Introduction to Correlated Matter

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Some bare numbers and unsettling questions

0.1 Goal of the game

Condensed matter physics is a remarkable domain where the effects of quantum mechanics combine with the presence of a very large ($\sim 10^{23}$) coupled degrees of freedom. The interplay between these two ingredients leads to the richness of phenomena that we observe in everyday's materials and which have led to things such useful in our daily life as semiconductors (transistors, computers !), liquid crystals (flat panel displays), superconductivity (cables and magnets used in today's MRI equipments) and more recently giant magnetoresistance (hard drive reading heads).

When looking at this type of problems, one important question is how should we model them. In particular one essential question that one has to address is whether the interaction among the particles is an important ingredient to take into account or not. The answer to that question is not innocent. If the answer is no, then all is well (but perhaps a little bit boring) since all we have to do is to solve the problem of one particle, and then we are done. This does not mean that all trivial effects disappear since fermions being indistinguishable have to obey the Pauli principle. But it means at least that the heart of the problem is a single particle problem and excitations. This is what is routinely done in all beginner's solid state physics course, where all the properties of independent electrons are computed.

If the answer to the above questions is no, then we have a formidable problem, where all degrees of freedom in the system are coupled. Solving a Schroedinger equation with 10^{23} variables is completely out of the question, so one should develop tools to be able to tackle such a problem with some chance of success.

What is the appropriate situation in most materials is thus something of importance, and one should address in turn the following points

- 1. Are the quantum effects important in a solid at the one particle level. Here there is no surprise, the answer for most metals is yes, given the ratio of the typical energy scale in a solid ($\sim 10000K$) due to the Pauli principle, compared to the standard thermal energy scale ($\sim 300K$)
- 2. From a purely empirical point of view, does the independent electron picture works to explain the properties of many solids.
- 3. From a more theoretical point of view can one estimate the ratio of the interaction energy (essentially the Coulomb interaction in a solid) to the kinetic energy and work out the consequences of such interactions.

The answer to the first question is without surprise, and can be found in all standard textbooks on solid state physics. The answer to the second question is much more surprising, since in practice the free electron theory works extremely well to describe most of the solids. When one is faced with such a fact the standard reaction is to think that the interactions are indeed negligible in most solid. Unfortunately (or rather quite fortunately), this naive interpretation of the data does not corresponds with a naive estimate of the value of the interactions. One is thus faced with the formidable puzzle to have to treat the interactions, and also to understand why, by some miracle they seem to magically disappear in the physical observables. The miracle is in fact called Fermi liquid theory and was discovered by L. D. Landau, and we will try to understand and explain the main features of this theory in these lectures.

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CHAPTER 1

Basics of solid state physics

The goal of this chapter is to review the salient features of noninteracting electrons. This will useful in order to determine whether the interactions lead or not to drastic changes in the physics. We will also estimate the order of magnitude of the interactions in a normal metal, starting from the Coulomb interaction and recall the main differences between Coulomb interactions in the vacuum and in a solid.

Most of the material in this chapter is classical knowledge of solid state physics (textbooks by Ziman, Kittel, Oupra, Ashcroft & Mermin). We will however use as soon as possible the proper technology to perform the calculations.

1.1 The jellium model

The simple case of free electrons allows us to introduce most of the quantities we will use. Let us consider free electrons described by the Hamiltonian

$$H = \frac{p^2}{2m} \tag{1.1}$$

The eigenstates are the plane waves $|\mathbf{k}\rangle$, defined by

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{\sqrt{\Omega}} e^{i \boldsymbol{k} \boldsymbol{r}}$$
(1.2)

where Ω is the volume of the system. The corresponding eigenvalue is

$$\varepsilon_{k} = \frac{\hbar^2 k^2}{2m} \tag{1.3}$$

In addition to the above orbital part, the electron possesses a spin 1/2. A complete basis of the spin degrees of freedom is provided by the two eigenstates of one of the spin component. One usually takes the S_z one, and we define the corresponding basis as $|\uparrow\rangle$ and $|\downarrow\rangle$ The ensemble α of quantum numbers needed to fully characterize the electrons is thus its momentum and its spin $\alpha = (\sigma, \mathbf{k})$.

For a system of finite size the values of \boldsymbol{k} are quantized by the boundary conditions. In the limit of a very large size the precise boundary condition does not matter so we will take periodic boundary conditions for simplicity. This means that for a system of linear dimensions L (the volume being $\Omega = L^d$ for a system in d dimensions), the wavefunction ψ must satisfy $\psi(x + L) = \psi(x)$ and similar relations in all directions. This imposes that each component of \boldsymbol{k} is of the form

$$k_l = \frac{2\pi m_l}{L} \tag{1.4}$$

where the m_l are integers for l = 1, ..., d with d the dimension of the system.

At zero temperature the Pauli principle states that each quantum state is occupied by at most one fermion. One thus starts to fill the lowest energy levels to accommodate the N electrons of the system. One thus fills the energy level up to the Fermi energy $E_{\rm F}$ and up to a momentum $k_{\rm F}$ such that $\varepsilon_{k_{\rm F}} = E_{\rm F}$. At finite temperature, the states are occupied with a probability that is given by the Fermi-Dirac factor

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}$$
(1.5)

where μ is the chemical potential. The total number of electrons in the system is given by

$$N(\mu) = \sum_{k\sigma} f(\varepsilon_k) \tag{1.6}$$

We consider now the system at the absolute zero temperature temperature. In this limit the Fermi-Dirac distribution becomes a step-function : $f(\varepsilon_{\mathbf{k}}) = \theta(\varepsilon - \varepsilon_{\mathbf{k}})$. We note that the total number of states with an energy lower than ε is given by

$$N(\varepsilon) = \sum_{k} \theta(\varepsilon - \varepsilon_{k})$$
(1.7)

The sum over the integers can be simplified in the large N limit since the values of k_i are nearly continuous. Using (1.4) one gets

$$\sum_{\boldsymbol{k}} \to \frac{\Omega}{(2\pi)^d} \int d\boldsymbol{k}$$
(1.8)

One has thus (the sum over the spin degrees of freedom simply giving a factor of two)

$$N(E_{\rm F}) = \frac{2\Omega}{(2\pi)^3} \frac{4\pi}{3} k_{\rm F}^3$$
(1.9)

one can therefore relate the density of particles to the Fermi wavevector

$$n = N/\Omega = k_{\rm F}^3/(3\pi^2) \tag{1.10}$$

The existence of a Fermi level is of prime importance for the properties of solids. Given the relative energies of $E_{\rm F}$ and, say, the temperature, most of the excitations will simply be blocked by the Pauli principle, and the ones that will play a role will be the ones close to the Fermi level. This simple fact is what gives to most solids their unusual properties, and allow for quantum effects to manifest themselves even at high (by human standards) temperature.

A specially important quantity is the density of states per unit volume $\rho(\varepsilon)$. $\rho(\varepsilon)d\varepsilon$ measures the number of states that have an energy between ε and $\varepsilon + d\varepsilon$. The density of states is obviously the derivative of $N(\varepsilon)$, leading to

$$\rho(\varepsilon) = \frac{1}{\Omega} \frac{\partial N(\varepsilon)}{\partial \varepsilon} = \frac{1}{\Omega} \sum_{\alpha} \delta(\varepsilon - \varepsilon_{\alpha})$$
(1.11)

As an illustration we will recompute the density of states for free fermions in any dimension. Since the energy depends only on k^2 it is convenient to use spherical coordinates. One has $\int d\mathbf{k} = \int_0^\infty k^{d-1} dk S_d$ where S_d is the surface of the unit sphere $[S_1 = 2, S_2 = 2\pi, S_3 = 4\pi$ and $1/S_d = 2^{d-1} \pi^{d/2} \Gamma(d/2)]$ and thus (with a factor 2 coming from the spin degeneracy)

$$N(\epsilon) = \frac{2\Omega}{(2\pi)^d} S_d \int_0^\infty k^{d-1} dk = \frac{2\Omega}{(2\pi)^d} \frac{S_d}{d} k^d = \frac{2\Omega}{(2\pi)^d} \frac{S_d}{d} \left(\frac{2m\varepsilon}{\hbar^2}\right)^{d/2}$$
(1.12)

for $\varepsilon > 0$ and zero otherwise. One thus sees that the density of states

$$\rho(\epsilon) = \frac{1}{\Omega} \frac{\partial N(\varepsilon)}{\partial \varepsilon} = \frac{S_d}{(2\pi)^d} \left(\frac{2m}{\hbar^2}\right)^{d/2} \varepsilon^{d/2-1}$$
(1.13)

behaves in three dimensions as

$$\rho(\epsilon) = \frac{\sqrt{2m^3}}{\pi^2 \hbar^3} \sqrt{\varepsilon} \tag{1.14}$$

while it is a constant in two dimensions and has a $1/\sqrt{\varepsilon}$ singularity at the bottom of the band in one dimension.

