta}\right)iq_n\chi_{ch,sp}\left(\mathbf{q},iq_n\right) &(48.4)\\ &= \frac{1}{N}\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}}-2\epsilon_{\mathbf{k}}\right)n_{\mathbf{k}\sigma} &(48.5)\end{aligned}$$

is satisfied with $n_{\mathbf{k}\sigma}=n_{\mathbf{k}\boldsymbol{\sigma}}^{(1)}$, the same as the Fermi function for the non-interacting case since it is computed from $\mathcal{G}^{(1)}$. [2]

Remark 147 *$U_{sp}\left\langle n_\uparrow\right\rangle\left\langle n_\downarrow\right\rangle=U\left\langle n_\uparrow n_\downarrow\right\rangle$ can be understood as correcting the Hatree-Fock factorization so that the correct double occupancy be obtained. Expressing the irreducible vertex in terms of an equal-time correlation function is inspired by the approach of Singwi [?] to the electron gas. But TPSC is different since it also enforces the Pauli principle and connects to a local correlation function, namely $\left\langle n_\uparrow n_\downarrow\right\rangle$.*

48.2 Mermin-Wagner, Kanamori-Brueckner

The functional form of the results that we found for spin and charge fluctuations have the RPA form but the renormalized interactions U_{sp} and U_{ch} must be computed from

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)}=n-2\left\langle n_\uparrow n_\downarrow\right\rangle \qquad (48.6)$$

and

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)}=n+2\left\langle n_\uparrow n_\downarrow\right\rangle-n^2. \qquad (48.7)$$

With the *ansatz* Eq.(48.3), the above system of equations is closed and the Pauli principle is enforced. The first of the above equations is solved self-consistently with the U_{sp} ansatz. This gives the double occupancy $\left\langle n_\uparrow n_\downarrow\right\rangle$ that is then used to obtain U_{ch} from the next equation. The fastest way to numerically compute $\chi^{(1)}(q)$ is to use fast Fourier transforms [?].

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[2] For the conductivity with vertex corrections [?], the f-sum rule with $n_{\mathbf{k}\sigma}$ obtained from $G^{(2)}$ is satisfied.

These TPSC expressions for spin and charge fluctuations were obtained by enforcing the conservations laws and the Pauli principle. In particular, TPSC satisfies the f-sum rule Eq.(48.5). But we obtain for free a lot more of the physical results, namely Kanamori-Brueckner renormalization and the Mermin-Wagner theorem.

Let us begin with Kanamori-Brueckner renormalization of U. Many years ago, Kanamori in the context of the Hubbard model [**?**], and Brueckner in the context of nuclear physics, introduced the notion that the bare U corresponds to computing the scattering of particles in the first Born approximation. In reality, we should use the full scattering cross section and the effective U should be smaller. From Kanamori's point of view, the two-body wave function can minimize the effect of U by becoming smaller to reduce the value of the probability that two electrons are on the same site. The maximum energy that this can cost is the bandwidth since that is the energy difference between a one-body wave function with no nodes and one with the maximum allowed number. Let us see how this physics comes out of our results. Far from phase transitions, we can expand the denominator of the local moment sum-rule equation to obtain

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi^{(1)}(q)\left(1+\frac{1}{2}U_{sp}\chi^{(1)}(q)\right)=n-2\frac{U_{sp}}{U}\left\langle n_{\uparrow}\right\rangle\left\langle n_{\downarrow}\right\rangle. \tag{48.8}$$

Since $\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_0(q)=n-2\left\langle n_{\uparrow}\right\rangle\left\langle n_{\downarrow}\right\rangle$, we are can solve for U_{sp} and obtain [3].

$$U_{sp} = \frac{U}{1+\Lambda U} \tag{48.9}$$

$$\Lambda \equiv \frac{1}{n^2}\frac{T}{N}\sum_{iq_n}\sum_{\mathbf{q}}\left(\chi^{(1)}\right)^2(\mathbf{q},iq_n). \tag{48.10}$$

We see that at large U, U_{sp} saturates to $1/\Lambda$, which in practice we find to be of the order of the bandwidth. For those that are familiar with diagrams, note that the Kanamori-Brueckner physics amounts to replacing each of the interactions U in the ladder or bubble sum for diagrams in the particle-hole channel by infinite ladder sums in the particle-particle channel [**?**]. This is not quite what we obtain here since $\left(\chi^{(1)}\right)^2$ is in the particle-hole channel, but in the end, numerically, the results are close and the Physics seems to be the same. One cannot make strict comparisons between TPSC and diagrams since TPSC is non-perturbative.

While Kanamori-Brueckner renormalization, or screening, is a quantum effect that occurs even far from phase transitions, when we are close we need to worry about the Mermin-Wagner theorem. To satisfy this theorem, approximate theories must prevent $\langle n_{\uparrow}n_{\downarrow}\rangle$ from taking unphysical values. This quantity is positive and bounded by its value for $U=\infty$ and its value for non-interacting systems, namely $0\leq\langle n_{\uparrow}n_{\downarrow}\rangle\leq n^2/4$. Hence, the right-hand side of the local-moment sum-rule Eq.(48.6) is contained in the interval $\left[n,n-\frac{1}{2}n^2\right]$. To see how the Mermin-Wagner theorem is satisfied, write the self-consistency condition Eq.(48.6) in the form

$$\frac{T}{N}\sum_{q}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U\frac{\langle n_{\uparrow}n_{\downarrow}\rangle}{\langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle}\chi^{(1)}(q)}=n-2\langle n_{\uparrow}n_{\downarrow}\rangle. \tag{48.11}$$

Consider increasing $\langle n_{\uparrow}n_{\downarrow}\rangle$ on the left-hand side of this equation. The denominator becomes smaller, hence the integral larger. To become larger, $\langle n_{\uparrow}n_{\downarrow}\rangle$ has to decrease on the right-hand side. There is thus negative feedback in this equation that will make the self-consistent solution finite. This, however, does not prevent

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[3] There is a misprint of a factor of 2 in Ref. [20]. It is corrected in Ref.[**?**].

the expected phase transition in three dimensions [**?**]. To see this, we need to look in more details at the phase space for the integral in the sum rule.

As we know from the spectral representation for χ,

$$\chi_{ch,sp}\left(\mathbf{q},iq_n\right) = \int \frac{d\omega'}{\pi}\frac{\chi''_{ch,sp}\left(\mathbf{q},\omega'\right)}{\omega'-iq_n} = \int \frac{d\omega'}{\pi}\frac{\omega'\chi''_{ch,sp}\left(\mathbf{q},\omega'\right)}{\left(\omega'\right)^2+\left(\omega_n\right)^2}. \tag{48.12}$$

the zero Matsubara frequency contribution is always the largest. There, we find the so-called Ornstein-Zernicke form for the susceptibility.

Ornstein-Zernicke form Let us focus on the zero Matsubara frequency contribution and expand the denominator near the point where $1-\frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0) = 0$. The wave vector $\mathbf{Q}$ is that where $\chi^{(1)}$ is maximum. We find [**?**],

$$\begin{aligned}\chi_{sp}\left(\mathbf{q}+\mathbf{Q},iq_n\right) &\simeq \frac{\chi^{(1)}(\mathbf{Q},0)}{1-\frac{1}{2}U_{sp}\chi^{(1)}-\frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}}{\partial\mathbf{Q}^2}q^2-\frac{1}{2}U_{sp}\frac{\partial\chi^{(1)}}{\partial(iq_n)}iq_n}\\ &\sim \frac{\xi^2}{1+\xi^2q^2+iq_n/\omega_{sp}},\end{aligned} \tag{48.13}$$

where all quantities in the denominator are evaluated at $(\mathbf{Q},0)$. On dimensional grounds,

$$-\frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}(\mathbf{Q},0)}{\partial\mathbf{Q}^2}/\left(1-\frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0)\right)$$

scales (noted $\sim$) as the square of a length, ξ, the correlation length. That length is determined self-consistently. Since, $\omega_{sp}\sim\xi^{-2}$, all finite Matsubara frequency contributions are negligible if $2\pi T/\omega_{sp}\sim 2\pi T\xi^2 \gg 1$. That condition in the form $\omega_{sp}\ll T$ justifies the name of the regime we are interested in, namely the renormalized classical regime. The classical regime of a harmonic oscillator occurs when $\omega \ll T$. The regime here is "renormalized" classical because at temperatures above the degeneracy temperature, the system is a free classical gas. As temperature decreases below the Fermi energy, it becomes quantum mechanical, then close to the phase transition, it becomes classical again.

Substituting the Ornstein-Zernicke form for the susceptibility in the self-consistency relation Eq.(48.6), we obtain

$$T\int\frac{d^d\mathbf{q}}{\left(2\pi\right)^d}\frac{1}{q^2+\xi^{-2}} = \widetilde{C} \tag{48.14}$$

where $\widetilde{C}$ contains non-zero Matsubara frequency contributions as well as $n-2\left\langle n_\uparrow n_\downarrow\right\rangle$. Since $\widetilde{C}$ is finite, this means that in two dimensions $(d=2)$, it is impossible to have $\xi^{-2}=0$ on the left-hand side otherwise the integral would diverge logarithmically. This is clearly a dimension-dependent statement that proves the Mermin-Wagner theorem. In two-dimensions, we see that the integral gives a logarithm that leads to

$$\xi\sim\exp\left(C'/T\right).$$

where in general, C' can be temperature dependent [**?**]. When C' is not temperature dependent, the above result is similar to what is found at strong coupling in the non-linear sigma model. The above dimensional analysis is a bit expeditive. A more careful analysis [**?**, **?**] yields prefactors in the temperature dependence of the correlation length.

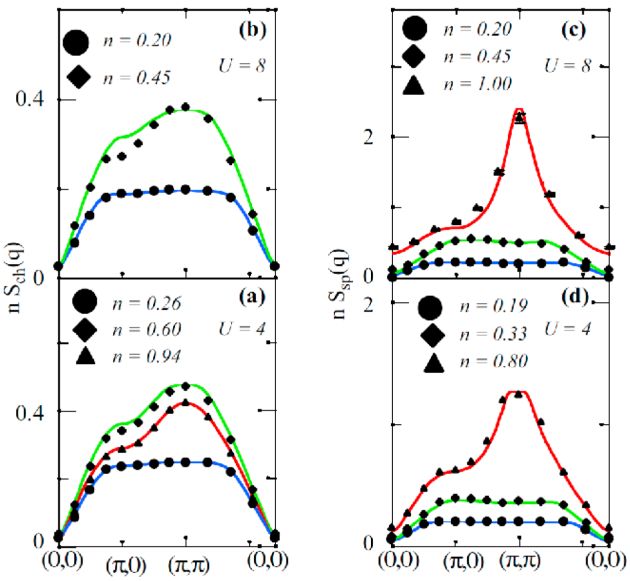

Figure 48-1 Wave vector $(\mathbf{q})$ dependence of the spin and charge structure factors for different sets of parameters. Solid lines are from TPSC and symbols are QMC data. Monte Carlo data for $n = 1$ and $U = 8t$ are for 6×6 clusters and $T = 0.5t$; all other data are for 8×8 clusters and $T = 0.2t$. Error bars are shown only when significant. From Ref. [?].

48.3 Benchmarking

Quantum Monte Carlo calculations, that we explain in a later Chapter of this book, can be considered exact within statistical sampling. Hence they can be used as benchmarks for any approximation scheme. In this section, we present a few benchmarks on spin and charge fluctuations, and then on self-energy. More comparisons may be found in Refs. [?] and [?, 20, ?, ?] and others quoted in these papers.

48.3.1 Spin and charge fluctuations

The set of TPSC equations for spin and charge fluctuations Eqs.(48.6,48.7,48.3) is rather intuitive and simple. The agreement of calculations with benchmark QMC calculations is rather spectacular, as shown in Fig.(48-1). There, one can see the results of QMC calculations of the structure factors, i.e. the Fourier transform of the equal-time charge and spin correlation functions, compared with the corresponding TPSC results.

This figure allows one to watch the Pauli principle in action. At $U = 4t$, Fig.(48-1a) shows that the charge structure factor does not have a monotonic dependence on density. This is because, as we approach half-filling, the spin fluctuations are becoming so large that the charge fluctuations have to decrease so that the sum still satisfies the Pauli principle, as expressed by Eq.(46.36). This kind of agreement is found even at couplings of the order of the bandwidth and when second-neighbor hopping t' is present [?, ?].

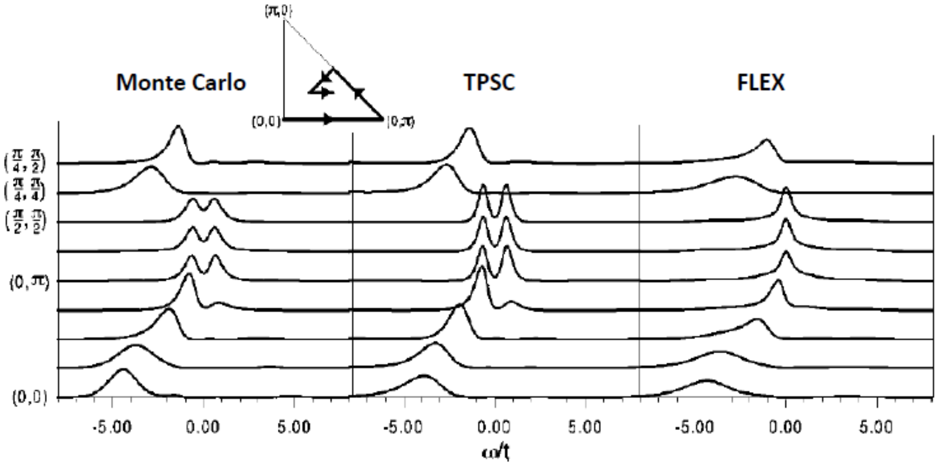

Figure 48-2 Single-particle spectral weight $A(\mathbf{k},\omega)$ for $U=4$, $\beta=5$, $n=1$, and all independent wave vectors $\mathbf{k}$ of an 8×8 lattice. Results obtained from maximum entropy inversion of Quantum Monte Carlo data on the left panel, from TPSC in the middle panel and form the FLEX approximation on the right panel. (Relative error in all cases is about 0.3%). Figure from Ref.[?]

Remark 148 *Even though the entry in the renormalized classical regime is well described by TPSC [?], equation (48.3) for* U_{sp} *fails deep in that regime because* $\Sigma^{(1)}$ *becomes too different from the true self-energy. At* $n=1$, $t'=0$, *deep in the renormalized classical regime,* U_{sp} *becomes arbitrarily small, which is clearly unphysical. However, by assuming that* $\langle n_\uparrow n_\downarrow\rangle$ *is temperature independent below* T_X, *a property that can be verified from QMC calculations, one obtains a qualitatively correct description of the renormalized-classical regime. One can even drop the ansatz and take* $\langle n_\uparrow n_\downarrow\rangle$ *from QMC on the right-hand side of the local moment sum-rule Eq.(48.6) to obtain* U_{sp}.

48.3.2 Self-energy

We check that the formula for the self-energy Eq.(47.13) is accurate by comparing in Fig. 48-2 the spectral weight (imaginary part of the Green's function) obtained from Eq.(47.13) with that obtained from Quantum Monte Carlo calculations. The latter are exact within statistical accuracy and can be considered as benchmarks. The meaning of the curves are detailed in the caption. The comparison is for half-filling in a regime where the simulations can be done at very low temperature and where a non-trivial phenomenon, the pseudogap, appears. This all important phenomenon is discussed further below in subsection 52.1 and in the first case study, Sect. 52.2. In the third panel, we show the results of another popular Many-Body Approach, the FLuctuation Exchange Approximation (FLEX) [?]. It misses [?] the physics of the pseudogap in the single-particle spectral weight because it uses fully dressed Green's functions and assumes that Migdal's theorem applies, i.e. that the vertex does not need to be renormalized consequently Ref.[20, ?]. The same problem exists in the corresponding version of the GW approximation. [?]