1.2 Particle density and chemical potential

For a band of electrons with a density of states described by $\rho(\epsilon)$, and given a certain value of the chemical potential μ , the electron density $(n = N/\Omega)$ is given by the integral over energy ϵ of the Fermi-Dirac distribution (giving the average occupation of each energy level ϵ) multiplied with the density of states (providing to the number of energy levels per unit volume $\rho(\epsilon)d\epsilon$ in the interval $\{\epsilon, \epsilon + d\epsilon\}$)

$$n = \int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \rho(\epsilon) d\epsilon$$
(1.15)

1.3 Chemical potential in two dimensions

The density of states in two dimensions is

$$\rho = \frac{m}{\pi\hbar^2} \quad (\epsilon \ge 0)$$

$$\rho(\epsilon) = 0 \quad (\epsilon < 0)$$
(1.16)

so that, using the substitution $x = \beta \epsilon$

$$\frac{\beta n}{\rho} = \int_0^\infty \frac{1}{e^{x - \beta \mu} + 1} dx \tag{1.17}$$

The integral on the righthand side has a simple solution in analytical closed form

$$-\left[\ln(1+e^{-x+\beta\mu})\right]_{0}^{\infty} = \ln(1+e^{\beta\mu})$$

hence

$$e^{\beta n/\rho} - 1 = e^{\beta \mu}$$

from which

$$\mu(n,T) = k_B T \ln \left(e^{\beta n/\rho} - 1 \right)$$

The chemical potential at T = 0 is by definition the Fermi energy, hence $E_{\rm F} = n/\rho$. It will be handy to rearrange the terms using the properties of logaritms $\ln(a \cdot b) = \ln(a) + \ln(b)$

$$\mu(n,T) = E_{\rm F} + k_B T \ln\left(1 - e^{-\beta E_{\rm F}}\right)$$
(1.18)

1.4 Maxwell relation

In the present section, as well as the following one we will make use of relation between $d\mu/dn$ and the compressibility, $\kappa = n^{-1}dn/dp$. This is an example of a so-called Maxwell relation, and we briefly explain where it comes from. The Helmholtz free energy $F(N, \Omega, T)$ is a smooth function of its parameters N, Ω, T . The chemical potential and the pressure are defined as $\mu = (\partial F/\partial N)_T$ and $p = -(\partial F/\partial \Omega)_T$. The smoothness of F implies that the order of differentiation doesn't matter, i.e. $(\partial^2 F/\partial \Omega \partial N)_T = (\partial^2 F/\partial N \partial \Omega)_T$. Consequently, multiplying both sides with N, we have

$$\left(N\frac{\partial\mu}{\partial\Omega}\right)_T = -\left(N\frac{\partial p}{\partial N}\right)_T \tag{1.19}$$

We now take advantage of the fact that, in the present situation, the dependence on volume and particle number only enters through the ratio $n = N/\Omega$, so that

$$\left(\frac{\partial\mu}{\partial(1/n)}\right)_T = -\left(n\frac{\partial p}{\partial n}\right)_T \tag{1.20}$$

Differentiating in parts gives the Maxwell relation

$$n\left(\frac{\partial\mu}{\partial n}\right)_T = \left(\frac{\partial p}{\partial n}\right)_T \tag{1.21}$$

1.5 Compressibility at zero temperature

Let us now move to another thermodynamic quantity namely the compressibility. Normally the compressibility (at constant temperature) of a system is the way the volume varies when one varies the pressure, namely

$$\kappa = \frac{1}{n} \left(\frac{dn}{dp} \right)_T \tag{1.22}$$

The dp/dn is related to $d\mu/dn$ by the Maxwell relation Eq. 1.21, which after substituting the definition of κ gives

$$\kappa = \frac{1}{n^2} \left(\frac{dn}{d\mu}\right)_T \tag{1.23}$$

At zero temperature the compressibility can be readily computed by noting that for this limit the Fermi-Dirac distribution is a step-function, and $\mu = \epsilon_F$, so that

$$n = \int_{-\infty}^{\epsilon_F} d\varepsilon \rho(\varepsilon) \tag{1.24}$$

(in the present example the density of states satisfies: $\rho(\varepsilon) = 0$ for $\varepsilon < 0$, but the above equation remains valid when the density of states is finites for negative energies) and thus

$$\kappa = \frac{\rho_F}{n^2} \tag{1.25}$$

as is obvious from Fig. 1.1.



Figure 1.1: Change of number of particles for a change of chemical potential



Figure 1.2: Temperature dependence of the chemical potential, pressure, entropy and specific heat of a 2 dimensional electron gas.

1.6 Temperature dependent compressibility in two dimensions

Clearly for $T \to 0$ the chemical potential converges toward $E_{\rm F}$. Hence we see that at T = 0 the chemical potential coincides with $n/\rho = E_{\rm F}$. In order to obtain the equation of state p(n,T) we can use the Maxwell relation, Eq. 1.21. We then obtain

$$\left(\frac{\partial p}{\partial n}\right)_T = \frac{n}{\rho} + \frac{n}{\rho} \frac{1}{e^{\beta n/\rho} - 1}$$
(1.26)

Combining both terms gives for the compressibility

$$\kappa(T) = \frac{\rho}{n^2} \left\{ 1 - e^{-n/(\rho k_B T)} \right\}$$
(1.27)

which for $T \to 0$ gives once again $\kappa(0) = \rho/n^2$, and in the opposite limit of high temperature corresponds to the result for the ideal gas: $\kappa(T \to \infty) \approx 1/(nk_BT)$.

1.7 Pressure in two dimensions

An expression for the pressure of n particles per unit volume is obtained by integration of both sides of Eq. 1.26 over the particle density n:

$$\int_0^n \left(\frac{\partial p}{\partial n'}\right)_T dn' = \int_0^n \left\{\frac{n'}{\rho} + \frac{n'}{\rho}\frac{1}{e^{\beta n'/\rho} - 1}\right\} dn'$$

with the result

$$p(n,T) - p(0,T) = \frac{n^2}{2\rho} + \int_0^n \frac{n'}{\rho} \frac{1}{e^{\beta n'/\rho} - 1} dn'$$

As to the second term of the lefthand side of the expression we can use the fact that in the absence of particles the pressure is zero, p(0,T) = 0. We carry out a transformation of integration variable $dn' \rightarrow dz$ with the help of the substitution $z = \beta n/\rho$. This way, and using the fact that $E_{\rm F} = n/\rho$, the equation of state becomes

$$p(n,T) = \frac{n^2}{2\rho} + \rho(k_B T)^2 \int_0^{\beta E_F} \frac{z}{e^z - 1} dz$$
(1.28)

Due to the first term on the right hand side, the pressure does not converge to zero when we take $T \rightarrow 0$! The fact that at absolute zero the pressure of a gas of fermions remains finite is a general property which reflects the fact that the Pauli-principle forces the electrons to occupy states of finite momentum and velocity.

1.8 Specific heat in two dimensions

With the help of the thermodynamical relation $F = \mu N - p\Omega$ we obtain the expression for the Helmholtz free energy density $f = F/\Omega$

$$f(n,T) = \frac{n^2}{2\rho} + nk_B T \ln\left(1 - e^{-\beta E_{\rm F}}\right) - \rho(k_B T)^2 \int_0^{\beta E_{\rm F}} \frac{z}{e^z - 1} dz \tag{1.29}$$

The entropy density is obtained as the partial derivative $s = -\partial f / \partial T |_n$. Consequently

$$s(n,T) = 2\rho k_B^2 T \int_0^{\beta E_F} \frac{z}{e^z - 1} dz - nk_B \ln\left(1 - e^{-\beta E_F}\right)$$

and, using $c_V = T \partial s / \partial T |_{\Omega,N}$ we obtain the expression for the specific heat at fixed volume

$$c_V(T) = 2\rho k_B^2 T \int_0^{\beta E_{\rm F}} \frac{z}{e^z - 1} dz - nk_B \frac{\beta E_{\rm F}}{e^{\beta E_{\rm F}} - 1}$$

Considering now temperatures $T \ll E_{\rm F}/k_B$ the specific heat becomes

$$c_V = 2\rho k_B^2 T \int_0^\infty \frac{z}{e^z - 1} dz + O(e^{-\beta E_{\rm F}})$$

Since $\int_0^\infty \frac{z}{e^z-1} dz = \pi^2/6$ we obtain for $T \ll E_{\rm F}/k_B$

$$c_V = \frac{\pi^2}{3}\rho k_B^2 T \tag{1.30}$$

As we will see in the sequel, the predicted linear temperature dependence of the specific heat of a metal at low temperatures is true for general density of states and dimensions, and it agrees with experimental results on a gas of fermions, as for example shown in Fig. 1.3.



Figure 1.3: Specific heat of URu₂Si₂ at low temperatures. (Source: J. Levallois, Ph D thesis, Université Paul Sabatier de Toulouse, 2008)

1.9 Specific heat in any dimensions

An intuitive way to obtain the linear temperature dependence of the specific heat of a metal, is by considering that the specific heat is simply the change in energy (heat) of the system with



Figure 1.4: The difference in energy between a system at T = 0 and T finite is due to the thermal excitations of particles within a slice of $k_{\rm B}T$ around the Fermi energy $E_{\rm F}$. All the others are blocked by the Pauli principle.

respect with the temperature. The total energy per spin degree of freedom is given by

$$E(T) = \sum_{k} f(\varepsilon_{k} - \mu)\varepsilon_{k}, \qquad (1.31)$$

while the chemical potential is given by the conservation of the total number of particles

$$N = \sum_{k} f(\varepsilon_{k} - \mu).$$
(1.32)

Notice that in these equations what is fixed is the number of particles, and therefore the chemical potential depends on temperature. Even if one normally uses the grand-canonical ensemble to obtain Eqs. (1.31) and (1.32), they are also valid in the canonical ensemble, by fixing N. Differentiating (1.31) with respect to T gives the specific heat. The full calculation is left to the reader as an exercise. We will here just give a qualitative argument, emphasizing the role of the Fermi surface.

When going from T = 0 to the small temperature T, particle in the system will gain an energy of the order of $k_{\rm B}T$ since they can be thermally excited. However the Pauli principle will block most of such excitations and thus only the particles that are within a slice of $k_{\rm B}T$ in energy around the Fermi energy can find the empty states in which they can be excited as indicated in Fig. 1.4. The number of such excitations is thus

$$\Delta N(T)/\Omega = k_{\rm B} T \rho \tag{1.33}$$

and the gain in energy is

$$\Delta E(T)/\Omega = k_{\rm B}^2 T^2 \rho \tag{1.34}$$

leading to a specific heat (at constant volume)

$$c_V(T) \propto k_{\rm B}^2 \rho T \tag{1.35}$$

which is, apart from a factor $\pi^2/3$, the exact result obtained in eq.1.30. The Pauli principle and the large Fermi energy compared to the temperature thus directly imply that the specific heat of an independent electron gas is linear in temperature. The proportionality coefficient γ is, up to nonimportant constants directly proportional to the density of states at the Fermi level. This is the first illustration of something that we will encounter often: because of the Pauli principle, most of the states are blocked and thus useless. Only a very small fraction of the electron, close to the Fermi level contributes to the physical observables. This is a very important point, since it means that we can essentially ignore, in most cases, most of the precise details of the band structure and kinetic energy, provided that we know what is the density of states at the Fermi level. In practice, because the energy scale that we are probing (here the temperature) is usually much smaller than the typical energy scale over which the density of state varies we can consider that this quantity is a constant.

The linear dependence of the specific heat of the fermions, is a spectacular manifestation of the Pauli principle. Indeed let us assume instead that our electrons were classical particles. Then we could compute the total energy using the equipartition, and the fact that this is $\frac{1}{2}k_{\rm B}T$ per degree of freedom. We would have

$$c_{\rm cl}(T) = \frac{Nk_{\rm B}}{2\Omega} \tag{1.36}$$

which using Eq. 1.30 would lead to

$$c_{\rm el}/c_{\rm cl} \equiv \frac{\pi^2}{3} \left(\frac{k_{\rm B}T}{E_{\rm F}}\right) \tag{1.37}$$

which would lead easily at temperatures of the order of 10K but even at ambient temperature to an error of several orders of magnitude.

1.10 Magnetic susceptibility in any dimensions

One notes, that only the density of states at the Fermi level enters in the value of the compressibility (up to non important factors, that are independent of the physical system considered). This is a consequence of the Pauli principle. Insulators for which the density of states is zero at the Fermi level are incompressible. If the chemical potential is varied no additional electron can enter the system. A naive picture of this could be to say that if we have already two electrons per site (a filled band) then there is no "place" where one could squeeze an additional electron. Alternatively a metal, which has a finite density of states at the Fermi level can accommodate additional electrons when the Fermi level is increased. The same image would apply since in that case the band would be partly filled and one would have places with zero or only one electro where one could insert additional particles.

Finally for a solid the last simple useful thermodynamic quantity is the magnetic susceptibility. Quite generally the magnetic susceptibility is the way the magnetization varies when an external magnetic field is applied on the system

$$\chi = \left(\frac{dM}{dH}\right)_T \tag{1.38}$$

The main source of magnetization in the solid is provided by the spins of the electrons (there are also orbital effects but let us ignore those for the moment). The magnetization per spin is given by

$$\boldsymbol{m} = g\mu_{\rm B}\boldsymbol{\sigma} \tag{1.39}$$

where $\mu_{\rm B}$ is the Bohr magneton, a quantity depending on the unit system, allowing the conversion of orbital moments into magnetic moments, and g the Lande factor is a dimensionless number telling for each particle how the orbital moment converts into a magnetic moment $(g \simeq 2 \text{ for the electron in a vacuum})$. The energy gained by the spins when coupled with an external magnetic field is thus

$$E_B = -\boldsymbol{B} \cdot \sum_i Ng\mu_{\rm B}\boldsymbol{\sigma}_i \tag{1.40}$$



Figure 1.5: Cartoon of incompressibility. A system with a half filled band has many sites where an additional electron could be added and is thus compressible (left). On the other hand a filled band corresponds to two electron per site. No additional electron could be added even if the chemical potential is increased. The system is incompressible.

Applying the field in the z direction and using the fact that for a spin 1/2 only two quantized values of the spin are possible one obtains

$$E_B = -\frac{g\mu_{\rm B}}{2}B(N_{\uparrow} - N_{\downarrow}) \tag{1.41}$$

The energies for each up (resp down) spins is thus shifted by $\varepsilon(k) \rightarrow \varepsilon(k) \mp (g\mu_{\rm B})B$. As shown in Fig. 1.6 this implies, since the chemical potential remains unchanged that more spin up and less spin downs will be present in the system. In a total similarity with the compressibility

$$\frac{\Delta N_{\uparrow}}{\Omega} = -\frac{\Delta N_{\downarrow}}{\Omega} = \rho_F \frac{g\mu_{\rm B}}{2}B \tag{1.42}$$

leading to a variation of magnetization due to the spins

$$\Delta M_z = \frac{(g\mu_{\rm B})}{2} \frac{\Delta N_{\uparrow} - \Delta N_{\downarrow}}{\Omega} = B \frac{(g\mu_{\rm B})^2}{4} \rho_F \tag{1.43}$$

and thus to a spin susceptibility

$$\chi = \frac{(g\mu_{\rm B})^2}{4}\rho_F \tag{1.44}$$

We again see that only the states very close to the Fermi level contribute, which implies that the spin susceptibility is again controlled by the density of states at the Fermi level.

This little survey of noninteracting electrons thus disclosed various important facts that constitute the essence of what a non-interacting electron gas looks like, and that we can summarize below. These properties will of course be crucial to set a frame of comparison with the case of interacting particles.

The ground state of the system is a Fermi sea with a certain number of states occupied, the other are empty at zero temperature. There is a *sharp* separation between these two set of

Sect. 1.11



Figure 1.6: Cartoon of susceptibility. Without field the up (left) and down spin states (right) are described by the green curves. The chemical potential for both species is indicated by the red line. Applying a magnetic field decreases the energies of the up spins and increases those of the down spins (dark blue curves). The energy of part of the down-electrons is now above E_F and part of the up electron states below E_F remains empty (grey aeras). Equilibrium is reestablished if we flip the spins of the extra up-electrons, so that the chemical potential for up-and down spins becomes once again the same (red line). These spin-flips create an imbalance of up and down spin populations, and thus a finite magnetization.

states and in particular a discontinuity in the occupation factor n(k) at the Fermi level $k_{\rm F}$. For a non interacting electron gas all states below the Fermi energy are occupied with probability one, all states above with probability zero.

The thermodynamics corresponding to this state, dominated by the Pauli principle, leads to

- 1. A specific heat that is linear in temperature $C_V \propto \gamma T$ for temperatures much smaller than the Fermi energy $(T \ll E_{\rm F})$
- 2. A charge compressibility that goes to a constant κ_0 at zero temperature.
- 3. A spin susceptibility that goes to a constant χ_0 at zero temperature.

For noninteracting electrons, these three constants γ , κ_0 and χ_0 are up to non system dependent constants simply the density of states at the Fermi level ρ_F .

Finally the excitations above the ground state are easy to identify for the case of independent electrons. They consist is adding an electron in an eigenstate of momentum \mathbf{k} and spin σ , or in removing one electron from the occupied states below the Fermi level (in other words creating a hole), again with a well defined momentum and spin.