Remark 149 *The dressing of one vertex in the second line of Fig. 47-1 means that we do not assume a Migdal theorem. Migdal's theorem arises in the case of electron-phonon interactions [**?**]. There, the small ratio m/M, where m is the electronic mass and M the ionic mass, allows one to show that the vertex corrections are negligible. This is extremely useful to formulate the Eliashberg theory of superconductivity.*

Remark 150 *In Refs. [20, **?**] we used the notation $\Sigma^{(1)}$ instead of $\Sigma^{(2)}$. The notation of the present paper is the same as that of Ref. [**?**]*

49. DYNAMICAL MEAN-FIELD THEORY AND MOTT TRANSITION-I

In this Chapter, we will see a physically motivated derivation of dynamical mean-field theory and discuss the results found by this method on the Mott transition. A more rigorous approach to the derivation will appear later in this book. There are many review articles. We quote from Ref.[7] amongs others.

The band picture of electrons explained very well the occurence of metals, with bands that are unfilled, and insulators, with filled bands, de Boer and Verwey (1937) reported that many transition-metal oxides with a partially filled d-electron band were exceptions. They were often poor conductors and indeed often insulators. NiO became the prototypical example. following their report, Peierls (1937) pointed out the importance of the electron-electron correlation: According to Mott (1937), Peierls noted

> "it is quite possible that the electrostatic interaction between the electrons prevents them from moving at all. At low temperatures the majority of the electrons are in their proper places in the ions. The minority which have happened to cross the potential barrier find therefore all the other atoms occupied, and in order to get through the lattice have to spend a long time in ions already occupied by other electrons. This needs a considerable addition of energy and so is extremely improbable at low temperatures."

Peierls is explaining that at half-filling, every unit cell is occupied by one carrier in the presence of strong Coulomb repulsion. And the electrons cannot move because of the large Coulomb repulsion it would cost. Later, Slater found another way to obtain an insulator at half-filling even when Coulomb interactions are weak. This is when long-range antiferromagnetic order leads to a doubling of the unit cell. We have already seen in the previous Chapter that perfect nesting could lead to a diverging antiferromagnetic susceptibility, and hence to a phase transition with arbitrarily weak interaction. In that case, the Brillouin zone becomes half the size so the band split in two and the lower band is now full. The Mott insulator and the antiferromagnetic insulator are conceptually very different. One has long-range order while the other does not.

In the 1970's vanadium oxide became an example of a material showing a Mott transition. The phase diagram appears in Fig. 49-1. The substitution of vanadium by another metal with d electrons is modeled here as pressure. The accuracy of this hypothesis is confirmed by real pressure experiments that appear on the same plot (see the top and bottom horizontal axis). Pressure increases the overlap between orbitals, hence the kinetic energy and tends to delocalize electrons. We see on this phase diagram a finite temperature first order transition between a metal and an insulator without long-range order. This material has a three-dimensional lattice structure.

Layered organic conductors are quasi two-dimensional materials with a half-filled band. These are soft materials, so one can apply pressure and have a sizeable effect on the electronic structure. One observes a first-order metal-insulator transition at high-temperature that ends at a critical point. For both materials there

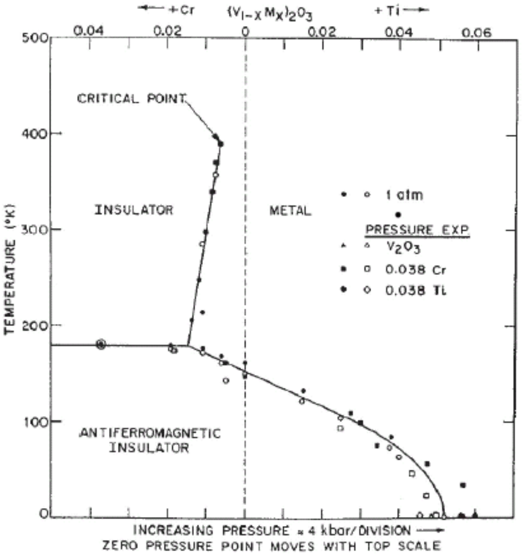

Figure: McWhan, PRB 1970; Limelette, Science 2003

Figure 49-1

is an antiferromagnetic phase at low temperature, suggesting the importance of electron-electron interactions.

Simple pictures of the Mott transition have been proposed. In the Brinkman-Rice scenario, the effective mass becomes infinite at the Mott transition. In the Mott picture, at large interaction and half-filling, the non-interacting band splits in two and there is an empty and a filled band, so no conduction. As the interaction strenght decreases, a metallic phase occurs when the bands overlap.

The modern view of this transition contains a bit of both of the above ideas. That view emerges from dynamical mean-field theory, that we explain in this Chapter. This theory was discovered after Vollhardt and Metzner proposed and exact solution for the Hubbard model in infinite dimension. Georges and Kotliar and independently Jarrell arrived at the same theory.

We begin with an apparently related problem, that of a single site with a Hubbard interaction, connected to a bath of non-interacting electrons. This is the so-called Anderson impurity model. The we will argue that in infinite dimension the self-energy depends only on frequency. That will allow us to establish a self-consistency relation.

49.1 Quantum impurities

We will only set up the problem of quantum impurities without solving it. The Numerical Renormalization Group approach (NRG) and Density Matrix Renormalization Group are examples of approaches that can be used to solve this problem.

We begin with the Anderson impurity problem. Including the chemical poten-

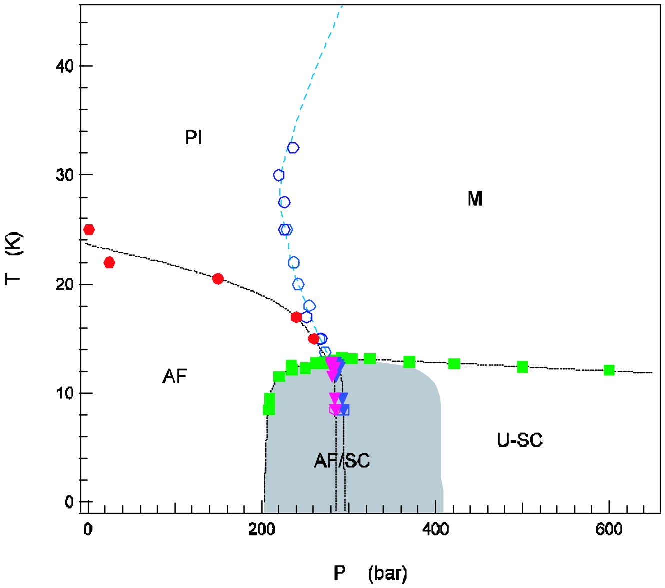

Figure 49-2

tial the model is defined by

$$K_I = H_f + H_c + H_{fc} - \mu N \tag{49.1}$$

$$K_f \equiv \sum_{\sigma} (\varepsilon - \mu) f^{\dagger}_{i\sigma} f_{i\sigma} + U \left(f^{\dagger}_{i\uparrow} f_{i\uparrow} \right) \left(f^{\dagger}_{i\downarrow} f_{i\downarrow} \right) \tag{49.2}$$

$$K_c \equiv \sum_{\sigma} \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{49.3}$$

$$H_{fc} \equiv \sum_{\sigma} \sum_{\mathbf{k}} \left(V_{\mathbf{k}i} c^{\dagger}_{\mathbf{k}\sigma} f_{i\sigma} + V^{*}_{i\mathbf{k}} f^{\dagger}_{i\sigma} c_{\mathbf{k}\sigma} \right) \tag{49.4}$$

To physically motivate this model, think of a single f level on an atom where the on-site interaction is very large. That site is hybridized through $V_{i\mathbf{k}}$ with conduction electrons around it. The sum over $\mathbf{k}$ in the hybridization part of the Hamiltonian H_{fc} basically tells us that it is the local overlap of the conduction band with the impurity that produces the coupling.

Suppose we want to know the properties of the impurity, such as the local density of states. It can be obtained from the Green function

$$\mathcal{G}_{ff}(\tau) = -\left\langle T_{\tau} f_{i\sigma}(\tau) f^{\dagger}_{i\sigma} \right\rangle . \tag{49.5}$$

We will proceed with the equations of motion method, following steps analogous to those in the exercise on non-interacting impurities. We first write the equations of motion for $c_{\mathbf{k}\sigma}$ and $f_{i\sigma}$

$$\frac{\partial}{\partial \tau} c_{\mathbf{k}\sigma} = [K_I, c_{\mathbf{k}\sigma}] \tag{49.6}$$

$$= -(\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma} - V_{\mathbf{k}i} f_{i\sigma} \tag{49.7}$$

$$\frac{\partial}{\partial \tau} f_{i\sigma} = [K_I, f_{i\sigma}] \tag{49.8}$$

$$= -(\varepsilon - \mu) f_{i\sigma} - U f^{\dagger}_{i-\sigma} f_{i-\sigma} f_{i\sigma} - \sum_{\mathbf{k}} V^{*}_{i\mathbf{k}} c_{\mathbf{k}\sigma} \tag{49.9}$$

Proceeding like our in our earlier derivation of the equations of motion we have

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{ff}(\tau) &= -\delta(\tau)\left\langle\left\{f_{i\sigma}(\tau), f_{i\boldsymbol{\sigma}}^{\dagger}\right\}\right\rangle \\
&\quad -\left\langle T_\tau\left(-(\varepsilon-\mu)f_{i\sigma}(\tau) - Uf_{i-\sigma}^{\dagger}(\tau)f_{i-\sigma}(\tau)f_{i\sigma}(\tau) - V_{\mathbf{k}i}^{*}c_{\mathbf{k}\sigma}\right)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle \qquad (49.10)\\
&= -\delta(\tau) - (\varepsilon-\mu)\mathcal{G}_{ff}(\tau) + U\left\langle T_\tau f_{i-\sigma}^{\dagger}(\tau)f_{i-\sigma}(\tau)f_{i\sigma}(\tau)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle - \sum_{\mathbf{k}}V_{i\mathbf{k}}^{*}\mathcal{G}_{cf}(\mathbf{k},i,\tau)
\end{aligned}$$

where we defined

$$\mathcal{G}_{cf}(\mathbf{k},i,\tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle. \qquad (49.11)$$

To eliminate this quantity, we write its equations of motion

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{cf}(\mathbf{k},i,\tau) &= -\delta(\tau)\left\langle\left\{c_{\mathbf{k}\sigma}(\tau), f_{i\boldsymbol{\sigma}}^{\dagger}\right\}\right\rangle \\
&\quad -\left\langle T_\tau\left(-(\varepsilon_{\mathbf{k}}-\mu)c_{\mathbf{k}\sigma}(\tau) - V_{\mathbf{k}i}f_{i\sigma}(\tau)\right)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle \\
&= -(\varepsilon_{\mathbf{k}}-\mu)\mathcal{G}_{cf}(\mathbf{k},i,\tau) - V_{\mathbf{k}i}\mathcal{G}_{ff}(\tau) \qquad (49.12)
\end{aligned}$$

that follows because $\left\{c_{\mathbf{k}\sigma}, f_{i\boldsymbol{\sigma}}^{\dagger}\right\} = 0$. It can be solved by going to Matsubara frequencies

$$\mathcal{G}_{cf}(\mathbf{k},i,ik_n) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}\mathcal{G}_{ff}(ik_n). \qquad (49.13)$$

Substituting in the equation for $\mathcal{G}_{ff}(ik_n)$ we obtain

$$\begin{aligned}
&\left[ik_n - (\varepsilon-\mu) - \sum_{\mathbf{k}}V_{i\mathbf{k}}^{*}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}\right]\mathcal{G}_{ff}(ik_n) \\
&= 1 - U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f_{i-\sigma}^{\dagger}(\tau)f_{i-\sigma}(\tau)f_{i\sigma}(\tau)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle. \qquad (49.14)
\end{aligned}$$

The last term on the right-hand side is related to the self-energy as usual by

$$\Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) \equiv -U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f_{i-\sigma}^{\dagger}(\tau)f_{i-\sigma}(\tau)f_{i\sigma}(\tau)f_{i\boldsymbol{\sigma}}^{\dagger}\right\rangle \qquad (49.15)$$

The equation to be solved has exactly the same Dyson equation structure as that which we would find for a single impurity

$$\begin{aligned}
\mathcal{G}_{ff}^{0}(ik_n)^{-1}\mathcal{G}_{ff}(ik_n) &= 1 + \Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) \qquad (49.16)\\
\mathcal{G}_{ff}(ik_n) &= \mathcal{G}_{ff}^{0}(ik_n) + \mathcal{G}_{ff}^{0}(ik_n)\Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n), \qquad (49.17)
\end{aligned}$$

except that now the "non-interacting" Green function is

$$\mathcal{G}_{ff}^{0}(ik_n)^{-1} = ik_n - (\varepsilon-\mu) - \sum_{\mathbf{k}}V_{i\mathbf{k}}^{*}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}. \qquad (49.18)$$

This is in fact exactly the non-interacting Green function that we would find with $U = 0$. One can propagate from the impurity site back to the impurity site by going through the bath. One often defines the hybridization function $\Delta_{ff}(ik_n)$ by

$$\Delta_{ff}(ik_n) = \sum_{\mathbf{k}}V_{i\mathbf{k}}^{*}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i}. \qquad (49.19)$$

The solution to this impurity problem is complicated. The structure in imaginary time is highly non-trivial. Wick's theorem does not apply to the effective impurity problem. Contrary to the atomic limit, the number of electrons on a site is not conserved, i.e. it is time-dependent, and the simplicity of the problem is lost. There is a complicated dynamics where electrons move in and out of the impurity site and what happens at a given time depends on what happened at earlier ones. For example, if there is a down electron on the impurity site, another down electron will not be able to come on the site unless the previous one comes out. The problem contains the rich Physics that goes under the name of Kondo and could be the subject of many chapters in this book. We will not for now expand further on this.

49.2 A simple example of a model exactly soluble by mean-field theory

Let us forget momentarily about quantum mechanics and consider a simpler problem of classical statistical mechanics. Mean-field theory is often taken as an approximate solution to a model. It can also be formulated as an exact solution of a different model. That helps understand the content of mean-field theory.

Mean-field theory is the exact solution of the following infinite range Ising model

$$H=-\frac{1}{2N}\left(\sum_{i=1}^{N}S_i\right)^2-h\sum_i S_i. \tag{49.20}$$

with $S_i=\pm1$. We have chosen the exchange $J=1$. The range of the interaction is extremely weak in the thermodynamic limit. The $1/N$ normalisation is necessary to have an energy that is extensive, i.e. proportional to the number of sites. In the usual Ising model, a given site interacts only with its neighbors so the energy is clearly extensive.

To compute the partition function, we use the Hubbard-Stratonovich transformation that represents $e^{-\beta H}$ as a Gaussian integral

$$e^{\left[\frac{\beta}{2N}\left(\sum_{i=1}^{N}S_i\right)^2+\beta h\sum_i S_i\right]}=\left(\frac{N\beta}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}d\lambda e^{\left[-\frac{\beta N}{2}\lambda^2+\beta(\lambda+h)\sum_i S_i\right]}. \tag{49.21}$$

The result can be checked by completing the square. Then, the partition function can be computed easily

$$\begin{aligned}
Z &= \sum_{\{S_i\}}e^{-\beta H}\\
&= \left(\frac{N\beta}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}d\lambda e^{-\frac{\beta N}{2}\lambda^2}\left[2\cosh\left(\beta\left(\lambda+h\right)\right)\right]^N\\
&= \left(\frac{N\beta}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}d\lambda e^{-N\beta F(\lambda)} \qquad (49.22)
\end{aligned}$$

where

$$F\left(\lambda\right)=\frac{\lambda^2}{2}-\frac{1}{\beta}\ln\left[2\cosh\left(\beta\left(\lambda+h\right)\right)\right]. \tag{49.23}$$

Because $N\rightarrow\infty$, we can evaluate the integral by steepest descent and the free energy per site is given by

$$f\left(h\right)=\min_{\lambda}F\left(\lambda\right)+O\left(\frac{1}{N}\right). \tag{49.24}$$

The value of λ which minimizes F has the meaning of magnetization density. Indeed, $\partial F/\partial\lambda = 0$ leads to

$$\lambda = \tanh[\beta(\lambda + h)] \tag{49.25}$$

and using the previous result,

$$m = \left(\frac{\partial F}{\partial h}\right)_\lambda = \tanh[\beta(\lambda + h)] = \lambda. \tag{49.26}$$

This is what is found in mean-field theory.