1.11 Electrons in periodic potentials: band theory

One of the most important features in solids is the presence of the potential imposed by the crystalline structure of the solids. The ions, charged positively act as a periodic potential on the electron and lead to the formation of energy bands.



Figure 1.7: a) independent electrons; b) small overlap between the wavefunctions which defines the hopping integral t.

There are two ways to view the formation of bands. The first one is to start from the free electrons and add a periodic potential on them. The total Hamiltonian of the system becomes

$$H = \frac{p^2}{2m} + V_0 \cos(Qx)$$
 (1.45)

where for simplicity we have written the periodic Hamiltonian in one dimension only. As explained in the previous section, the solutions of the $\frac{P^2}{2m}$ term are plane waves with a given momentum k. In order to understand the effect of the perturbation V_0 one can use simple perturbation theory. The perturbation is important when it couples states that have degenerate energy, which means that the states -Q/2 and Q/2 will be strongly coupled.

We will not follow this route here but look at the second way to obtain the main features of bands, namely to start from the opposite limit where the electrons are tightly bound to one site. Around the atom the electron is characterized by a certain atomic wavefunction $\langle r | \phi_i \rangle = \phi(r - r_i)$ that is not very important here. If the wave function is tightly bound around the atom then the overlap between the wavefunctions is essentially zero

$$\langle \phi_i | \phi_j \rangle = \delta_{ij} \tag{1.46}$$

we assume in the following that the energy corresponding to this atomic wavefunction is E_0 . This is shown in Fig. 1.7

In the following we will forget the notation $|\phi_i\rangle$ and simply denote the corresponding wavefunction by $|i\rangle$ to denote that this is the wavefunction around the *i*-th atom (centered on point r_i). The full state of the system is thus described by the basis of all the functions $|i\rangle$ and the energy of the problem would be

$$H = \sum_{i} E_0 |i\rangle \langle i| \tag{1.47}$$

Of course the wave functions between different sites are not completely orthogonal and there is a small overlap. The dominant one is of course the one between nearest neighbors but this can depend also on the shape of the individual atomic functions that could also favor some directions. This small overlap ensures that $|i\rangle$ is not an eigenstate of the Hamiltonian but that the matrix element $t_{ij} = \langle i|H|j\rangle$ is finite. The tight binding approximation consists in keeping this matrix element while still assuming that the direct overlap between the wavefunctions is zero (1.46). Physically t_{ij} describes the amplitude of tunnelling of a particle from the site r_i to the site r_j . It is important to note that systems such as cold atomic gases in optical lattices are excellent realizations of such a tight binding model. The Hamiltonian becomes

$$H = \sum_{i} E_0 |i\rangle \langle i| - t \sum_{\langle i,j\rangle} |i\rangle \langle j|$$
(1.48)

where we have here for simplicity only retained the overlap between nearest neighbors (denoted by $\langle i, j \rangle$). The first term is the energy of the degenerate atomic levels while the second term t describes the tunnelling between the different sites. The particles will thus delocalize to gain energy from the second term.

In order to solve the Hamiltonian (1.48) one notices that this Hamiltonian is invariant by translation. This means that the momentum is a conserved quantity, and one can simultaneously diagonalize the momentum operator and the Hamiltonian. The eigenstates of the momentum being plane waves, it means that it will be convenient to work in the Fourier space to get a simpler, and hopefully diagonal Hamiltonian. We use

$$|k\rangle = \frac{1}{\sqrt{N_s}} \sum_{j=0}^{N_s - 1} e^{ikr_j} |j\rangle$$

$$|j\rangle = \frac{1}{\sqrt{N_s}} \sum_{k \in BZ} e^{-ikr_j} |k\rangle$$
(1.49)

where N_s is the number of lattice sites. For simplicity we have confined ourselves to one dimension, the generalization being obvious.

Two conditions constraint the allowed values of k. One is the usual quantification condition inside the box $k = \frac{2\pi n}{L}$ where n is a relative integer. As usual in Fourier transform large distances give a condition on the small values of k. Contrarily to the case of the continuum there is here a second condition coming from the fact that the space is discrete and that $r_j = aj$ where j is an integer can only take a set of discrete values. In order to get vectors $|j\rangle$ that are different from the second relation in (1.49) it is necessary for the coefficients in the sum to be different. It is easy to see that translating the value of k by $\frac{2\pi p}{a}$ where p is an integer leaves the exponentials unchanged and thus correspond in fact to identical $|k\rangle$. One must thus restrict the values of k in an interval of size $2\pi/a$. Here it is the small values of r that block the large values of k. One can take any interval. In order to have the symmetry $k \to -k$ obvious it is convenient to choose $[-\pi/a, +\pi/a]$ which is known as the first Brillouin zone. All other values of the k can be deduced by periodicity. The total number of allowed k values is

$$\frac{2\pi}{a}\frac{L}{2\pi} = \frac{L}{a} = N_s \tag{1.50}$$

which is indeed the number of independent states in the original state basis.

Using this new basis we can work out the Hamiltonian. Let us first look at the term

$$H_{\mu} = -\mu \sum_{j=0}^{N_s - 1} |j\rangle\langle j| \tag{1.51}$$

Using (1.49) this becomes

$$H_{\mu} = -\mu \frac{1}{N_s} \sum_{j=0}^{N_s - 1} \sum_{k_1} \sum_{k_2} e^{i(k_1 - k_2)r_j} |k_1\rangle \langle k_2|$$
(1.52)

The sum over j can now be done

$$\frac{1}{N_s} \sum_{j=0}^{N_s - 1} e^{i(k_1 - k_2)r_j} \tag{1.53}$$

If $k_1 = k_2$ the result is obviously 1. If $k_1 \neq k_2$ then one has a geometric series and the sum is

$$\frac{e^{i(k_1-k_2)aN_s}-1}{e^{i(k_1-k_2)a}-1} \tag{1.54}$$

which is always zero given the quantization condition on k. One has thus that the sum is δ_{k_1,k_2} . This gives

$$H_{\mu} = -\mu \sum_{k} |k\rangle \langle k| \tag{1.55}$$

as could be expected the Hamiltonian is diagonal. This could have been even directly written since this is just a chemical potential term counting the total number of particle which can be expressed in the same way regardless of the base (this is just the closure relation).

Let us now look at

$$H = -t \sum_{j=0}^{N_s - 1} |j\rangle \langle j + 1| + \text{h.c.}$$
(1.56)

a similar substitution now leads to

$$H = -t \frac{1}{N_s} \sum_{j=0}^{N_s - 1} \sum_{k_1} \sum_{k_2} e^{i(k_1 - k_2)r_j} e^{ik_2 a} |k_1\rangle \langle k_2| + \text{h.c.}$$
(1.57)

which after the sum over j has been made leads to

$$H = -t\sum_{k} 2\cos(ka)|k\rangle\langle k|$$
(1.58)

The transformed Hamiltonian, known as the tight-binding Hamiltonian thus reads

$$H = -t\sum_{k} 2\cos(ka)|k\rangle\langle k| + E_0\sum_{k}|k\rangle\langle k|$$
(1.59)

As could be expected it is diagonal in k. This is because the initial Hamiltonian is invariant by translation and we have here only one state per unit cell. Thus the number of eigenstates in each k sector is only one. If one has had two atoms per unit cell, going to Fourier space would have reduced the $N_s \times N_s$ matrix to a 2 × 2 to diagonalize and so on. It is thus very important to notice the symmetries of the Hamiltonian and to use them to find the proper base.

The Hamiltonian (1.59) contains the atomic energy E_0 . In the absence of hybridization the ground state is N_s times degenerate since the electrons can be put on each site. When there is hybridization t the electrons can gain energy by delocalizing (another expression of the uncertainty principle), which leads to the formation of energy bands. The tight binding is thus a very simple description that encompasses all the properties of the bands: counting the number of states, the proper analytical properties for the energy etc.

The generalization of the above formula to a square or cubic lattice is straightforward and gives

$$\varepsilon(\mathbf{k}) = -2\sum_{l} t_l \cos(k_l a_l) \tag{1.60}$$

where l denotes each coordinate axis. Close to the bottom of the band one can expand the cosine to get an energy of the form

$$\varepsilon(k) = E_0 - 2t + \sum_l t_l a_l^2 k_l^2 \tag{1.61}$$

this allows to define an effective mass tensor $m_l^* = 1/(2t_l a_l^2)$ by analogy with the energy of free electrons. Here the "mass" has nothing to do with the real mass of the electron but simply describes the facility with which the electron is able to move from one site to the next. The mass can (and in general will) of course be anisotropic since there is no reason why the overlap of atomic orbital in different directions be the same.

It is worth noticing that the filling of the band is crucial for the electronic properties of the system. A system which has one electron per site will fill half of the allowed values of k in the band (because of the spin one value of k can accommodate two electrons of opposite spins). One has thus a half filled band, which usually gives a very good density of states at the Fermi level. One can thus expect, based on independent electrons, in general systems with one electron per site to be good metals. On the contrary a system with two electrons per site will fill all values of k and thus correspond to an insulator, or a semiconductor if the gap to the next band is not too large. It was a tremendous success of band theory to predict based on band filling which elements should conduct or not.

1.12 Theoretical assumptions and experimental realities

How much of the previous estimates and calculation corresponds to the actual solids? Let us start with measurements of the specific heat. Results are shown in Fig. 1.8 where the coefficient of the linear term of the specific heat is given for simple elements. The first observation is that even for the realistic systems the specific heat is still linear in temperature. This is already a little bit surprising since the linear behavior of the temperature is coming from the existence of a sharp discontinuity at the Fermi surface. One could have naively expected that since the energy of the interaction is of the order of the Fermi energy, this discontinuity would be replaced by something else. It is thus surprising to still have a linear T dependence of the specific heat. The independent electron results seem to be much more robust than anticipated. One can nevertheless see from Fig. 1.8 that although the picture of independent electrons works qualitatively it does not work quantitatively and that the coefficient γ can be quite different from the one from the free electron picture.

For the electron gas various factors can enter in this change of γ . First the bandstructure of the material can lead, as we saw, to a strong change of the dispersion relation, and thus to a quite different γ . Second to estimate the effects of the interactions is difficult given their long range nature (with the screening) in solids. An very nice alternative to electrons is provided by ³He. Indeed the ³He atom is a fermion, since it is made of three nucleons. It is neutral, and since the scattering potentials of two 3 He atoms are very well known the interactions are short range and perfectly characterized. In addition the kinetic energy is simply of the form $p^2/(2M)$ so the density of states at the Fermi level are perfectly known. The specific heat coefficient, compressibility and spin susceptibility are shown in Fig. 1.9 Here again one has the surprising result that the independent fermion theory works qualitatively very well. In addition to the specific heat that is linear in temperature, the compressibility is a constant at low temperatures and the spin susceptibility is also a constant. Both these last properties are also strongly dependent on the existence of a sharp discontinuity at the Fermi surface at zero temperature, and it is thus very surprising to see the hold in the presence of interactions. But as for the electron case, one sees that the values of these three quantities are not given by the independent fermion theory, where these three quantities are simply the density of states at the Fermi level. Here we have three independent numbers, which clearly vary as a function of the interaction, as can be seen by the pressure dependence of these quantities. Indeed increasing the pressure changes the density of particles, and thus the interaction between them (the change in kinetic energy and density of states can be computed very precisely in that case). We will thus have to understand this very puzzling experimental fact.

ELEMENT	FASE ELECTRON 7 (in 10 ⁻⁴ cal-m	MEASURED y ole ⁻¹ -K ⁻²)	RATIO* (m*/m)
Li	1.8	4.2	23
Na	2.6	3.5	13
K	4.0	4.7	1.2
Rb	4.6	5.8	1.3
Cs	5.3	7.7	15
Cu	1.2	1.6	13
Ag	1.5	1.6	1.1
Au	1.5	1.6	1.1
Be	1.2	0.5	0.42
Mg	24	3.2	13
Ca	3.6	6.5	1.8
Sr	4.3	8.7	20
Ba	4.7	6.5	1.4
Nb	1.6	20	12
Fe	1.5	12	8.0
Mn	1.5	40	27
Za	1.8	1.4	0.78
Cd	2.3	1.7	0.74
Hg	2.4	5.0	21
A	2.2	3.0	1.4
Ga	24	1.5	0.62
In	2.9	43	15
n	3.1	3.5	1.1
Sn	3.3	4.4	13
Pb	3.6	7.0	1.9
Bi	4.3	0.2	0.047
Sb	3.9	1.5	0.38

Figure 1.8: Coefficient γ of the linear term in temperature for the specific heat, both from free electron calculations and measured for simple elements (From the textbook on solid state physics by Ashcroft & Mermin). This shows that for realistic systems, the specific heat still exhibits a linear temperature dependence at low temperatures, just like for free electrons. The slope γ is different from the one of free electrons and allows to define an effective mass m^* .



Figure 1.9: Effective mass m^* normalized to the bare mass m of the ³He atom, as extracted from the specific heat measurements and as a function of pressure P. The notation $(1 + F_0^a)^{-1}$ is the ratio between the spin susceptibility and the effective mass. κ/κ_0 is the normalized (with respect to free particles) compressibility. One sees that although the basic properties of free fermions still work (specific heat linear in temperature, constant compressibility, constant susceptibility at low temperature), the coefficients characterizing these three quantities are three different numbers, dependent on the pressure, hence on the interactions.

CHAPTER 2

Quantum many-body theory

In much of what has been treated until now, we have only tried to solve the Schroedinger equation of one particle at a time. While in some cases the problem at stake involves more than one particle, we always try to invent tricks such as to simplify to a single-particle problem. However, this is not always possible of course, and so it is important to learn how to formulate and solve many-body physics in quantum mechanics. The purpose of this chapter is to familiarize the student with the quantum mechanics of fields in the context of condensed matter physics. While in many respects equivalent to quantum-field theory of elementary particle physics, the electrons in a solid move relatively slowly, hence relativistic effects are small and can be treated perturbatively. A well-known example is spin-orbit coupling.

Assume that we have a system with two particles, let's say one electron and one neutron, each separately trapped in some potential well, the electron in a state with wavefunction $\psi_a(r_1)$ and the neutron in $\psi_b(r_2)$. The wavefunction describing the two particles together will be something of the form

$$\Psi(r_1, r_2) = \psi_a(r_1)\psi_b(r_2) \tag{2.1}$$

Suppose now that we have two ⁴He atoms instead of an electron and a neutron. We will discover below, that in this case the wavefunction of the two particles together is *not* given by $\psi_a(r_1)\psi_b(r_2)$.

2.1 Bosons

In order to show this, let us first talk about a different type of boson, namely quanta of vibration. For this purpose we choose the example of a nitrogen molecule. Since eighty percent of what you have been breathing in and out since you were born is nitrogen molecules, it seems reasonable enough that we spend a little thought on that from time to time. The molecule consists of two nitrogen nuclei consisting of 7 protons and 7 neutrons, and each atom surrounded by 7 electrons. Four of those are deeply bound by the nuclear potential. The other three form the covalent bond between the two nitrogen atoms of the molecule. Electronic excitations are rather costly in energy, the lowest one occurring at about 8 eV. The low energy scale properties have therefor to do with the vibration of the two nuclei against each other in the background of their electronic clouds. In equilibrium the distance between the two nuclei is $r_0 = 0.15$ nm. This distance represents the minimum of the effective potential energy for the nuclear coordinates, defined as the sum of the electron energies and the Coulomb interaction between the nuclei. For small displacements $x = r - r_0$ away from this minimum we can expand the potential energy as $E_p(x) = E(r_0) + fx^2/2 + gx^3$, where m is the reduced mass of the relative motion of the two nuclei, and f represents the effective force constant. Neglecting the terms gx^3 and higher

order, the vibrational motion is then described by the Hamiltonian

$$\hat{H} = E(r_0) - \frac{\hbar^2}{2m}\hat{\partial}_x^2 + \frac{m\omega^2}{2}\hat{x}^2$$
(2.2)

where m is the reduced mass of the relative motion (0.5*14=7 times the proton mass), and $\omega = \sqrt{f/m}$ is the vibrational frequency of the classical equations of motion. The Schroedinger equation can be solved straightforwardly of course, but for the present discussion we use an ingeneous trick of quantum mechanics, which is to substitute the following expression for \hat{x} and $\hat{\partial}_x$:

$$\hat{\partial}_x = \sqrt{\frac{m\omega}{2\hbar}} \{a - a^{\dagger}\}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \{a + a^{\dagger}\}$$
(2.3)

It is easy to verify that the operators a and a^{\dagger} satisfy the commutation relations

$$[a, a^{\dagger}] = 1$$

$$[a^{\dagger}, a^{\dagger}] = 0$$

$$[a, a] = 0$$

$$(2.4)$$

The transformed Hamiltion is

$$H = E(r_0) + \frac{\hbar\omega}{2} + \hbar\omega a^{\dagger}a \tag{2.5}$$

The set of eigenstates of this Hamiltonian consists of a series of equidistant energy levels

$$\langle n|H|n\rangle = E(r_0) + \frac{\hbar\omega}{2} + n\hbar\omega$$
 (2.6)