49.3 The self-energy is independent of momentum in infinite dimension

It took a long time to find a variant of the Hubbard model that could be solved by a mean-field theory. That the Hubbard model was exactly soluble in infinite dimension was discovered by Metzner and Vollhardt. Kotliar and George and Jarrell found that is was possible to formulate a mean-field theory based on these ideas. The key result is that in infinite dimension, the self-energy depends only on frequency.

First we need to formulate the Hubbard model in such a way that in infinite dimension it gives a non-trivial and physical result, somewhat in the way that we did for the Ising model above. The possibly troublesome term is the kinetic energy. Consider the value of $\left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle$ for nearest neighbors. In the ground state, that quantity can be interpreted as the matrix element $\langle\psi_{i\sigma}\left|\psi_{j\sigma}\right\rangle$ where $\left|\psi_{j\sigma}\right\rangle$ is the ground state with one less particle at site j and $\langle\psi_{i\sigma}|$ the ground state where we add a particle at site i. Hence $\left|\langle\psi_{i\sigma}\left|\psi_{j\sigma}\right\rangle\right|^2$ is the probability for a particle to go from j to i. It has to scale like $1/d$ if we want particle-number to be conserved. This means that $\left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle$ scales as $1/\sqrt{d}$ so if we want a finite number for the kinetic energy, we need to multiply t by $\sqrt{d}$. Taking into account that there are Z neighbors, with $Z = 2d$ for a hypercubic lattice, we need an additional factor of $1/d$. The kinetic energy in the end is thus written as

$$E_{kin} = -\left(t^*\sqrt{d}\right)\frac{1}{d}\sum_{\langle i,j\rangle}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right). \tag{49.27}$$

The interaction term does not need to be scaled since it is local. The quantity $t^*/\sqrt{d}$ thus plays the role of the usual t entering the kinetic energy, with t^* finite in the $d \to \infty$ limit

We can find the same result by requiring that the bandwidth remains finite in the infinite dimensional limit. Consider the single-particle density of states

$$N(\omega) = \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\dots\int_{-\pi}^{\pi}\frac{dk_d}{2\pi}\delta(\omega - \varepsilon_1 - \varepsilon_2 - \dots\varepsilon_d) \tag{49.28}$$

with $\varepsilon_i = -2t\cos k_i$. This has the structure of a probability density for a variable that is the sum of identically distributed statistically independent variables. One can make the change of variables from $P(k_i) = 1/(2\pi)$ to $P(\varepsilon_i)$ so that

$$N(\omega) = \int d\varepsilon_1\int d\varepsilon_2\dots\int d\varepsilon_d P(\varepsilon_1)P(\varepsilon_2)\dots P(\varepsilon_d)\,\delta(\omega - \varepsilon_1 - \varepsilon_2 - \dots\varepsilon_d). \tag{49.29}$$

The resulting probability density is a Gaussian with mean zero since $\int d\varepsilon_1 P(\varepsilon_1)\varepsilon_1 = 0$ and variance $2t^2 d$ because $\int d\varepsilon_1 P(\varepsilon_1)\varepsilon_1^2 = \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}(2t\cos(k_1))^2 = (2t)^2/2$. More specifically,

$$N(\omega) = \frac{1}{\sqrt{\pi (2t)^2 d}}\exp\left[-\left(\frac{\omega}{2t\sqrt{d}}\right)^2\right]. \tag{49.30}$$

This means that in the limit $d \to \infty$, we need to choose

$$t = t^*/\sqrt{d}$$

with t^* finite if we want a density of states with a finite width in that limit. In the same way that we had to take an effective exchange interaction smaller in our Ising model example, here we need to take an effective hopping that is smaller, $t^*/\sqrt{d}$, in the infinite dimensional limit.

The fact that $\left\langle c_{i\sigma}^\dagger c_{j\sigma}\right\rangle$ scales as $1/\sqrt{d}$ in the $d \to \infty$ limit has important consequences on the self energy. Indeed, $\mathcal{G}$ will also scale as $1/\sqrt{d}$. Hence, if we consider the real space expression for Σ_{12} where 1 and 2 are near-neighbor sites, then apart from the Hartree-Fock term that arises in first order perturbation theoty, we find from second order that the contribution is proportional to $\mathcal{G}_{1,2}^3$ which is proportional to $1/d^{3/2}$. There is an additional factor $1/\sqrt{d}$ in the Green's function every time the distance increases by one so Σ_{ij} for more distant ij is even smaller. In the end, this means that the self-energy depends only on frequency.

49.4 The dynamical mean-field self-consistency relation

Since the self-energy depends only on frequency, the Green's function on the infinite lattice reads in Fourier-Matsubara space

$$\mathcal{G}(\mathbf{k}, ik_n) = \frac{1}{ik_n - \varepsilon_{\mathbf{k}} - \Sigma(ik_n)}. \tag{49.31}$$

The Green's function in real space, on the same lattice site, is obtained from Fourier transformation

$$\begin{aligned}
\mathcal{G}_{ii}(ik_n) &= \int \frac{d^d\mathbf{k}}{(2\pi)^d}\frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu) - \Sigma(ik_n)} \\
&= \int \frac{d^d\mathbf{k}}{(2\pi)^d}\int d\varepsilon\,\delta(\varepsilon - (\varepsilon_{\mathbf{k}} - \mu))\frac{1}{ik_n - \varepsilon - \Sigma(ik_n)} \\
&= \int d\varepsilon N(\varepsilon)\frac{1}{ik_n - \varepsilon - \Sigma(ik_n)}.
\end{aligned} \tag{49.32}$$

We give more detailed justification in a later chapter, but for now, we just ask that this result be the same as that obtained for a single site in the presence of a bath. In other words, we assume that the influence of the rest of the lattice is to transfer electrons in and out of the lattice site. But we know that for a single site in a bath,

$$\mathcal{G}_{ii}^{-1}(ik_n) = \left(\mathcal{G}_{ii}^0(ik_n)\right)^{-1} - \Sigma(ik_n). \tag{49.33}$$

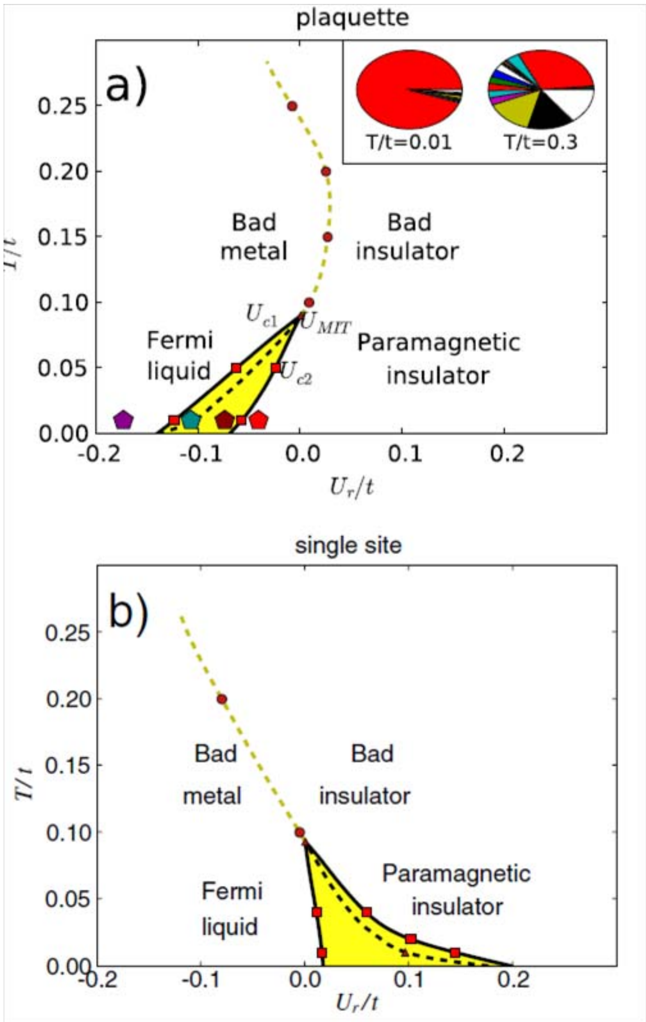

Figure 49-3 First order transition for the Mott transition. (a) shows the result fro two dimensions obtained for a 2×2 plaquette in a bath. In (b), the result obtained for a single site. The horizontal axis is $U_r = (U - U_{MIT})/U_{MIT}$ with $U_{MIT} = 6.05t$ in the plaquette case and $U = 9.35t$ in the single site case.

So we solve the problem iteratively as follows. Take a $\left(\mathcal{G}^0_{ii}(ik_n)\right)^{-1}$ and compute $\Sigma(ik_n)$ for the single-site Anderson impurity problem. Substitute that self-energy in the expression for the infinite lattice Green's function and ask that the projected Green's function found from Eq.(49.32) be equal to the impurity Green's function Eq.(49.33). If this is not the case, change $\mathcal{G}^0_{ii}(ik_n)$ until the condition is satisfied. The difficult part of the problem resides in finding the solution of the impurity problem. There are a number of methods to do that. So usually, it is not enough to say that one is working with dynamical mean-field theory. One also has to specify the "impurity solver".

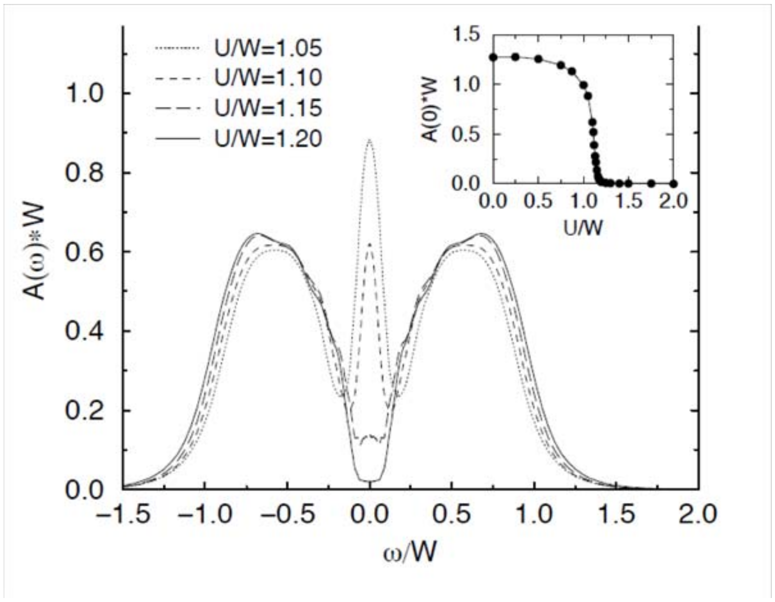

Figure 49-4 decrease for U 1:1 W; from Ref. [78] in Vollhardt in Mancini.

49.5 The Mott transition

Clausius-Clapeyron

$$dE = TdS + \mu dN + DdU \tag{49.34}$$

$$d(E - TS - \mu N) = -SdT - Nd\mu + DdU \tag{49.35}$$

Set $d\mu = 0$,then along the phase boundary

$$-S_M dT_c + D_M dU_c = -S_I dT_c + D_I dU_c. \tag{49.36}$$

Hence

$$\frac{dT_c}{dU_c} = \frac{D_I - D_M}{S_I - S_M} \tag{49.37}$$

49.6 Doped Mott insulators

$$\frac{dT_c}{d\mu_c} = \frac{n_{\mathrm{UD}} - n_{\mathrm{OD}}}{S_{\mathrm{OD}} - S_{\mathrm{UD}}}. \tag{49.38}$$

The calculation shows that T_c increases as μ_c increases (i.e. the first-order line bends toward the Mott insulator). This implies that the UD phase has a lower entropy than the OD phase. In an analogous way, by taking a constant T plane, one obtains

$$\frac{dU_c}{d\mu_c} = \frac{n_{\mathrm{UD}} - n_{\mathrm{OD}}}{D_{\mathrm{UD}} - D_{\mathrm{OD}}}. \tag{49.39}$$

The calculations show that μ_c decreases as U_c increases. Hence, the UD phase has lower double occupancy than the OD phase. This is as expected and suggests again that in the UD phase the correlations are stronger.

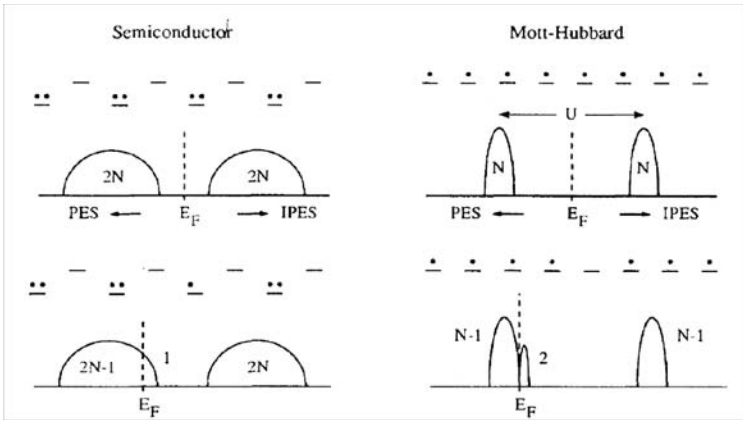

Figure 49-5

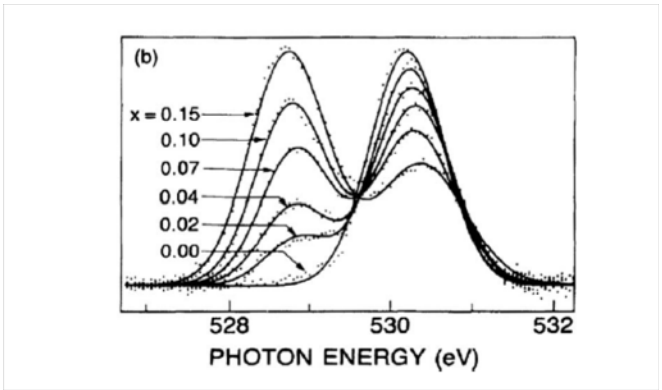

Figure 49-6

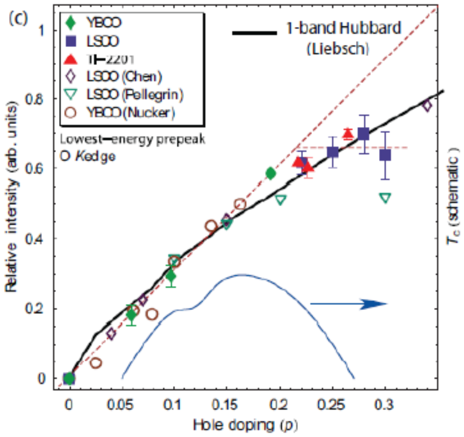

Figure 49-7

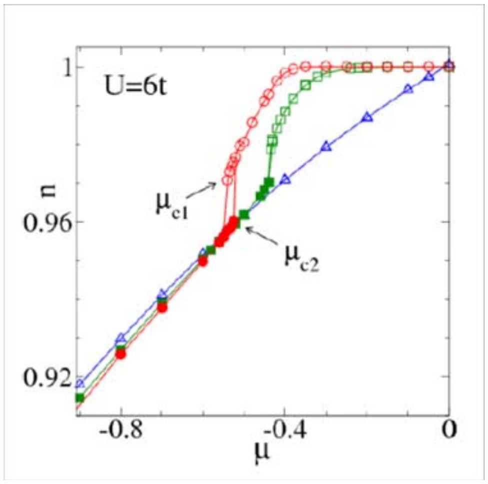

Figure 49-8

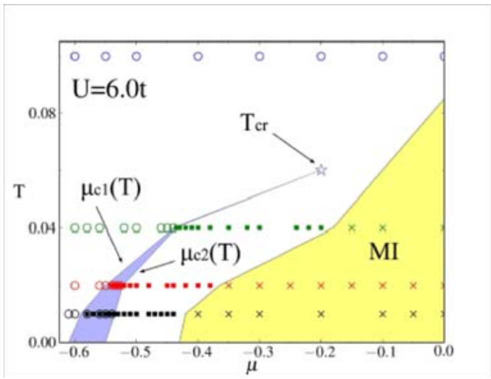

Figure 49-9

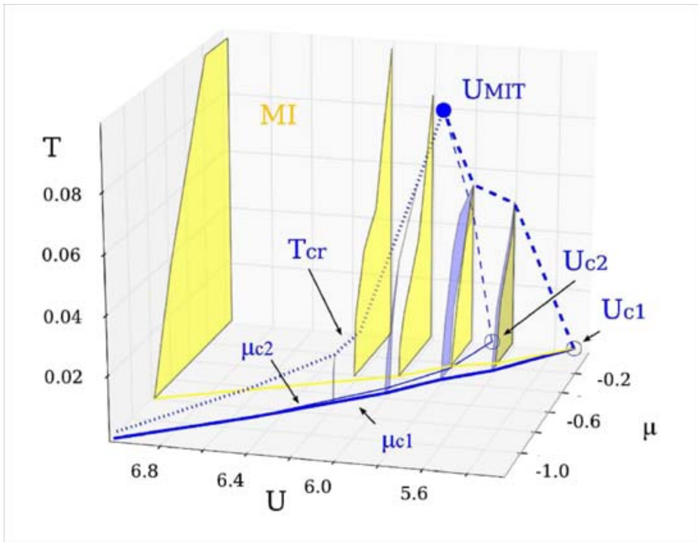

Figure 49-10

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Part VII

Broken Symmetry

From now on, these are very sketchy notes that will evolve towards a more structured text with time.

In this chapter we encounter the limits of our first principle of *adiabatic continuity,* mentioned in the introduction. That principle is in competition with another one. Indeed. interactions may lead to divergent perturbation theory that cannot be resummed in any way. This breakdown reflects a deep fact of nature, that interactions may lead to new phases of matter, and these phases may be characterized sometimes by broken symmetries. This is the principle of *broken symmetry.* It is a principle because it is an empirically observed fact of very broad applicability. We will see how it arises in the simplest manner in a model of ferromagnetism proposed many years ago by Stoner. Original ideas go back to Weiss. This will allow us to develop most of the concepts and approaches we will need to study superconductivity. One of the lessons of this chapter will be that it is impossible to reach a broken symmetry phase from the phase without the broken symmetry by using perturbation theory. And vice-versa. The transition point, whether as a function of interaction strength or as a function of temperature, is a singularity. Our main example will be ferromagnetism. At the end of the chapter we will touch upon many problems of mean-field theories.

50. 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.

50.1 Simple arguments, the Stoner model

In the Hartree Fock approximation,

$$\widetilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + U\left\langle n_{-\sigma}\right\rangle \tag{50.1}$$

The idea of Stoner, illustrated in Figs.() and () for two and three dimensions, is best illustrated in the limiting case where U is very large. Then by taking all the spins to be up, one increases the kinetic energy, but there is no potential energy. Clearly, if U is large enough (Nagaoka ferromagnetism) it seems that this will always be the lowest energy solution since the kinetic energy is the same whatever the value of U .

The above solution breaks the rotational symmetry of the original Hamiltonian, yet it is a lower energy state. The proper way to consider this problem is to put an infinitesimal magnetic field pointing in one direction in the original Hamiltonian, then take the infinite volume limit, then take the field to zero. In pratical situations, this is how symmetry is broken anyway.

At the threshold for the instability, when the two wave vectors become different, the energies for up and down spins are still identical, so

$$\varepsilon_{\mathbf{k}_F\uparrow} - \varepsilon_{\mathbf{k}_{F\downarrow}} = U\left(\left\langle n_\downarrow\right\rangle - \left\langle n_{F\uparrow}\right\rangle\right). \tag{50.2}$$

Expanding the left-hand side in powers of $\left\langle n_\downarrow\right\rangle - \left\langle n_\uparrow\right\rangle$ we have, using that $\frac{\partial\varepsilon_{k_{F\sigma}}}{\partial k_{F\sigma}}\frac{\partial k_{F\sigma}}{\partial n_\sigma}$ is independent of spin,

$$\begin{aligned}
\frac{\partial\varepsilon_{k_F}}{\partial k_F}\frac{\partial k_F}{\partial n}\left(\left\langle n_\downarrow\right\rangle - \left\langle n_\uparrow\right\rangle\right) &= U\left(\left\langle n_\downarrow\right\rangle - \left\langle n_{F\uparrow}\right\rangle\right) &(50.3)\\
\frac{\partial\varepsilon_{k_F}}{\partial n} &= U &(50.4)\\
1 &= U\frac{\partial n}{\partial\varepsilon_{k_F}} = U\frac{\partial}{\partial\varepsilon_{k_F}}\int^{\varepsilon_{k_F}} N\left(\varepsilon\right)d\varepsilon &(50.5)\\
1 &= UN\left(\varepsilon_{k_F}\right) &(50.6)
\end{aligned}$$

where $N(E)$ is the density of states for a given spin species. The last formula is the celebrated Stoner criterion for antiferromagnetism.

50.2 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

$$|\Psi\rangle = \Pi_{\mathbf{k}\uparrow}\theta\left(k_{F\uparrow} - |\mathbf{k}|\right)\Pi_{\mathbf{k}\downarrow}\theta\left(k_{F\downarrow} - |\mathbf{k}|\right)c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}_{\downarrow}}|0\rangle . \tag{50.7}$$

Using Ritz's variational principle, we need to minimize

$$\langle\Psi| H - \mu N |\Psi\rangle = \sum_{\mathbf{k},\boldsymbol{\sigma}}(\varepsilon_{\mathbf{k}} - \mu)\langle n_{\mathbf{k},\boldsymbol{\sigma}}\rangle + NU\langle n_{-\sigma}\rangle\langle n_{\sigma}\rangle . \tag{50.8}$$

We will not proceed further since this is a special case ($T = 0$) of the more general equations treated in the following section.

50.3 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

$$\begin{aligned}
\widetilde{H}_0 &= \sum_{\mathbf{k},\boldsymbol{\sigma}}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + U\sum_i\left(\langle n_{i\uparrow}\rangle n_{i\downarrow} + \langle n_{i\downarrow}\rangle n_{i\uparrow}\right) && (50.9)\\
&= \sum_{\mathbf{k},\boldsymbol{\sigma}}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + U\sum_{\mathbf{k}}\left(\langle n_{\uparrow}\rangle c^{\dagger}_{\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow} + \langle n_{\downarrow}\rangle c^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}\right) && (50.10)
\end{aligned}$$

In other words, it is as if we had written in the interaction term $n_{i\uparrow} \to \langle n_{i\uparrow}\rangle + \delta n_{i\uparrow}$ and neglected the terms quadratic in δn_i (with at the end $\delta n_{i\uparrow} \to n_{i\uparrow}$).

The calculation then proceeds as usual by using Feynman's variational principle

$$-T\ln Z \leq -T\ln Z_{\widetilde{0}} + \left\langle\left(H - \widetilde{H}_0\right)\right\rangle_{\widetilde{0}} \tag{50.11}$$

to minimize the right-hand side, which can be written, using the usual definition $\zeta_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$

$$\begin{aligned}
&-T\ln\left[\prod_{\mathbf{k}}\left(1 + e^{-\beta(\zeta_{\mathbf{k}} + U\langle n_{\uparrow}\rangle)}\right)\left(1 + e^{-\beta(\zeta_{\mathbf{k}} + U\langle\langle n_{\downarrow}\rangle\rangle)}\right)\right]\\
&+UN\langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle - 2UN\langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle . && (50.12)
\end{aligned}$$

Defining

$$n = \langle n_{\uparrow}\rangle + \langle n_{\downarrow}\rangle \tag{50.13}$$

and the “order parameter”

$$m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle \tag{50.14}$$

that measures the magnetization, or spin polarization, we set the derivative with respect of m equalt to zero to obtain the extremum. This leads to

$$\sum_\sigma \left\{ \left[-T \sum_{\mathbf{k}} \frac{e^{-\beta(\zeta_{\mathbf{k}}+U\langle n_{-\sigma}\rangle)}}{1+e^{-\beta(\zeta_{\mathbf{k}}+U\langle n_{-\sigma}\rangle)}} \left(\beta U \frac{\partial \langle n_{-\sigma}\rangle}{\partial m} \right) \right] - UN \left(\frac{\partial \langle n_\sigma \rangle}{\partial m} \langle n_{-\sigma}\rangle \right) \right\} = 0 \tag{50.15}$$

which, using the derfinition of the magnetization Eq.(50.14) and of the Fermi function, can be written

$$-\sum_{\mathbf{k}} f\left(\zeta_{\mathbf{k}} + U\left\langle n_\downarrow \right\rangle\right) + \sum_{\mathbf{k}} f\left(\zeta_{\mathbf{k}} + U\langle n_\uparrow \rangle\right) - N\langle n_\downarrow \rangle + N\langle n_\uparrow \rangle = 0. \tag{50.16}$$

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

$$\langle n_\downarrow \rangle + \langle n_\uparrow \rangle = \frac{1}{N} \sum_{\mathbf{k}} \left(f\left(\zeta_{\mathbf{k}} + U\langle n_\uparrow\rangle\right) + f\left(\zeta_{\mathbf{k}} + U\left\langle n_\downarrow\right\rangle\right)\right). \tag{50.17}$$

50.4 The gap equation and Landau theory in the ordered state

Using our definition of the magnetization Eq.(50.14) and the equation for the minimum Eq.(50.16), we obtain an equation (also called the gap equation) for the order parameter m,

$$m = \frac{1}{N} \sum_{\mathbf{k}} \left(f\left(\zeta_{\mathbf{k}} + U\frac{n}{2} - U\frac{m}{2}\right) - f\left(\zeta_{\mathbf{k}} + U\frac{n}{2} + U\frac{m}{2}\right)\right). \tag{50.18}$$

Suppose we are close to the transition where m is small. Expanding the right-hand side, we have

$$\begin{aligned} m &= \frac{1}{N} \sum_{\mathbf{k}} \frac{\partial f(\zeta_{\mathbf{k}})}{\partial \zeta_{\mathbf{k}}} (-Um) + O\left(m^3\right) && (50.19) \\ &= UN\left(\varepsilon_{k_F}\right) m + O\left(m^3\right), && (50.20) \end{aligned}$$

where we have used that as $T \to 0$ the derivative of the Fermi function becomes minus a delta function.

The last equation may also be written

$$\left(1 - UN\left(\varepsilon_{k_F}\right)\right) m = bm^3 \tag{50.21}$$

where a more detailed calculation gives that

$$b = \frac{N''\left(\varepsilon_{k_F}\right)}{24} - \frac{\left(N'\left(\varepsilon_{k_F}\right)\right)^2}{8N\left(\varepsilon_{k_F}\right)}. \tag{50.22}$$

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.(50.21) 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.(50.21)? 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 151 *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.(50.19) is temperature dependent. In Eq.(50.20) we have taken the zero temperature limit.*

50.5 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 $\widetilde{H}_0$ is spin dependent

$$\widetilde{H}_0 = \sum_{\mathbf{k},\boldsymbol{\sigma}} \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \tag{50.23}$$

Starting from the diagrams in Fig.(39-2) and recalling that only the Hartree diagram survives because up electrons interact only with down, the effective medium equations are obtained for each spin component

$$\widetilde{\Sigma}_{\sigma} = U\langle n_{-\sigma}\rangle + \varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} = 0 \tag{50.24}$$

so that we recover the Stoner result $\widetilde{\varepsilon}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} + U\langle n_{-\sigma}\rangle$. The gap equation is obtained from

$$G_{\sigma}(\mathbf{k}, ik_n) = \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} + \mu} \tag{50.25}$$

from which we extract the spin-dependent density

$$\begin{aligned} \langle n_\sigma \rangle &= T \sum_n e^{ik_n \eta} \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} + \mu} \qquad (50.26) \\ &= \frac{1}{N} \sum_{\mathbf{k}} f\left(\varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle - \mu\right). \qquad (50.27) \end{aligned}$$

Adding the previous equations to $\langle n_\downarrow \rangle + \langle n_\uparrow \rangle$, we recover all the previous results for the magnetization etc.

51. 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

$$\begin{aligned}
\left.\frac{\partial\left\langle S_z\right\rangle}{\beta\partial h}\right|_{h=0} &= \left.\frac{\partial}{\beta\partial h}\frac{\operatorname{Tr}\left[e^{-\beta(K-hS_z)}S_z\right]}{\operatorname{Tr}\left[e^{-\beta(K-hS_z)}\right]}\right|_{h=0} &(51.1)\\
&= \left\langle S_zS_z\right\rangle-\left\langle S_z\right\rangle\left\langle S_z\right\rangle\equiv\left\langle S_zS_z\right\rangle_c. &(51.2)
\end{aligned}$$

51.1 The noninteracting limit and rotational invariance

The spin susceptibility is obtained from the spin-spin correlation function. Very schematically, consider the connected part of the time-ordered product,

$$\begin{aligned}
\left\langle T_\tau S_zS_z\right\rangle_c &= \left\langle T_\tau\left(n_\uparrow-n_\downarrow\right)\left(n_\uparrow-n_\downarrow\right)\right\rangle_c &(51.3)\\
&= \left\langle T_\tau n_\uparrow n_\uparrow\right\rangle_c+\left\langle T_\tau n_\downarrow n_\downarrow\right\rangle_c-\left\langle T_\tau n_\uparrow n_\downarrow\right\rangle_c-\left\langle T_\tau n_\downarrow n_\uparrow\right\rangle_c &(51.4)
\end{aligned}$$

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

$$\begin{aligned}
\left\langle T_\tau\rho\rho\right\rangle_c &= \left\langle T_\tau\left(n_\uparrow+n_\downarrow\right)\left(n_\uparrow+n_\downarrow\right)\right\rangle_c &(51.5)\\
&= \left\langle T_\tau n_\uparrow n_\uparrow\right\rangle_c+\left\langle T_\tau n_\downarrow n_\downarrow\right\rangle_c+\left\langle T_\tau n_\uparrow n_\downarrow\right\rangle_c+\left\langle T_\tau n_\downarrow n_\uparrow\right\rangle_c. &(51.6)
\end{aligned}$$

Since the last two terms do not contribute, we are left for both spin and charge with

$$\begin{aligned}
\chi_0\left(\mathbf{q},iq_n\right) &= -\frac{1}{N}\sum_{\mathbf{p},\sigma}T\sum_n G_\sigma^0\left(\mathbf{p}+\mathbf{q},ip_n+iq_n\right)G_\sigma^0\left(\mathbf{p},ip_n\right) &(51.7)\\
&= -\frac{2}{N}\sum_{\mathbf{p}}\frac{f\left(\zeta_{\mathbf{p}}\right)-f\left(\zeta_{\mathbf{p}+\mathbf{q}}\right)}{iq_n+\zeta_{\mathbf{p}}-\zeta_{\mathbf{p}+\mathbf{q}}}. &(51.8)
\end{aligned}$$

Rotational invariance should give us in general, ven in the presence of interactions,

$$\begin{aligned}\left\langle T_\tau S^+S^-\right\rangle_c+\left\langle T_\tau S^-S^+\right\rangle_c &= \frac{1}{4}\left\langle T_\tau\left(S_x+iS_y\right)\left(S_x-iS_y\right)\right\rangle_c &(51.9)\\ &+\frac{1}{4}\left\langle T_\tau\left(S_x-iS_y\right)\left(S_x+iS_y\right)\right\rangle_c &(51.10)\\ &= \frac{1}{2}\left(\left\langle T_\tau S_xS_x\right\rangle_c+\left\langle T_\tau S_yS_y\right\rangle_c\right)\\ &= \left\langle T_\tau S_zS_z\right\rangle_c . &(51.11)\end{aligned}$$

This comes out indeed from considering the diagrams in Fig.(). At the outer vertices, the spin must now flip as indicated because of the presence of the operators S^+S^-.