Since the operators a^{\dagger} and a have the property to raise and lower the energy of the harmonic oscillator by increments of $\hbar\omega$

$$a^{\dagger} |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$
(2.7)

they are called raising and lowering operators. Now there exists an interesting analogy here with the situation of indistinguishable particles. Suppose that we wouldn't know that we are actually dealing with a nitrogen molecule because we have put it in a box. We could make several of such boxes, each containing a nitrogen molecule. We would also be able to measure the weight of these boxes. So let's say, that we have a few hundred boxes, and we have measured the weight of each of them. We would notice that each box has a weight $M_{box} + nM_{particle}$, where n is an integer number which is different from one box to another. If we can't look inside the boxes, we have no way to tell that in fact $M_p c^2 = \hbar \omega$, corresponding to a quantum of vibrational energy of the nitrogen molecule in it. We would probably arrive at the conclusion that a box with weight $M_{box} + nM_{particle}$ must contain n particles with the same mass, $M_{particle}$. If we bring two boxes in contact with each other it will be possible to exchange a quantum of energy between them. If we than measure the weight again, we would conclude that one of the particles has tunneled from one box to another. So for all practical purposes the vibrational quanta behave as if they are particles. Now for the following discussion it is important to emphasize that these particles are intrinsically indistinguishable. That is to say: We start with box 1 having mass M_{box} and box 2 with mass $= M_{box} + 5M_{particle}$. We now put them in contact, such as to enable tunneling of energy quanta between the boxes. For example, after some time box 1 might have mass

 $= M_{box} + M_{particle}$, and box 2 would than have mass $= M_{box} + 4M_{particle}$. If the mass $M_{particle}$ would come from distinguishable particles (let's say marbles, each with a different color), 5 different possibilities exist, according to the color of the marble that has tunneled from one box to another. However, in reality we have just changed the energy of the molecule in box 2 from $5\hbar\omega$ to $4\hbar\omega$, and the one in box 1 from 0 to $\hbar\omega$, and there is only one way in which one can do this. So the energy quanta are indistinguishable particles, where *indistinguishable* has very strong consequences for the entropy of the system.

We take the description one step further by associating the position of the j'th box, r_j , to the raising and lowering operators of the molecules inside them. This leads to the Hamiltonian

$$H = E_0 + \sum_j \hbar \omega a^{\dagger}(r_j) a(r_j)$$
(2.8)

with the commutation relations

$$[a(r_i), a^{\dagger}(r_j)] = \delta_{i,j}$$

$$[a^{\dagger}(r_i), a^{\dagger}(r_j)] = 0$$

$$[a(r_i), a(r_j)] = 0$$
(2.9)

In a next step we could take into account the tunneling probability between the boxes. If they form a regular array the result would be solutions in the form of Bloch-waves,

$$H = E_0 + \sum_k \hbar \omega_k a_k^{\dagger} a_k \tag{2.10}$$

where $a_k = N_s^{-1/2} \sum_j e^{ikr_j} a(r_j)$ with the commutation relations

$$[a_k, a_p^{\dagger}] = \delta_{k, p+Q}$$

$$[a_k^{\dagger}, a_p^{\dagger}] = 0$$

$$[a_k, a_p] = 0$$
(2.11)

where Q is a reciprocal lattice vector. Interestingly, certain elementary particles such as photons, W-bosons or Z-bosons behave in exactly this way. For the electromagnetic field in vacuum one has for example

$$\hat{H} = \int d^3r \left(\frac{\hat{B}(r)^2}{2\mu_0} + \frac{\hat{E}(r)^2}{2\epsilon_0} \right)$$
(2.12)

where $\hat{B}(r)$ and $\hat{E}(r)$ are non-commuting operators. The details of this treatment are outside the scope of these lecture notes, and can be found in textbooks on electromagnetism. Properly weighted linear combinations of \hat{B}_k and \hat{E}_k correspond again to raising and lowering operators, so that

$$\hat{H} = E_0 + \hbar c \sum_{k} |\mathbf{k}| a_{k}^{\dagger} a_{k}$$
(2.13)

Notice an important difference with the previous case: The vibrational modes of the nitrogen molecule are described by a wavefunction of x which exists in coordinate space. In the case of the electromagnetic field it is not the coordinate that is described by a quantum mechanical wavefunction, but components of the electromagnetic fields \hat{B} and \hat{E} . One can in a way regard the electromagnetic field amplitude as a quantum harmonic oscillator in an extra dimension orthogonal to x,y,z and t.

The indistinguishable particles defined above satisfy a particular set of commutation relations, by virtue of which they are classified as bosons. We will come to the (only) other type (fermions) in the next section. Let us take a closer look now at the raising and lowering operators. From the earlier expressions in this section one easily obtains after Fourier transformation the following properties

$$a_{k}^{\dagger} |n_{k}\rangle = \sqrt{n_{k} + 1} |n_{k} + 1\rangle$$

$$a_{k} |n_{k}\rangle = \sqrt{n_{k}} |n_{k} - 1\rangle$$
(2.14)

These properties completely define the operators by their matrix elements between all the elements of a complete basis. Let us check that the operators a_k^{\dagger} and a_k are indeed hermitian conjugate. The only non-zero matrix element for a_k^{\dagger} is

$$\langle n_k + 1 | a_k^{\dagger} | n_k \rangle = \sqrt{n_k + 1} \tag{2.15}$$

Taking the complex conjugate of the above expression one thus gets

$$\langle n_k | a_k | n_k + 1 \rangle = \sqrt{n_k + 1} \tag{2.16}$$

which is indeed exactly the definition of the operator a_k in (2.14) (with the replacement of n_k by $n_k + 1$). Another important properties of the operators, is that they only span the Fock space (i.e. the space of all many-particle states of all possible numbers of particles). Indeed although it seems formally from (2.14) that the operator a_k could operate on a state that has $n_k = 0$ particles in the state k the prefactor in the definition ensures that the corresponding matrix element is zero

$$a_k \left| n_k = 0 \right\rangle = 0 \tag{2.17}$$

and thus if one tries to apply the annihilation operator on a state that has no particle in the corresponding quantum state one cannot generate unphysical states.

If we define the state that contains no particles in any of the quantum states (sometimes referred to as the vacuum)

$$|0\rangle = |n_1 = 0, n_2 = 0, \dots, n_\Omega = 0\rangle$$
(2.18)

it is easy to see that from this vacuum $|0\rangle$ and the operators a_i^{\dagger} we can construct all the vectors of the complete basis of the Fock space, since

$$|n_1, \dots, n_i, \dots, n_{\Omega}\rangle = \frac{(a_1^{\dagger})^{n_1} \dots (a_{\Omega}^{\dagger})^{n_{\Omega}}}{\sqrt{n_1!} \dots \sqrt{n_{\Omega}!}} |0\rangle$$
(2.19)

Thus one can completely describe the Fock space from the single state $|0\rangle$ and the creation (and annihilation since they are hermitian conjugate) operators. Note that the vacuum verifies the property that for any i

$$a_i \left| 0 \right\rangle = 0 \tag{2.20}$$

Note also that one should not mix up the number 0 with $|0\rangle$. The latter is a vector in Fock space. Operators can act upon it resulting in other vectors in Fock space. To illustrate the difference: $0 \times 0 = 0$, whereas $\langle 0|0\rangle = 1$.

The creation and annihilation operators constitute thus a very convenient way of describing the Fock space. Rather than defining them from their matrix elements in a given basis, it is more convenient do define them from their intrinsic properties.

Let us give some examples. Elementary particles such as photons, W- or Z- bosons, or composite particles such as helium atoms are bosons. We begin by the question as to how to represent the wavefunction in coordinate space of a boson, using the field-theoretical language of quantized fields that we have introduced above. Suppose that the boson occupies a specific space coordinate \mathbf{r} . Note that such a state is usually not an eigenstate of the Hamiltonian. We indicate the corresponding wavefunction describing the particle coordinate \mathbf{r}' as $\psi_{\mathbf{r}}(\mathbf{r}')$. In fact, $|\psi_{\mathbf{r}}(\mathbf{r}')|^2$ should be a Dirac δ -function: $|\psi_{\mathbf{r}}(\mathbf{r}')|^2 = \delta(\mathbf{r}' - \mathbf{r})$. We indicate the corresponding Bosons

vector in Hilbert space as $|r\rangle$. In field-theoretical language we need the following notation for the operators which create and annihilate a particle at a particular space coordinate r:

$$\begin{aligned} a^{\dagger}(\boldsymbol{r}) \left| 0 \right\rangle &= \left| \boldsymbol{r} \right\rangle \\ a(\boldsymbol{r}) \left| \boldsymbol{r} \right\rangle &= \left| 0 \right\rangle \\ \left[a(\boldsymbol{r}), a^{\dagger}(\boldsymbol{r}') \right] &= \delta(\boldsymbol{r} - \boldsymbol{r}') \end{aligned}$$
 (2.21)