51.2 Effect of interactions, the Feynman way

You can read the next section immediatly if you have read the previous part.

In the Hubbard model, we took into account the Pauli principle so that up electrons interact only with down electrons. If we return to the original problem where up can interact with down, we need to sum at the same time ladders and bubbles in the way indicated in Fig.(?) to recover rotational invariance in an RPA-like approximation. Since the interaction U is independent of momentum, the two diagrams in Fig.(?a) cancel each other exactly and we are left only with Fig.(?b) which corresponds to the theory where up interacts only with down.

In that theory, the set of diagrams that contributes to $\left\langle T_\tau S_zS_z\right\rangle_c$ is given in Fig.(?). It is different from the set of diagrams that contributes to $\left\langle T_\tau S^+S^-\right\rangle_c+\left\langle T_\tau S^-S^+\right\rangle_c$ but the final answer is the same in the paramgnetic state with no broken symmetry. Bubbles only contribute to $\left\langle T_\tau S_zS_z\right\rangle_c$ but the odd terms have one extra minus sign because the minus sign in $-\left\langle T_\tau n_\uparrow n_\downarrow\right\rangle_c-\left\langle T_\tau n_\downarrow n_\uparrow\right\rangle_c$. Hence, the result is exacly the same as for $\left\langle T_\tau S^+S^-\right\rangle_c+\left\langle T_\tau S^-S^+\right\rangle_c$ that we compute with the ladder sum in Fig.(?). Consider for example $\left\langle T_\tau S^+S^-\right\rangle_c$. There is one minus sign for each order in perturbation theory, hence a factor $(-U)$ and since there are no extra fermion loops included and U is momentum independent, it is the quantity $-\chi_0/2$ that is multiplied when we increase the order by one. More specifically, we obtain

$$\begin{aligned}\left\langle T_\tau S^+S^-\right\rangle_c &= \frac{\chi_0}{2}+\frac{\chi_0}{2}(-U)\left(-\frac{\chi_0}{2}\right)+\frac{\chi_0}{2}(-U)^2\left(-\frac{\chi_0}{2}\right)^2+\ldots &(51.12)\\ &= \frac{\chi_0/2}{1-\frac{U}{2}\chi_0}. &(51.13)\end{aligned}$$

We thus obtain in Fourier space where the above equation is algebraic,

$$\chi=\left\langle T_\tau S^+S^-\right\rangle_c+\left\langle T_\tau S^-S^+\right\rangle_c=\left\langle T_\tau S_zS_z\right\rangle_c=\frac{\chi_0}{1-\frac{U}{2}\chi_0}. \qquad (51.14)$$

At finite frequency, a retarded response function can be positive or negative because of resonnances. 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

$$\begin{aligned}\chi(\mathbf{q},iq_n) &= \int\frac{d\omega}{\pi}\frac{\chi''(\mathbf{q},\omega)}{\omega-iq_n}\\ &= \int\frac{d\omega}{\pi}\frac{\omega\chi''(\mathbf{q},\omega)}{(\omega)^2+(q_n)^2} &(51.15)\end{aligned}$$

hence *a fortiori* $\chi(\mathbf{q},0)$ is positive. Hence, the RPA result Eq.(51.14) is non-physical when $1<\frac{U}{2}\chi_0(\mathbf{q},0)$. There is a phase transition when the generalized Stoner criterion

$$\boxed{1=\frac{U}{2}\chi_0(\mathbf{q},0)} \tag{51.16}$$

is satisfied. Note that the first wave vector for which the above result is satisfied is the one that becomes unstable. It does not necessarily correspond to a uniform ferromagnet ($\mathbf{q}=\mathbf{0}$). We will see a specific example below with the antiferromagnet. In the special ferromagnetic case

$$\lim_{\mathbf{q}\to\mathbf{0}}\chi_0(\mathbf{q},0)=\lim_{\mathbf{q}\to\mathbf{0}}-\frac{2}{N}\sum_{\mathbf{p}}\frac{f(\zeta_{\mathbf{p}})-f(\zeta_{\mathbf{p}+\mathbf{q}})}{\zeta_{\mathbf{p}}-\zeta_{\mathbf{p}+\mathbf{q}}}=-\frac{2}{N}\sum_{\mathbf{p}}\frac{\partial f(\zeta_{\mathbf{p}})}{\partial\zeta_{\mathbf{p}}} \tag{51.17}$$

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.(50.6).

51.3 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

$$\chi(\mathbf{q},0)\approx\frac{\chi_0(\mathbf{0},0)}{1-\frac{U}{2}\chi_0(\mathbf{q},0)-\left(\frac{U}{2}\right)^2\frac{\partial^2\chi_0(\mathbf{q},0)}{\partial^2q^2}q^2}\sim\frac{A}{\xi^{-2}+q^2} \tag{51.18}$$

which shows an exponential decrease in real space with correlation length $\xi^{-2}\sim 1-\frac{U}{2}\chi_0(\mathbf{q},0)$. The above functional form is known by the name of Ornstein-Zernicke. At the transition point, the system becomes "critical". The transition point itself is called a critical point. The presence of this long correlation length also manifests itself in the existence of "critical slowing down". In the present case, we will discover an overdamped collective mode whose typical frequency decreases as we approach the critical point.

Consider for example, the zero temperature transverse magnetic structure factor

$$S_\perp(\mathbf{q},\omega)=\frac{2}{1-e^{-\beta\omega}}\chi_\perp''(\mathbf{q},\omega). \tag{51.19}$$

In the paramagnetic state there is rotational invariance so there is in fact no difference between longitudinal and transverse. We see that $T=0$, $S_\perp(\mathbf{q},\omega)=2\chi_\perp''(\mathbf{q},\omega)$ for $\omega>0$. The RPA prediction is thus,

$$S_\perp(\mathbf{q},\omega)=2\,\mathrm{Im}\left[\frac{\chi_0^R}{1-\frac{U}{2}\chi_0^R}\right]=\frac{2\chi_0''(\mathbf{q},\omega)}{\left(1-\frac{U}{2}\chi_0'(\mathbf{q},\omega)\right)^2+\left(\frac{U}{2}\chi_0''(\mathbf{q},\omega)\right)^2} \tag{51.20}$$

$$\approx\frac{2\chi_0''(\mathbf{q},\omega)}{\left(1-UN(\varepsilon_{k_F})\right)^2+\left(\frac{U}{2}\chi_0''(\mathbf{q},\omega)\right)^2}. \tag{51.21}$$

To evaluate $\chi_0''(\mathbf{q},\omega)$, it suffices to analytically continue our general result for the non-interacting spin susceptibility Eq.(51.8) in the small $\mathbf{q}$ limit

$$\begin{aligned}
\chi_0^R(\mathbf{q},\omega) &= -\frac{2}{N}\sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} && (51.22)\\
&\approx -\frac{2}{N}\sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \frac{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} && (51.23)
\end{aligned}$$

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 $\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}} \approx -\mathbf{v}_F \cdot \mathbf{q}$

$$\chi_0^R(\mathbf{q},\omega) = 2\int d\varepsilon N(\varepsilon) \int_{-1}^{1} \frac{d(\cos\theta)}{2} \frac{\partial f(\varepsilon-\mu)}{\partial \varepsilon} \frac{v_F q\cos\theta}{\omega + i\eta - v_F q\cos\theta} \qquad (51.24)$$

$$\begin{aligned}
\chi_0''(\mathbf{q},\omega) &= -2\pi \int d\varepsilon N(\varepsilon) \int_{-1}^{1} \frac{d(\cos\theta)}{2} \frac{\partial f(\varepsilon-\mu)}{\partial \varepsilon} v_f q\cos(\theta)\,\delta(\omega - v_F q\cos\theta) && (51.25)\\
&= \pi N(\varepsilon_{k_F}) \frac{\omega}{v_F q} \equiv C\frac{\omega}{v_F q} && (51.26)
\end{aligned}$$

Substituting in the RPA expression Eq.(51.20) we find

$$S_\perp(\mathbf{q},\omega) = 2\chi_\perp''(\mathbf{q},\omega) = \frac{2C\frac{\omega}{v_F q}}{(1 - UN(\varepsilon_{k_F}))^2 + \left(C\frac{\omega}{v_F q}\right)^2}. \qquad (51.27)$$

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

$$\chi_\perp(\mathbf{q},\omega) = \frac{A}{\xi^{-2} + aq^2 + bh^{2/3} - c\frac{i\omega}{v_F q}}. \qquad (51.28)$$

51.4 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 colletive 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 smalll by continuity.

51.4.1 Tranverse susceptibility

The longitudinal susceptibility is always gapped in the ordered state since it corresponds to changing the magnetization. The transverse susceptibility on the other hand is given by a RPA formula analogous to above Eq.(51.14). Being careful that $\chi_{\perp}^{R-+}(\mathbf{q},\omega) \equiv \langle T_\tau S^+ S^- \rangle_c$ has one less factor of two in its definition we find,

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \tag{51.29}$$

with, given the new excitation spectrum in the ordered state, a new definition of the "non-interacting" susceptibility $\chi_{0\perp}^{R-+}(\mathbf{q},\omega)$

$$\chi_{0\perp}^{R-+}(\mathbf{q},\omega) = -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p+q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta + \widetilde{\zeta}_{\mathbf{p+q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow}}. \tag{51.30}$$

that corresponds to the diagram in Fig.(?). Expanding as before in the small $\mathbf{q}$ limit, we have for small wave vector

$$\widetilde{\zeta}_{\mathbf{p+q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow} \approx \mathbf{v}_F \cdot \mathbf{q} + U\left(\langle n_\downarrow\rangle - \langle n_\uparrow\rangle\right) = \mathbf{v}_F \cdot \mathbf{q} - \Delta \tag{51.31}$$

so that for $\mathbf{v}_F \cdot \mathbf{q} \ll \Delta$ we can expand,

$$\begin{aligned}
\chi_{0\perp}^{R-+}(\mathbf{q},\omega) &\approx -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p+q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta - \Delta} \\
&\quad \times \left[1 - \frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F \cdot \mathbf{q}}{\omega + i\eta - \Delta}\right)^2 + \cdots\right] && (51.32) \\
&\approx -\frac{\left(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle\right)}{\omega + i\eta - \Delta}\left(1 + O\left(q^2\right)\right) = \frac{-\Delta/U}{\omega + i\eta - \Delta}\left[1 + \frac{C}{(\omega + i\eta - \Delta)^2} q^2\right] && (51.33)
\end{aligned}$$

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 $|\omega| < \Delta$

$$\begin{aligned}
\chi_{\perp}^{R-+}(\mathbf{q},\omega) &= \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \approx \frac{\frac{-\Delta/U}{\omega + i\eta - \Delta}}{1 - \frac{-\Delta}{\omega + i\eta - \Delta} + U\frac{C}{(\omega + i\eta - \Delta)^2} q^2} && (51.34) \\
&\approx \frac{-\Delta/U}{\omega + i\eta - Dq^2}. && (51.35)
\end{aligned}$$

The complete transverse spin susceptibility is obtained by combining the two results

$$\begin{aligned}\chi_{\perp}^{R-+}(\mathbf{q},\omega)+\chi_{\perp}^{R+-}(\mathbf{q},\omega) &= \frac{-\Delta/U}{\omega+i\eta-Dq^{2}}+\frac{\Delta/U}{\omega+i\eta+Dq^{2}} \\ &= -\frac{\Delta}{U}\frac{2Dq^{2}}{(\omega+i\eta)^{2}-(Dq^{2})^{2}}.\end{aligned} \tag{51.36}$$

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 $D = \frac{U}{2\Delta}C$. 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

$$\operatorname{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega)+\chi_{\perp}^{R+-}(\mathbf{q},\omega)\right)=\pi\frac{\Delta}{U}\delta\left(\omega-Dq^{2}\right)-\pi\frac{\Delta}{U}\delta\left(\omega+Dq^{2}\right). \tag{51.37}$$

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 $\operatorname{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega)+\chi_{\perp}^{R+-}(\mathbf{q},\omega)\right)\omega>0$ is violated.

51.4.2 Thermodynamics and the Mermin-Wagner theorem

The thermodynamic transverse susceptibility is obtained from the usual thermodynamic sum rule (Note that $\operatorname{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega')+\chi_{\perp}^{R+-}(\mathbf{q},\omega')\right)$ is odd but not each of the terms individually).

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega=0)+\chi_{\perp}^{R+-}(\mathbf{q},\omega=0)=\int\frac{d\omega'}{\pi}\frac{\operatorname{Im}\left(\chi_{\perp}^{R-+}(\mathbf{q},\omega')+\chi_{\perp}^{R+-}(\mathbf{q},\omega')\right)}{\omega'} \tag{51.38}$$

The contribution of the Goldstone mode to that susceptibility is easy to obtain from our previous results

$$\chi_{\perp}^{R-+}(\mathbf{q},\omega=0)+\chi_{\perp}^{R+-}(\mathbf{q},\omega=0)=\frac{\Delta}{U}\frac{2}{Dq^{2}}. \tag{51.39}$$

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 $\langle S_xS_y\rangle = 0$. This means that the following quantity

$$T\sum_{iq_n}\frac{1}{N}\sum_{\mathbf{q}}\chi_{\perp}^{-+}(\mathbf{q},iq_n)\,e^{\pm iq_n\eta} \tag{51.40}$$

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.(51.35) that the spin-wave contribution to that susceptibility is

$$\chi_{\perp}^{-+}(\mathbf{q}, iq_n) = \frac{-\Delta/U}{iq_n - Dq^2}. \tag{51.41}$$

Substituting this in our previous condition and using the usual result

$$\lim_{\eta \to 0} T \sum_n \frac{e^{iq_n\eta}}{iq_n - x} = \frac{-1}{e^{\beta x} - 1} \tag{51.42}$$

for performing the sum over bosonic Matsubara frequencies, we obtain in the long wavelength limit

$$T \sum_{iq_n} \frac{1}{N} \sum_{\mathbf{q}} \frac{-\Delta/U}{iq_n - Dq^2} e^{iq_n\eta} = \frac{\Delta}{U} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^{\beta Dq^2} - 1} \tag{51.43}$$

$$\sim \frac{\Delta}{U} \int \frac{d^dq}{(2\pi)^d} \frac{T}{Dq^2} \tag{51.44}$$

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 152 *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* $\int \frac{d^dq}{(2\pi)^d} \langle S_{x\mathbf{q}} S_{x-\mathbf{q}} \rangle$ *we recover the previous result Eq.(51.44) concerning the divergence of local fluctuations in two dimensions.*

51.4.3 Kanamori-Brückner screening: Why Stoner ferromagnetism has problems

Very early on, Kanamori in the context of Solid State Physics and Brückner in the context of nuclear matter, found in the low density limit that interactions U are renormalized by quantum fluctuations. Said in a less mysterious manner, the cross section for two electrons scattering off each other should be calculated beyond the Born approximation. As we have seen in the problem of one electron scattering off and impurity in Fig.(?), in the case of only two electrons scattering off each other, summing the Born series, or the analog of the Lipmann-Schwinger equation, corresponds to summing the ladder diagrams in Fig. (?). This means that in the calculation of the diagram in Fig.(?) that contributes to the transverse spin susceptibility, we should use instead the diagram in Fig.(?). By flipping the lines, one also sees that this is identical to computing the "fan diagrams" illustrated in Fig.(?). In other words, everywhere U appears in the summationn of the ladder diagrams to compute the transverse susceptibiloity, we should instead use

$$U_{eff}(\mathbf{Q}, iQ_n) = \frac{U}{1 + U\Lambda(\mathbf{Q}, iQ_n)} \tag{51.45}$$

where Λ is given by the diagram in Fig.(?). To recover a simple momentum independent U_{eff}, we average the above expression over $\mathbf{Q}$. In addition, we assume that the $iQ_n = 0$ piece dominates. It was shown by Chen *et al.* (1991) by comparing the results of the above approximation with essentially exact quantum Monte Carlo calculations, that this is a good approximation. It does not seem to work however for the charge fluctuations.

The consequences of this effect are important. Indeed, there is a maximum value of U_{eff} given by the average of $1/\Lambda\left(\mathbf{Q},0\right)$. This gives roughly the bandwidth since physically this effect comes about from making the two-body wave function small where U is large.This is more or less like making a 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 $N\left(\varepsilon_{k_F}\right)$ is proportional to $1/W$. So at best the product $U_{eff}N\left(\varepsilon_{k_F}\right)$ can become equal to unity with difficulty at large U. In more exact calculations, one sees that ferromagnetism does not generally occur in the one-band Hubbard model, because of this effect, except perhaps in special cases where there is a Van Hove singularity in the density of states that is not located at half-filling (otherwise antiferromagnetism dominates), a possibility that arises when $t' \neq 0$. (Hankevych et al. 2004).

A more systematic way of taking these effects into account, including the charge channel and the absence of ferromagnetism unless one is close to the Van Hove singularity, is the TPSC that we introduced in the previous part.

52. ANTIFERROMAGNETISM CLOSE TO HALF-FILLING AND PSEUDOGAP IN TWO DIMENSIONS

We return to the normal state and look at the dominant instability in the half-filled case $n = 1$. In that case, the Fermi surface of the Hubbard model with nearest-neighbor hopping exhibits the phenomenon of nesting. For example, the Fermi surface in the two-dimensional case is a diamond, as illustrated in Fig. (?). All the points of the flat surfaces are connected by the same wave vector $\mathbf{Q} = (\pi, \pi)$ which leads to a very large susceptibility. Whereas at low filling the maximum susceptibility is at $q = 0$, in the present case it is a local maximum that is smaller than the maximum at $\mathbf{Q}$, as we will see.

Let us compute the spin susceptibility at that nesting wave vector. Nesting in the present case means that

$$\zeta_{\mathbf{p}+\mathbf{Q}} = -2t\left(\cos\left(k_x + \pi\right) + \cos\left(k_y + \pi\right)\right) = -\zeta_{\mathbf{p}}. \tag{52.1}$$

Using this result we find that the zero-frequency susceptibility at that wave vector $\mathbf{Q}$ is

$$\begin{aligned} \chi_0^R\left(\mathbf{Q}, 0\right) &= -\frac{2}{N}\sum_{\mathbf{p}} \frac{f\left(\zeta_{\mathbf{p}}\right) - f\left(\zeta_{\mathbf{p}+\mathbf{Q}}\right)}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{Q}}} = -\frac{2}{N}\sum_{\mathbf{p}} \frac{f\left(\zeta_{\mathbf{p}}\right) - f\left(-\zeta_{\mathbf{p}}\right)}{2\zeta_{\mathbf{p}}} & (52.2) \\ &= \frac{1}{N}\sum_{\mathbf{p}} \frac{1 - 2f\left(\zeta_{\mathbf{p}}\right)}{\zeta_{\mathbf{p}}} = \frac{1}{2}\int d\varepsilon N\left(\varepsilon\right) \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{2\varepsilon}. & (52.3) \end{aligned}$$

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 $\ln\left(W/T\right)$ where W is the bandwidth. This means that at sufficiently low temperature, the criterion $1 - \frac{U}{2}\chi_0^R\left(\mathbf{Q}, 0\right) = 0$ will always be satisfied whatever the value of U and there will be a transition to a state characterized by the wave vector $\mathbf{Q}$. This is the antiferromagnetic state where spins alternate in direction from one site to the other. In two dimensions for example, the chemical potential at $n = 1$ sits right at a logarithmic van Hove singularity in $N\left(\varepsilon\right)$ so that in fact $\chi_0^R\left(\mathbf{Q}, 0\right)$ scales like $\ln^2\left(W/T\right)$, which is larger than the single power of ln that one would obtain at $q = 0$.

When there is no nesting, like when the next-nearest neighbor hopping t' contributes, the susceptibility does not diverge at low temperature. In that case, the transition will occur only if U is large enough.

52.1 Pseudogap in the renormalized classical regime

When we compared TPSC with Quantum Monte Carlo simulations and with FLEX in Fig. 48-2 above, perhaps you noticed that at the Fermi surface, the

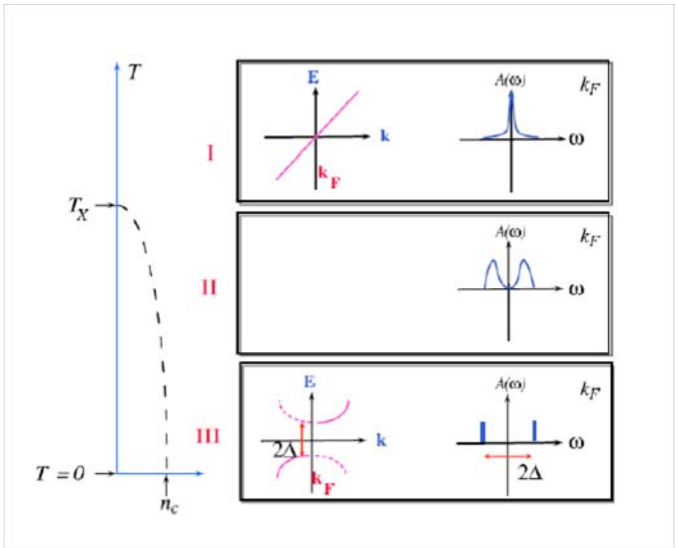

Figure 52-1 Cartoon explanation of the pseudogap due to precursors of long-range order. When the antiferromagnetic correlation length ξ becomes larger than the thermal de Broglie wavelength, there appears precursors of the $T=0$ Bogoliubov quasi-particles for the long-range ordered antiferromagnet. This can occur only in the renormalized classical regime, below the dashed line on the left of the figure.

frequency dependent spectral weight has two peaks instead of one. In addition, at zero frequency, it has a minimum instead of a maximum. That is called a pseudogap. A cartoon explanation [?] of this pseudogap is given in Fig. 52-1. At high temperature we start from a Fermi liquid, as illustrated in panel I. Now, suppose the ground state has long-range antiferromagnetic order as in panel III, in other words at a filling between half-filling and n_c. In the mean-field approximation we have a gap and the Bogoliubov transformation from fermion creation-annihilation operators to quasi-particles has weight at both positive and negative energies. In two dimensions, because of the Mermin-Wagner theorem, as soon as we raise the temperature above zero, long-range order disappears, but the antiferromagnetic correlation length ξ remains large so we obtain the pseudogap illustrated in panel II. As we will explain analytically below, the pseudogap survives as long as ξ is much larger than the thermal de Broglie wave length $\xi_{th} \equiv v_F/(\pi T)$ in our usual units. At the crossover temperature T_X, the relative size of ξ and ξ_{th} changes and we recover the Fermi liquid.

We now proceed to sketch analytically where these results come from starting from finite T. Details and more complete formulae may be found in Refs. [?, ?, 20, ?][1]. We begin from the TPSC expression (47.13) for the self-energy. Normally one has to do the sum over bosonic Matsubara frequencies first, but the zero Matsubara frequency contribution has the correct asymptotic behavior in fermionic frequencies iq_n so that, as in Sect.48.2, one can once more isolate on the right-hand side the contribution from the zero Matsubara frequency. In the renormalized classical regime then, we have [2]

$$\Sigma(\mathbf{k}_F, iq_n) \propto T \int q^{d-1} dq \frac{1}{q^2+\xi^{-2}} \frac{1}{iq_n - \varepsilon_{\mathbf{k}_F+\mathbf{Q}+\mathbf{q}}} \tag{52.4}$$

where $\mathbf{Q}$ is the wave vector of the instability. This integral can be done analytically

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[1] Note also the following study from zero temperature [?]

[2] This formula is similar to one that appeared in Ref.[?]

in two dimensions [20, **?**]. But it is more useful to analyze limiting cases [**?**]. Expanding around the points known as hot spots where $\varepsilon_{\mathbf{k}_F+\mathbf{Q}}=0$, we find after analytical continuation that the imaginary part of the retarded self-energy at zero frequency takes the form

$$\Sigma''^R(\mathbf{k}_F,0) \propto -\pi T\int d^{d-1}q_\perp dq_{||}\frac{1}{q_\perp^2+q_{||}^2+\xi^{-2}}\delta(v_F' q_{||}) \tag{52.5}$$

$$\propto \frac{\pi T}{v_F'}\xi^{3-d}. \tag{52.6}$$

In the last line, we just used dimensional analysis to do the integral.

The importance of dimension comes out clearly [**?**]. In $d=4$, $\Sigma''^R(\mathbf{k}_F,0)$ vanishes as temperature decreases, $d=3$ is the marginal dimension and in $d=2$ we have that $\Sigma''^R(\mathbf{k}_F,0)\propto \xi/\xi_{th}$ that diverges at zero temperature. In a Fermi liquid the quantity $\Sigma''^R(\mathbf{k}_F,0)$ vanishes at zero temperature, hence in three or four dimensions one recovers the Fermi liquid (or close to one in $d=3$). But in two dimensions, a diverging $\Sigma''^R(\mathbf{k}_F,0)$ corresponds to a vanishingly small $A(\mathbf{k}_F,\omega=0)$ as we can see from

$$A(\mathbf{k},\omega)=\frac{-2\Sigma''^R(\mathbf{k}_F,\omega)}{(\omega-\varepsilon_{\mathbf{k}}-\Sigma'^R(\mathbf{k}_F,\omega))^2+\Sigma''^R(\mathbf{k}_F,\omega)^2}. \tag{52.7}$$

Fig. 31 of Ref.[**?**] illustrates graphically the relationship between the location of the pseudogap and large scattering rates at the Fermi surface. At stronger U the scattering rate is large over a broader region, leading to a depletion of $A(\mathbf{k},\omega)$ over a broader range of **k** values.

Remark 153 *Note that the condition $\xi/\xi_{th}\gg 1$, necessary to obtain a large scattering rate, is in general harder to satisfy than the condition that corresponds to being in the renormalized classical regime. Indeed, $\xi/\xi_{th}\gg 1$ corresponds $T/v_F\gg \xi^{-1}$ while the condition $\omega_{sp}\ll T$ for the renormalized classical regime corresponds to $T\gg\xi^{-2}$, with appropriate scale factors, because ω_{sp} scales as ξ^{-2} as we saw in Eq. (48.13) and below.*

To understand the splitting into two peaks seen in Figs. 48-2 and 52-1 consider the singular renormalized contribution coming from the spin fluctuations in Eq. (52.4) at frequencies $\omega\gg v_F\xi^{-1}$. Taking into account that contributions to the integral come mostly from a region $q\leq\xi^{-1}$, one finds

$$\Sigma'^R(\mathbf{k}_F,\omega)=\left(T\int q^{d-1}dq\frac{1}{q^2+\xi^{-2}}\right)\frac{1}{ik_n-\varepsilon_{\mathbf{k}_F+\mathbf{Q}}}$$

$$\equiv\frac{\Delta^2}{\omega-\varepsilon_{\mathbf{k}_F+\mathbf{Q}}} \tag{52.8}$$

which, when substituted in the expression for the spectral weight (52.7) leads to large contributions when

$$\omega-\varepsilon_{\mathbf{k}}-\frac{\Delta^2}{\omega-\varepsilon_{\mathbf{k}_F+\mathbf{Q}}}=0 \tag{52.9}$$

or, equivalently,

$$\omega=\frac{(\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k}_F+\mathbf{Q}})\pm\sqrt{(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}_F+\mathbf{Q}})^2+4\Delta^2}}{2}, \tag{52.10}$$

which, at $\omega=0$, corresponds to the position of the hot spots[3]. At finite frequencies, this turns into the dispersion relation for the antiferromagnet [**?**].

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[3] For comparisons with paramagnon theory see [**?**].

It is important to understand that analogous arguments hold for any fluctuation that becomes soft because of the Mermin-Wagner theorem,[20, ?] including superconducting ones [20, ?, ?]. The wave vector $\mathbf{Q}$ would be different in each case.

To understand better when Fermi liquid theory is valid and when it is replaced by the pseudogap instead, it is useful to perform the calculations that lead to $\Sigma''^R(\mathbf{k}_F, 0) \propto \xi/\xi_{th}$ in the real frequency formalism. The details may be found in Appendix D of Ref. [20].

52.2 Pseudogap in electron-doped cuprates

High-temperature superconductors are made of layers of CuO_2 planes. The rest of the structure is commonly considered as providing either electron or hole doping of these planes depending on chemistry. At half-filling, or zero-doping, the ground state is an antiferromagnet. As one dopes the planes, one reaches a doping, so-called optimal doping, where the superconducting transition temperature T_c is maximum. Let us start from optimal hole or electron doping and decrease doping towards half-filling. That is the underdoped regime. In that regime, one observes a curious phenomenon, the pseudogap. What this means is that as temperature decreases, physical quantities behave as if the density of states near the Fermi level was decreasing. Finding an explanation for this phenomenon has been one of the major challenges of the field [?, ?].

To make progress, we need a microscopic model for high-temperature superconductors. Band structure calculations [?, ?] reveal that a single band crosses the Fermi level. Hence, it is a common assumption that these materials can be modeled by the one-band Hubbard model. Whether this is an oversimplification is still a subject of controversy [?, ?, ?, ?, ?, ?]. Indeed, spectroscopic studies [?, ?] show that hole doping occurs on the oxygen atoms. The resulting hole behaves as a copper excitation because of Zhang-Rice [?] singlet formation. In addition, the phase diagram [?, ?, ?, ?, ?, ?] and many properties of the hole-doped cuprates can be described by the one-band Hubbard model. Typically, the band parameters that are used are: nearest-neighbor hopping $t = 350$ to 400 meV and next-nearest-neighbor hopping $t' = -0.15$ to $-0.3t$ depending on the compound [?, ?]. Third-nearest-neighbor hopping $t'' = -0.5t'$ is sometimes added to fit finer details of the band structure [?]. The hoppings beyond nearest-neighbor mean that particle-hole symmetry is lost even at the band structure level.