where the third line is a consequence of the orthogonality of the set $\{|\mathbf{r}_{j}\rangle\}$ (j = 1, ...) of vectors in Hilbert-space describing bosons localized at space coordinates \mathbf{r}_{j} . Consider now a boson which occupies a state $|\beta\rangle$ described by some wavefunction, which we will indicate as $\psi_{\beta}(\mathbf{r})$. We can define a creation operator a_{β}^{\dagger} , which creates such as state from the vacuum

$$\beta \rangle = a_{\beta}^{\dagger} \left| 0 \right\rangle \tag{2.22}$$

We now ask the question what the inner product $\langle \boldsymbol{r}|\beta\rangle$ corresponds to. In fact, this is the projection on the state $|\beta\rangle$ of the state $|\boldsymbol{r}\rangle$ where the particle is localized at coordinate \boldsymbol{r} . In other words,

$$\langle \boldsymbol{r}|\beta\rangle = \psi_{\beta}(\boldsymbol{r}) \tag{2.23}$$

and the absolute square of this is just the probability to find the particle at this space coordinate. This identification implies a useful property of the corresponding creation and annihilation operators. We know that operating with an annihilation operator on the vacuum gives $a_{\beta} |0\rangle = 0$. We can therefore write

$$\langle \boldsymbol{r}|\beta\rangle = \langle 0|a(\boldsymbol{r})a^{\dagger}_{\beta}|0\rangle - \langle 0|a^{\dagger}_{\beta}a(\boldsymbol{r})|0\rangle$$
(2.24)

Of course, it makes no difference which sign we write in front of the second term on the righthand side, since it is zero. However, we like to generalize the definition of the single-particle wave-function, to states where other bosons are present as well, in other words if we wish to replace $|0\rangle$ in the above expression by an arbitrary state vector $|\Psi\rangle$. This generalization is the following:

$$[a(\boldsymbol{r}), a_{\beta}^{\dagger}] = \psi_{\beta}(\boldsymbol{r}) \qquad \text{for bosons}$$
(2.25)

Note, that on the left hand side we have two operators. Their commutator renders the <u>scalar</u> value on the righthand side of the expression, corresponding to the single particle wavefunction. In the following section we will see, that for fermions we have to replace the commutators with anticommutators in these expressions. Let us now investigate the following two-particle state

$$|1,2\rangle = a_1^{\dagger} a_2^{\dagger} |0\rangle \tag{2.26}$$

Obviously the function contains two bosons. One can reconstruct the expression of the wavefunction $\langle \mathbf{r}, \mathbf{r}' | 1, 2 \rangle$. With the help of the operators which create and annihilate a particle at a particular space coordinate \mathbf{r} :

$$\langle \boldsymbol{r}, \boldsymbol{r}' | 1, 2 \rangle = \langle 0 | \boldsymbol{a}(\boldsymbol{r}) \boldsymbol{a}(\boldsymbol{r}') \boldsymbol{a}_1^{\dagger} \boldsymbol{a}_2^{\dagger} | 0 \rangle \tag{2.27}$$

We now proceed by moving the two creation operators to the left hand side of the expression step by step. In the first step we have to interchange $a(\mathbf{r}')$ and a_1^{\dagger} . To do so we can insert the identity $a(\mathbf{r}')a_1^{\dagger} = a_1^{\dagger}a(\mathbf{r}') + \psi_1(\mathbf{r}')$. This leaves the expression

$$\langle \boldsymbol{r}, \boldsymbol{r}' | 1, 2 \rangle = \langle 0 | \boldsymbol{a}(\boldsymbol{r}) \boldsymbol{a}_{1}^{\dagger} \boldsymbol{a}(\boldsymbol{r}') \boldsymbol{a}_{2}^{\dagger} | 0 \rangle + \psi_{1}(\boldsymbol{r}') \langle 0 | \boldsymbol{a}(\boldsymbol{r}) \boldsymbol{a}_{2}^{\dagger} | 0 \rangle$$
(2.28)

In the bracket of the second term we recognize immediately $\langle 0|a(\mathbf{r})a_2^{\dagger}|0\rangle = \psi_2(\mathbf{r})$. We proceed in the same way by exchanging $a(\mathbf{r}')$ and a_2^{\dagger} in the first term, yielding

$$\langle \boldsymbol{r}, \boldsymbol{r}' | 1, 2 \rangle = \langle 0 | a(\boldsymbol{r}) a_1^{\dagger} a_2^{\dagger} a(\boldsymbol{r}') | 0 \rangle + \psi_2(\boldsymbol{r}') \langle 0 | a(\boldsymbol{r}) a_1^{\dagger} | 0 \rangle + \psi_1(\boldsymbol{r}') \psi_2(\boldsymbol{r})$$
(2.29)

The first term gives zero, since $a(\mathbf{r}')|0\rangle = 0$, and the bracket in the second term is $\psi_1(\mathbf{r})$. Together we obtain therefore

$$\langle \mathbf{r}, \mathbf{r}' | 1, 2 \rangle = \psi_2(\mathbf{r}')\psi_1(\mathbf{r}) + \psi_1(\mathbf{r}')\psi_2(\mathbf{r})$$
 (2.30)

We discover, that the wavefunction is even for the interchange of the coordinates of two bosons. It is easy to generalize this, and show that the wavefunction of N identical bosons satisfies:

$$\Psi(r_1, .., r_j, .., r_m, .., r_N) = \Psi(r_1, .., r_m, .., r_j, .., r_N)$$
(2.31)

in other words: the many-body wavefunction of N identical bosons has even parity under the exchange of coordinates of any pair of bosons. Note also, that this function is not normalized. The interest of the second quantization however is to stick with the operators and avoid coming back to the quite untractable wavefunctions. We see that we can deduce many things directly from the commutation relations. For example since $a_1^{\dagger}a_2^{\dagger} = a_2^{\dagger}a_1^{\dagger}$ from the commutation relation we see that

$$a_1^{\dagger} a_2^{\dagger} \left| 0 \right\rangle = a_2^{\dagger} a_1^{\dagger} \left| 0 \right\rangle \tag{2.32}$$

and thus the wavefunction $|1,2\rangle$ is obviously symmetric by permutation of the particles. The creation and annihilation operators are thus directly engineered to take properly care of the symmetrization of the wavefunctions and the indiscernibility of the particles. One can in fact extract a lot more directly from the commutation relations. In particular averages can be computed easily directly.

Let us illustrate it by looking at the normalization of the function $|1,2\rangle$. We want to compute

$$\langle 1, 2|1, 2\rangle = \langle 0|a_2a_1a_1^{\dagger}a_2^{\dagger}|0\rangle \tag{2.33}$$

although this is here a specific example, we will see that quite generally all physical observables reduce to the average in the vacuum of a certain product of creation and annihilation operators, so the method illustrated here can be applied generally. In order to compute the average, the only thing we need to use is the fact that the vacuum is destroyed by the a_i . We should thus bring back, using the commutation relations the operator a_i to act on the vacuum. Here we use $a_1a_1^{\dagger} = 1 + a_1^{\dagger}a_1$ from the commutation relation. One has thus

The second term is simple. We can use the commutation relation $a_1a_2^{\dagger} = a_2^{\dagger}a_1$ to rewrite the second term as $\langle 0|a_2a_1^{\dagger}a_2^{\dagger}a_1|0\rangle$ which immediately gives zero. $\langle 1,2|1,2\rangle$ is thus only given by the first term. Using again the commutation relations one obtains

$$\langle 1, 2|1, 2 \rangle = \langle 0|a_2a_2'|0 \rangle = \langle 0|(1 + a_2'a_2)|0 \rangle$$

= $\langle 0|1|0 \rangle$ (2.35)
= 1

Although the calculations can become tedious when the number of operator grows, the mechanics is always the same. With a little bit of habit one can speed up the calculations.

To come back to the ⁴He atoms. Here now we have real particles, which we can hold in our hand so to speak. So it would seem a bit weird that they would be indistinguishable in just the same way as the vibrational quanta and electromagnetic field quanta of the preceding discussion. Yet, it turns out that for all practical purposes they actually do behave as indistinguishable particles, more precisely, as bosons. Due to the fact that the two ⁴He atoms are indistinguishable particles, we have to take into account the fact that it is fundamentally impossible to tell them apart. One of the consequences is the occurrence of superfluidity at 2.17 Kelvin. Replacing ⁴He with ³He renders the atoms fermion-like, and the experimental consequences are huge. In particular superfluidity occurs at a 3 orders of magnitude lower temperature of 2.7 mK.