In electron-doped cuprates, the doping occurs on the copper, hence there is little doubt that the single-band Hubbard model is even a better starting point in this case. Band parameters [?] are similar to those of hole-doped cuprates. It is sometimes claimed that there is a pseudogap only in the hole-doped cuprates. The origin of the pseudogap is indeed probably different in the hole-doped cuprates. But even though the standard signature of a pseudogap is absent in nuclear magnetic resonance [?] (NMR) there is definitely a pseudogap in the electron-doped case as well [?], as can be seen in optical conductivity [?] and in Angle Resolved Photoemission Spectroscopy (ARPES) [?]. As we show in the rest of this section, in electron-doped cuprates strong evidence for the origin of the pseudogap is provided by detailed comparisons of TPSC with ARPES as well as by verification with neutron scattering [?] that the TPSC condition for a pseudogap, namely $\xi > \xi_{th}$, is satisfied. The latter length makes sense from weak to intermediate coupling when quasi-particles exist above the pseudogap temperature. In strong coupling,

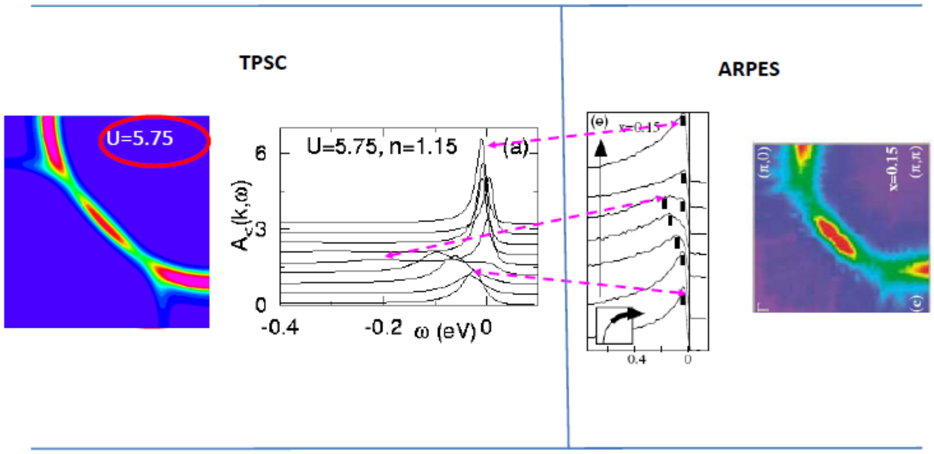

Figure 52-2 On the left, results of TPSC calculations [?, ?] at optimal doping, $x = 0.15$, corresponding to filling 1.15, for $t = 350$ meV, $t' = -0.175t$, $t_J = 0.05t$, $U = 5.75t$, $T = 1/20$. The left-most panel is the magnitude of the spectral weight times a Fermi function, $A(\mathbf{k}, \omega) f(\omega)$ at $\omega = 0$, so-called momentum-distribution curve (MDC). Red (dark black) indicates larger value and purple (light grey) smaller value. The next panel is $A(\mathbf{k}, \omega) f(\omega)$ for a set of fixed $\mathbf{k}$ values along the Fermi surface. These are so-called energy-dispersion curves (EDC). The two panels to the right are the corresponding experimental results [?] for $Nd_{2-x}Ce_xCuO_4$. Dotted arrows show the correspondence between TPSC and experiment.

i.e. for values of U larger than that necessary for the Mott transition, there is evidence that there is another mechanism for the formation of a pseudogap. This is discussed at length in Refs. [?, ?] [4]. The recent discovery [?] that at sufficiently large U there is a first order transition in the paramagnetic state between two kinds of metals, one of which is highly anomalous, gives a sharper meaning to what is meant by strong-coupling pseudogap.

Let us come back to modeling of electron-doped cuprates. Evidence that these are less strongly coupled than their hole-doped counterparts comes from the fact that a) The value of the optical gap at half-filling, ~ 1.5 eV, is smaller than for hole doping, ~ 2.0 eV [?]. b) In a simple Thomas-Fermi picture, the screened interaction scales like $\partial\mu/\partial n$. Quantum cluster calculations [?] show that $\partial\mu/\partial n$ is smaller on the electron-doped side, hence U should be smaller. c) Mechanisms based on the exchange of antiferromagnetic calculations with U/t at weak to intermediate coupling [?, ?] predict that the superconducting T_c increases with U/t. Hence T_c should decrease with increasing pressure in the simplest model where pressure increases hopping t while leaving U essentially unchanged. The opposite behavior, expected at strong coupling where $J = 4t^2/U$ is relevant [?, ?], is observed in the hole-doped cuprates. d) Finally and most importantly, there is detailed agreement between TPSC calculations [?, ?, ?] and measurements such as ARPES [?, ?], optical conductivity [?] and neutron [?] scattering.

To illustrate the last point, consider Fig. 52-2 that compares TPSC calculations with experimental results for ARPES. Apart from a tail in the experimental results, the agreement is striking. [5]. In particular, if there was no interaction, the Fermi surface would be a line (red) on the momentum distribution curve (MDC).

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[4] See also conclusion of Ref.[?].

[5] Such tails tend to disappear in more recent laser ARPES measurements on hole-doped compounds [?].

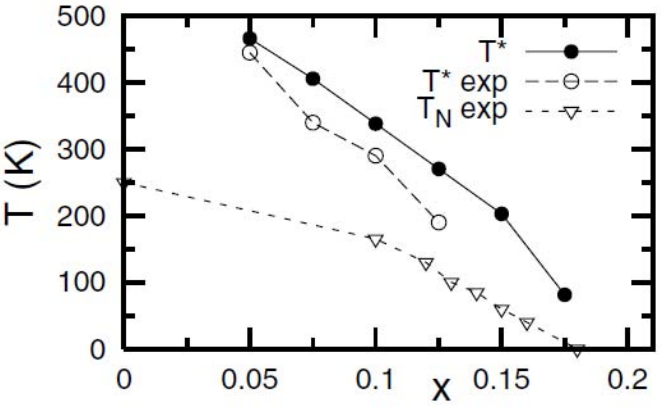

Figure 52-3

Instead, it seems to disappear at symmetrical points displaced from $(\pi/2, \pi/2)$. These points, so-called hot spots, are linked by the wave vector (π, π) to other points on the Fermi surface. This is where the antiferromagnetic gap would open first if there was long-range order. The pull back of the weight from $\omega = 0$ at the hot spots is close to the experimental value: 100 meV for the 15% doping shown, and 300 meV for 10% doping (not shown). More detailed ARPES spectra and comparisons with experiment are shown in Ref. [**?**]. The value of the temperature T^* at which the pseudogap appears [**?**] is also close to that observed in optical spectroscopy [**?**]. In addition, the size of the pseudogap is about ten times T^* in the calculation as well as in the experiments. For optical spectroscopy, vertex corrections (see Sect. **??**) have to be added to be more quantitative. Experimentally, the value of T^* is about twice the antiferromagnetic transition temperature up to $x = 0.13$. That can be obtained [**?**] by taking $t_z = 0.03t$ for hopping in the third direction. Recall that in strictly two dimensions, there is no long-range order. Antiferromagnetism appears on a much larger range of dopings for electron-doped than for hole-doped cuprates.

These TPSC calculations have predicted the value of the pseudogap temperature at $x = 0.13$ before it was observed experimentally [**?**] by a group unaware of the theoretical prediction in Fig.52-3. In addition, the prediction that ξ should scale like ξ_{th} at the pseudogap temperature has been verified in neutron scattering experiments [**?**] in the range $x = 0.04$ to $x = 0.15$. The range of temperatures and doping explored in that work is shown in Fig. 52-4. Note that the antiferromagnetic phase boundary, that occurs here because of coupling in the third dimension, is at a location different from earlier estimates that appear in Fig. 52-3. However, the location of the pseudogp temperature has not changed. At the doping that corresponds to optimal doping, T^* becomes of the order of 100 K, more than four times lower than at $x = 0.04$. The antiferromagnetic correlation length ξ beyond optimal doping begins to decrease and violate the scaling of ξ with ξ_{th}. In that doping range, T^* and the superconducting transition temperature are close. Hence it is likely that there is interference between the two phenomena [**?**], an effect that has not yet been taken into account in TPSC.

An important prediction that one should verify is that inelastic neutron scattering will find over-damped spin fluctuations in the pseudogap regime and that the characteristic spin fluctuation energy will be smaller than $k_B T$ whenever a pseudogap is present. Equality should occur above T^*.

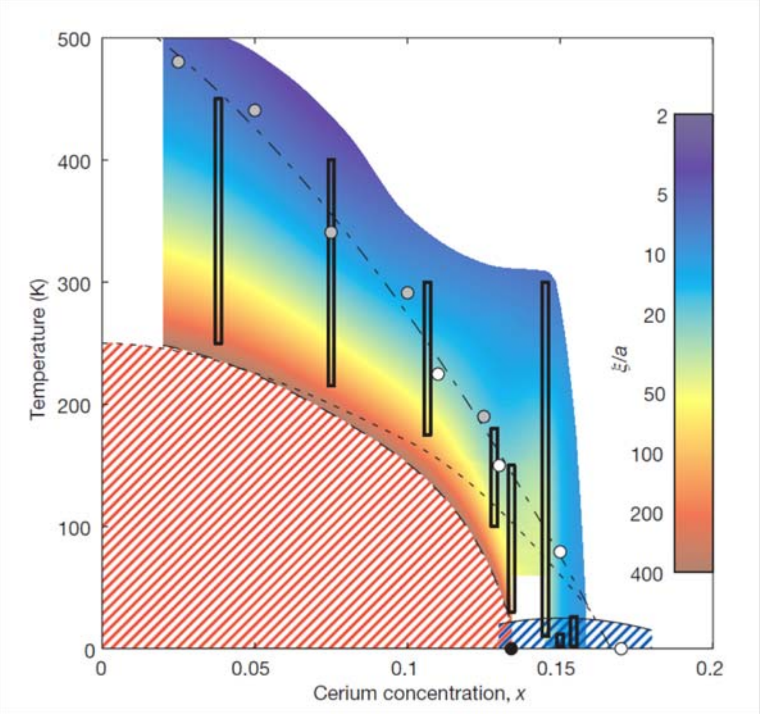

Figure 52-4

Finally, note that the agreement found in Fig. 52-2 between ARPES and TPSC is for $U \sim 6t$. At smaller values of U the antiferromagnetic correlations are not strong enough to produce a pseudogap in that temperature range. For larger U, the weight near $(\pi/2, \pi/2)$ disappears, in disagreement with experiments. The same value of U is found for the same reasons in strong coupling calculations with Cluster Perturbation Theory (CPT) [**?**] and with slave boson methods [**?**]. Recent first principle calculations [**?**] find essentially the same value of U. In that approach, the value of U is fixed, whereas in TPSC it was necessary to increase U by about 10% moving towards half-filling to get the best agreement with experiment. In any case, it is quite satisfying that weak and strong coupling methods agree on the value of U for electron-doped cuprates. This value of U is very near the critical value for the Mott transition at half-filling [**?**]. Hence, antiferromagnetic fluctuations at finite doping can be very well described by Slater-like physics (nesting) in electron-doped cuprates.

For recent calculations including the effect of the third dimension on the pseudogap see [**?**]. Finally, note that the analog of the above mechanism for the pseudogap has also been seen in two-dimensional charge-density wave dichalcogenides [**?**].

53. ADDITIONAL REMARKS: HUBBARD-STRATONOVICH TRANSFORMATION AND CRITICAL PHENOMENA

Part VIII

Appendices

A. FEYNMAN'S DERIVATION OF THE THERMODYNAMIC VARIATIONAL PRINCIPLE FOR QUANTUM SYSTEMS

For quantum systems, the general result Eq.(30.60) applies but it is more difficult to prove because there is in general no basis that diagonalizes simultaneously each and every term in the expansion of $T_\tau \exp\left[-\int_0^\beta d\tau \widetilde{V}(\tau)\right]$. If $\widetilde{V}$ was not time dependent, as in the classical case, then matters would be different since $\widetilde{V}^n$ would be diagonal in the same basis as $\widetilde{V}$ and one could apply our inequality Eq.(30.58) in this diagonal basis and prove the theorem. The proof of the variational principle in the quantum case is thus more complicated because of the non-commutation of operators. The proof given in Sec. 30.3.2 is simpler than this one. As far as I know, the following proof is due to Feynman [17].

Proof: First, let

$$\begin{aligned} H(\alpha) &= \widetilde{H}_0 + \alpha\left(H - \widetilde{H}_0\right) && \text{(A.1)} \\ &= \widetilde{H}_0 + \alpha\widetilde{V} && \text{(A.2)} \end{aligned}$$

then

$$H(0) = \widetilde{H}_0 \tag{A.3}$$

and

$$H(1) = H \tag{A.4}$$

The exact free energy corresponding to $H(\alpha)$ is then written as $F(\alpha)$. If for any α we can prove that $\partial^2 F(\alpha)/\partial\alpha^2 \leq 0$ then the function $F(\alpha)$ is concave downward and we can write

$$F(1) \leq F(0) + \left.\frac{\partial F(\alpha)}{\partial\alpha}\right|_{\alpha=0} \tag{A.5}$$

as illustrated in Fig.(A-1). Eq.(A.5) is the variational principle that we want Eq.(30.60). Indeed, let us compute the first derivative of $F(\alpha)$ by going to the interaction representation where $\widetilde{H}_0$ plays the role of the unperturbed Hamiltonian and use the result for F in terms of connected graphs Eq.(30.57) to obtain

$$\begin{aligned} \left.\frac{\partial F(\alpha)}{\partial\alpha}\right|_{\alpha=0} &= \frac{\partial}{\partial\alpha}\left\{-T\left[\left\langle T_\tau\left[e^{-\alpha\int_0^\beta d\tau\left(\widehat{H}(\tau)-\widetilde{H}_0\right)}\right]\right\rangle_{\widetilde{0}c} - 1\right]\right\}_{\alpha=0} && \text{(A.6)} \\ &= T\left\langle\int_0^\beta d\tau\left(\widehat{H}(\tau) - \widetilde{H}_0\right)\right\rangle_{\widetilde{0}} && \text{(A.7)} \\ &= \left\langle H - \widetilde{H}_0\right\rangle_{\widetilde{0}} && \text{(A.8)} \end{aligned}$$

The second line follows simply by expanding the time-ordered product to first order while the last line follows if we use the cyclic property of the trace

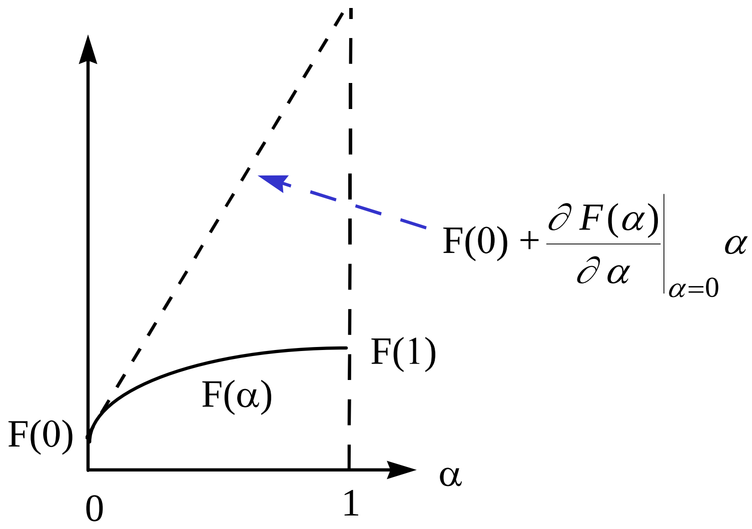

Figure A-1 Geometrical significance of the inequalities leading to the quantum thermodynamic variational principle.

to eliminate the imaginary-time dependence of the Hamiltonian. All that we have to do now is to evaluate the second derivative $\partial^2 F(\alpha)/\partial\alpha^2 \leq 0$ for an arbitrary value of α. This is more painful and will occupy us for the rest of this proof. It is important to realize that this concavity property of the free-energy is independent on the form of the Hamiltonian in general and of the interactions in particular, as long as the Hamiltonian is time-independent. The generalization to the time-dependent case is not obvious. The second derivative may be evaluated by going to the interaction representation where $H(\alpha)$ is the unperturbed Hamiltonian and $\gamma\left(H-\widetilde{H}_0\right)$ is the perturbation. Then,

$$F(\alpha+\gamma) = -T\left[\left\langle T_\tau\left[e^{-\gamma\int_0^\beta d\tau\left(\widehat{H}(\tau)-\widetilde{H}_0\right)}\right]\right\rangle_{\alpha,c} - 1\right] - T\ln Z(\alpha) \qquad (A.9)$$

and the second derivative of $F(\alpha)$ may be obtained from the second-order term in γ in the above expression. Note that the average is taken with the density matrix $\exp\left(H(\alpha)-\mu N\right)/Z(\alpha)$. Expanding the exponential to second order in γ and returning to our definition of $\widetilde{V}$ Eq.(A.2) we find

$$\begin{aligned}
F(\alpha+\gamma) &= F(\alpha)+\gamma\left\langle\widetilde{V}\right\rangle_\alpha - \frac{1}{2}\gamma^2\left(\frac{1}{\beta}\left\langle T_\tau\left[-\gamma\int_0^\beta d\tau\widetilde{V}(\tau)\right]^2\right\rangle_{\alpha,c}\right)+\ldots \\
F(\alpha+\gamma) &= F(\alpha)+\frac{\partial F(\alpha)}{\partial\alpha}+\frac{1}{2}\gamma^2\frac{\partial^2 F(\alpha)}{\partial\alpha^2}+\ldots \qquad (A.10)
\end{aligned}$$

so that the second derivative, using the expression we found above for the second cumulant Eq.(30.55) is,

$$\begin{aligned}
\frac{\partial^2 F(\alpha)}{\partial\alpha^2} &= -\frac{1}{\beta}\left\langle T_\tau\left[\left(-\int_0^\beta d\tau\widetilde{V}(\tau)\right)^2\right]\right\rangle_{\alpha,c} \qquad (A.11) \\
&= -\frac{1}{\beta}\left\langle T_\tau\left[\left(-\int_0^\beta d\tau\widetilde{V}(\tau)\right)^2\right]\right\rangle_{\alpha}+\frac{1}{\beta}\left\langle\int_0^\beta d\tau\widetilde{V}(\tau)\right\rangle_\alpha^2
\end{aligned}$$

This is where we need to roll up our sleeves and do a bit of algebra. Using the cyclic property of the trace and the definition of time-ordered product, we can rewrite the above result as follows,

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} = -2\frac{1}{\beta}\left\langle \int_0^\beta d\tau \widetilde{V}(\tau) \int_0^\tau d\tau' \widetilde{V}(\tau') \right\rangle_\alpha + \beta \left\langle \widetilde{V} \right\rangle_\alpha^2 \tag{A.12}$$

Let us work a bit on the first term by going to the basis where $H(\alpha)$ is diagonal. We obtain, using also the cyclic property of the trace,

$$\begin{aligned}
&\left\langle \int_0^\beta d\tau \widetilde{V}(\tau) \int_0^\tau d\tau' \widetilde{V}(\tau') \right\rangle_\alpha && \text{(A.13)}\\
=\ & \frac{1}{Z(\alpha)} \sum_{m,n} e^{-K_n\beta} \int_0^\beta d\tau \int_0^\tau d\tau' e^{K_n(\tau-\tau')} e^{-K_m(\tau-\tau')} \left| \langle n | \widetilde{V} | m \rangle \right|^2 \\
=\ & \frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \int_0^\beta d\tau e^{(K_n-K_m)\tau} \left. \frac{e^{(K_m-K_n)\tau'}}{K_m-K_n} \right|_0^\tau \left| \langle n | \widetilde{V} | m \rangle \right|^2 \\
& + \frac{1}{Z(\alpha)} \sum_n e^{-K_n\beta} \int_0^\beta d\tau \tau \left| \langle n | \widetilde{V} | n \rangle \right|^2 && \text{(A.14)}\\
=\ & \frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \int_0^\beta d\tau \frac{1-e^{(K_n-K_m)\tau}}{K_m-K_n} \left| \langle n | \widetilde{V} | m \rangle \right|^2 && \text{(A.15)}\\
& + \frac{\beta^2}{2Z(\alpha)} \sum_n e^{-K_n\beta} \left| \langle n | \widetilde{V} | n \rangle \right|^2 && \text{(A.16)}
\end{aligned}$$

The first term on the right-hand side is easily evaluated as follows

$$\begin{aligned}
& \frac{1}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \left[\frac{\beta}{K_m-K_n} + \frac{e^{(K_n-K_m)\beta}-1}{(K_m-K_n)^2} \right] \left| \langle n | \widetilde{V} | m \rangle \right|^2 \\
=\ & \frac{\beta}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \frac{\left| \langle n | \widetilde{V} | m \rangle \right|^2}{K_m-K_n} && \text{(A.17)}
\end{aligned}$$

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.(A.12) we finally obtain

$$\begin{aligned}
\frac{\partial^2 F(\alpha)}{\partial \alpha^2} =\ & -\frac{2}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \frac{\left| \langle n | \widetilde{V} | m \rangle \right|^2}{K_m-K_n} && \text{(A.18)}\\
& -\beta \left(\frac{\sum_n e^{-K_n\beta} \left| \langle n | \widetilde{V} | n \rangle \right|^2}{Z(\alpha)} - \left(\frac{\sum_n e^{-K_n\beta} \langle n | \widetilde{V} | n \rangle}{Z(\alpha)} \right)^2 \right)
\end{aligned}$$

The terms on the last line gives a negative contribution, as can be seen from the Cauchy-Schwarz inequality

$$\left[\sum_n |a_n|^2 \right] \left[\sum_n |b_n|^2 \right] \geq \left| \sum_n a_n b_n \right|^2 \tag{A.19}$$

when we substitute

$$a_n = \sqrt{\frac{e^{-K_n\beta}}{Z(\alpha)}} \tag{A.20}$$

$$b_n = \sqrt{\frac{e^{-K_n\beta}}{Z(\alpha)}} \langle n|\, \widetilde{V}\, |n\rangle \tag{A.21}$$

This allows us to prove that the sign of the second derivative is negative for any α. It suffices to rewrite the first term in Eq.(A.18) in the form

$$-\frac{2}{Z(\alpha)} \sum_{m\neq n} e^{-K_n\beta} \frac{\left|\langle n|\, \widetilde{V}\, |m\rangle\right|^2}{K_m - K_n} = -\frac{1}{Z(\alpha)} \sum_{m\neq n} \frac{e^{-K_n\beta} - e^{-K_m\beta}}{K_m - K_n} \left|\langle n|\, \widetilde{V}\, |m\rangle\right|^2 \tag{A.22}$$

and to use the Cauchy-Schwartz inequality to obtain

$$\frac{\partial^2 F(\alpha)}{\partial \alpha^2} \leq -\frac{1}{Z(\alpha)} \sum_{m\neq n} \frac{e^{-K_n\beta} - e^{-K_m\beta}}{K_m - K_n} \left|\langle n|\, \widetilde{V}\, |m\rangle\right|^2 \leq 0 \tag{A.23}$$

QED

B. NOTATIONS

C. DEFINITIONS

1. Canonical average

$$\frac{\sum_i e^{-\beta E_i}\left\langle i\right|\mathcal{O}\left|i\right\rangle}{\sum_i e^{-\beta E_i}} = \frac{\sum_i \left\langle i\right| e^{-\beta H}\mathcal{O}\left|i\right\rangle}{\sum_i e^{-\beta E_i}} = \frac{Tr\left[e^{-\beta H}\mathcal{O}\right]}{Tr\left[e^{-\beta H}\right]} = \left\langle \mathcal{O}\right\rangle \tag{C.1}$$

2. We often define the density matrix by

$$\widehat{\varrho} = e^{-\beta H}/\mathrm{Tr}\left[e^{-\beta H}\right]. \tag{C.2}$$

Then, we can write

$$\left\langle A_s\left(t\right)A_s\right\rangle = \mathrm{Tr}\left[\widehat{\varrho}A_s\left(t\right)A_s\right] \tag{C.3}$$

3. Conductivity sum rule

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}Re\left[\sigma_{xx}(q_x,\omega)\right] = \frac{ne^2}{2m} = \frac{\omega_p^2}{8\pi} \tag{C.4}$$

4. Dielectric constants

$$\overleftrightarrow{\epsilon}^T(\mathbf{q},\omega) = \left(1-\frac{\omega_p^2}{(\omega+i\eta)^2}\right)\overleftrightarrow{I} + \frac{4\pi}{(\omega+i\eta)^2}\left(\overleftrightarrow{\chi}^R_{\mathbf{jj}}(\mathbf{q},\omega)\right)^T. \tag{C.5}$$

$$\frac{1}{\epsilon^L(\mathbf{q},\omega)} = 1-\frac{4\pi}{q^2}\chi^R_{\rho\rho}(\mathbf{q},\omega). \tag{C.6}$$

5. Equalities.

$$\approx Asymptotically \quad equal \tag{C.7}$$

$$\sim Scales \quad as \tag{C.8}$$

$$\equiv Is \quad equal \quad by \quad definition$$

6. f sum rule

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{k},\omega) = \frac{n\mathbf{k}^2}{m}. \tag{C.9}$$

7. Fluctuation-dissipation theorem

$$S_{A_iA_j}(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega) \tag{C.10}$$

8. Fourier transforms

$$f_{\mathbf{k}} = \int d^3r\; f(\mathbf{r})\mathbf{e}^{-i\mathbf{k}\cdot\mathbf{r}}$$

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

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

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

(note the difference in sign in the exponent for space and time Fourier transforms.)

Convolution theorem:

$$\int dte^{i\omega t}\left[\int dt' a(t')b(t-t')\right] \equiv a_\omega b_\omega$$

Parseval's theorem is obtained by taking $\int \frac{d\omega}{2\pi}$ on both sides of the previous equality

$$\int dt' a(t')b(-t') \equiv \int \frac{d\omega}{2\pi} a_\omega b_\omega$$

The above two theorems may also be written in a reciprocal manner

$$\int \frac{d\omega}{2\pi} e^{-i\omega t}\left[\int \frac{d\omega'}{2\pi} a_{\omega'} b_{\omega-\omega'}\right] = a(t)b(t)$$

$$\int \frac{d\omega'}{2\pi} a_{\omega'} b_{-\omega'} = \int dte^{i\omega t} a(t)b(t)$$

9. Heisenberg representation

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

10. Interaction representation

$$\begin{aligned} \mathcal{O}_I(t) &= e^{iH_0t/\hbar}\mathcal{O}_S e^{-iH_0t/\hbar} \\ i\hbar\frac{\partial}{\partial t}U_I(t,t_0) &= \mathcal{H}_I(t)U_I(t,t_0) \qquad \text{(C.11)} \\ U_I(t,0) &= T_c e^{-i\int_0^t \mathcal{H}_I(t')dt'} \end{aligned}$$

$$U_I(t_0,t_0) = 1$$

1. Kramers-Krönig relations

$$Re\left[\chi^R_{A_iA_j}(\omega)\right] = \mathcal{P}\int \frac{d\omega'}{\pi}\frac{Im\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}$$

$$Im\left[\chi^R_{A_iA_j}(\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi}\frac{Re\left[\chi^R_{A_iA_j}(\omega')\right]}{\omega'-\omega}.$$

2. Kubo formula for longitudinal conductivity

$$\sigma_{xx}(q_x,\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right] = \left[\frac{1}{iq_x}\chi^R_{j_\mu\rho}(q_x,\omega)\right]. \qquad \text{(C.12)}$$

for transverse conductivity

$$\sigma_{yy}(q_x,\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_yj_y}(q_x,\omega) - \frac{ne^2}{m}\right]. \qquad \text{(C.13)}$$

3. Mathematical identities

$$\lim_{\eta\to 0}\frac{1}{\omega+i\eta}=\lim_{\eta\to 0}\frac{\omega-i\eta}{\omega^2+\eta^2}=\lim_{\eta\to 0}\left[\frac{\omega}{\omega^2+\eta^2}-\frac{i\eta}{\omega^2+\eta^2}\right]=\mathcal{P}\frac{1}{\omega}-i\pi\delta(\omega)$$

$$\lim_{\eta\to 0}\frac{1}{\omega-i\eta}=\lim_{\eta\to 0}\frac{\omega+i\eta}{\omega^2+\eta^2}=\lim_{\eta\to 0}\left[\frac{\omega}{\omega^2+\eta^2}+\frac{i\eta}{\omega^2+\eta^2}\right]=\mathcal{P}\frac{1}{\omega}+i\pi\delta(\omega)$$

4. Normalization:

   Continuum normalization for plane waves:

$$\langle\mathbf{R}|\,|\mathbf{k}_i\rangle=\frac{1}{\Omega^{1/2}}e^{i\mathbf{k}_i\cdot\mathbf{R}} \tag{C.14}$$

$$\int\frac{d\mathbf{k}}{(2\pi)^3}=\frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\quad;\quad\mathcal{V}=L_xL_yL_z\quad;\quad k_x=\frac{\pi n_x}{L_x}...\quad;\quad n_x=-\frac{L_x}{a}+1,...,-1,0,1,...,\frac{L_x}{a} \tag{C.15}$$

$$\int d\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}|=1 \tag{C.16}$$

$$\langle\mathbf{r}|\,|\mathbf{r}'\rangle=\delta\left(\mathbf{r}-\mathbf{r}'\right) \tag{C.17}$$

$$\langle\mathbf{r}|\,|\mathbf{k}\rangle=e^{i\mathbf{k}\cdot\mathbf{r}} \tag{C.18}$$

$$\int\frac{d\mathbf{k}}{(2\pi)^3}\,|\mathbf{k}\rangle\,\langle\mathbf{k}|=1 \tag{C.19}$$

$$\langle\mathbf{k}|\,|\mathbf{k}'\rangle=(2\pi)^3\,\delta\left(\mathbf{k}-\mathbf{k}'\right)$$

5. Plasma frequency

$$\omega_p^2=\frac{4\pi ne^2}{m} \tag{C.20}$$

6. Response function (Susceptibility)

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

   or in short hand,

$$\chi"_{A_iA_j}(t-t')=\frac{1}{2\hbar}\left\langle[A_i(t),A_j(t')]\right\rangle.$$

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

   For operators with the same signature under time reversal,

$$Im\left[\chi^R_{A_iA_j}(\omega)\right]=\chi"_{A_iA_j}(\omega)$$

   while two operators A_i, A_j with opposite signatures under time reversal

$$Re\left[\chi^R_{A_iA_j}(\omega)\right]=\chi"_{A_iA_j}(\omega).$$

   Spectral representation

$$\chi_{A_iA_j}(z)=\int\frac{d\omega'}{\pi}\frac{\chi"_{A_iA_j}(\omega')}{\omega'-z} \tag{C.21}$$

7. Tensors. Multiplication by a vector

$$\left(\overleftrightarrow{\sigma^T} \cdot \mathbf{A}\right)_{\mu} = \sum_{\nu} \sigma^T_{\mu\nu} A_{\nu}. \tag{C.22}$$

   Transverse part

$$\overleftrightarrow{\sigma^T}(\mathbf{q},\omega) = \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \cdot \overleftrightarrow{\sigma}(\mathbf{q},\omega) \cdot \left(\overleftrightarrow{\mathbf{I}} - \widehat{\mathbf{q}}\widehat{\mathbf{q}}\right) \tag{C.23}$$

   Longitudinal part

$$\overleftrightarrow{\sigma^L}(\mathbf{q},\omega) = \widehat{\mathbf{q}}\widehat{\mathbf{q}} \cdot \overleftrightarrow{\sigma}(\mathbf{q},\omega) \cdot \widehat{\mathbf{q}}\widehat{\mathbf{q}} \tag{C.24}$$

8. Thermal average (see canonical average)
9. Theta function (Heaviside function)

$$\theta(t) = \frac{1 \text{ if } t > 0}{0 \text{ if } t < 0}$$