2.2 Fermions

Let us now turn to the creation and annihilation operators for Fermions. In a similar way as for bosons (2.14) we define

$$c |1\rangle = |0\rangle$$

$$c^{\dagger} |0\rangle = |1\rangle$$

$$c |0\rangle = 0$$

$$c^{\dagger} |1\rangle = 0$$
(2.36)

Since for Fermions the Pauli principle prevents two fermions to be in the same quantum number, it means that the occupation numbers n are restricted to be either 0 or 1. It is thus important that the creation operator is not able to create two particles in one state. Just as for the bosons, we can use labels to attribute creation operators to identify a particular state in Hilbert space. In particular, in what follows labels i, j refer to a set of orthogonal states in Hilbert space. Instead of the commutation relations that we found for the bosons, the fermion creation and annihilation operators satisfy the following anti-commutation relations

$$\begin{cases} \{c_i, c_j^{\dagger}\} = \delta_{i,j} \\ \{c_i^{\dagger}, c_j^{\dagger}\} = 0 \\ \{c_i, c_j\} = 0 \end{cases}$$

$$(2.37)$$

where $\{\hat{a}, \hat{b}\} = \hat{a}\hat{b} + \hat{b}\hat{a}$, all the aforementioned properties are immediately achieved. We leave it as an exercise for the reader to demonstrate this !! In the same way as for the bosons the c_i and c_i^{\dagger} can be used to construct all the states of the Fock space from a vacuum $|0\rangle$ which is destroyed by all the c_i ($c_i |0\rangle = 0$) using the relation (2.19).

Wavefunctions and averages can be computed by exactly the same techniques that were given for the bosons. As an example let us look at the function with two fermions in the states 1 and 2

$$|1,2\rangle = c_1^{\dagger} c_2^{\dagger} |0\rangle \tag{2.38}$$

In order to do so, we use the notation for the operators which create and annihilate a fermion at a particular space coordinate r:

†() (o) ()

$$c^{\dagger}(\boldsymbol{r}) |0\rangle = |\boldsymbol{r}\rangle$$

$$c(\boldsymbol{r}) |\boldsymbol{r}\rangle = |0\rangle$$

$$\{c(\boldsymbol{r}), c^{\dagger}(\boldsymbol{r}')\} = \delta(\boldsymbol{r} - \boldsymbol{r}')$$
(2.39)

A single particle wave-function is described by the anti-commutator

$$\{c_{\beta}^{\dagger}, c(\boldsymbol{r})\} = \psi_{\beta}(\boldsymbol{r})$$
 for fermions (2.40)

which is similar to the boson-case, except that we now have an anti-commutator instead of a commutator. To see what this means in terms of single particle wavefunctions, we proceed in a similar way as for the bosons (i.e. the method which resulted in Eq. 2.30) by moving the creation operators to the left of the expression. The important difference is, that for fermions we create a minus sign every-time we exchange the order of two creation- or annihilation operators. After a few manipulations similar to the boson case we arrive at

$$\langle \boldsymbol{r}, \boldsymbol{r}' | 1, 2 \rangle = \psi_1(\boldsymbol{r}) \psi_2(\boldsymbol{r}') - \psi_1(\boldsymbol{r}') \psi_2(\boldsymbol{r})$$
(2.41)

where $\psi_j(\mathbf{r}_i) = \langle \mathbf{r}_i | \psi_j \rangle$. We discover, that the wavefunction is odd for the interchange of the coordinates of two fermions. It is easy to generalize this, and show that the wavefunction of N identical fermions satisfies in general:

$$\Psi(r_1, ..., r_j, ..., r_m, ..., r_N) = -\Psi(r_1, ..., r_m, ..., r_j, ..., r_N)$$
(2.42)

in other words: the many-body wavefunction of N identical fermions has odd parity under the exchange of coordinates of any pair of fermions. Note also, that, as was the case for the bosons, the two-particle wave-function defined in this way is not normalized: in the present case $\int \int |\langle \mathbf{r}, \mathbf{r}' | 1, 2 \rangle|^2 d\mathbf{r}\mathbf{r}' = 2$. On the other hand it remains true that $\langle \mathbf{r}, \mathbf{r}' | \mathbf{r}\mathbf{r}' \rangle = 1$ and $\langle 1, 2 | 1, 2 \rangle = 1$. In general proper attention needs to be given to normalization of the wavefunction when calculating quantum averages with many-body wavefunctions. Without going to the wavefunction one can directly see the antisymmetrization at the operator level. Using the anticommutation relation $\{c_1, c_2\} = 0$ one sees that

$$c_1^{\dagger}c_2^{\dagger}\left|0\right\rangle = -c_2^{\dagger}c_1^{\dagger}\left|0\right\rangle \tag{2.43}$$

and thus the wavefunction $|1,2\rangle$ is obviously antisymmetric by permutation of the particles.

The fact that the antisymmetrization is taken care of automatically by the operator c_i makes it very convenient to write even complicated functions. For example the Fermi sea corresponds to a state where all states with a lower energy that the Fermi energy are occupied. To describe the one particle state we introduce a complete basis. For the orbital part we can take the momentum basis $|\mathbf{k}\rangle$. We can take the two eigenstates of S_z denoted either $|\uparrow\rangle$ or $|\downarrow\rangle$ or $|\sigma_z = \pm\rangle$, for the complete basis in the spin sector. The states m are thus $m = (\mathbf{k}, \sigma_z = \pm)$. We can define the corresponding creation operators $c^{\dagger}_{\mathbf{k},\sigma}$ which creates an electron with the momentum \mathbf{k} and the spin $\sigma = \uparrow, \downarrow$. In terms of these operators the Fermi sea is simply

$$|\mathbf{F}\rangle = \prod_{\boldsymbol{k},\varepsilon_{\boldsymbol{k}}<\varepsilon_{F}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{\boldsymbol{k}\downarrow} |0\rangle$$
(2.44)

Averages in the void can be computed by exactly the same technique than described for the bosons. For example, if we take $|\beta\rangle = c_{\beta}^{\dagger} |0\rangle$, then (using the anticommutation relations)

$$\langle \beta | \beta \rangle = \langle 0 | c_{\beta} c_{\beta}^{\dagger} | 0 \rangle$$

= $\langle 0 | (1 - c_{\beta}^{\dagger} c_{\beta}) | 0 \rangle$
= $\langle 0 | 1 | 0 \rangle = 1$ (2.45)

Generalizing the above calculation we see that $\langle F|F \rangle = 1$.

2.3 One body operators

Now that we have operators that allow to construct the whole Fock space, what remains to be done is to express the physical observables we want to compute in terms of these operators. In order to do that we have to take into account that the physical observables have to act on indistinguishable particles, which sets some constraints on what they can be. To give the expression of the observables in second quantization we have to sort out observables in terms of how many particles are involved. Indeed there are physical observables that measure only the quantum numbers of *one* particle at a time (such as measuring the momentum, density, etc. of the particles) and others that need to deal with the quantum numbers of two of the particles to determine the matrix elements. This is for example the case of the operator measuring the interactions between the particles. The first type is called one body operators, while the second one is two body operators. One can have in principle operators that involve more than two particles to get the matrix elements (such as three body collisions and up) but they are of little use in practice in solid state physics, so we will mostly discuss here the one and two body operators. The formulas given here can be easily generalized if need be.

Let us start with the operator measuring the density of particles at a point r in coordinate space. The operator giving such a density for one particle is

$$\rho^{(1)}(\boldsymbol{r}) = |\boldsymbol{r}\rangle\langle\boldsymbol{r}| \tag{2.46}$$

In first quantization $\langle \psi | \rho^{(1)}(\boldsymbol{r}) | \psi \rangle = |\psi(\boldsymbol{r})|^2$. In second quantization the form of the operator will depend on the choice of the complete basis m we take. Let us start by taking the basis of the position $|\boldsymbol{r}\rangle$. In that case the operator $c^{\dagger}(\boldsymbol{r})$ is the operator creating a particle at point \boldsymbol{r} . Using this basis one obtains

$$\hat{\rho}(\boldsymbol{r}) = \sum_{\boldsymbol{r}''\boldsymbol{r}'} \langle \boldsymbol{r}' | \boldsymbol{r} \rangle \langle \boldsymbol{r} | \boldsymbol{r}'' \rangle c^{\dagger}(\boldsymbol{r}') c(\boldsymbol{r}'')$$

$$= \sum_{\boldsymbol{r}'\boldsymbol{r}''} \delta(\boldsymbol{r} - \boldsymbol{r}') \delta(\boldsymbol{r} - \boldsymbol{r}'') c^{\dagger}(\boldsymbol{r}') c(\boldsymbol{r}'')$$

$$= c^{\dagger}(\boldsymbol{r}) c(\boldsymbol{r})$$
(2.47)

The expression $c^{\dagger}(\mathbf{r})c(\mathbf{r})$ is particularly simple to understand. The operator $c^{\dagger}(\mathbf{r})c(\mathbf{r})$ destroys and recreate a particle in the same quantum state. Thus it has changed nothing on the system. However the action of the operator $c(\mathbf{r})$ will give zero if there is no particle in the corresponding quantum state (here a particle at the point \mathbf{r}) to destroy. The operator $c^{\dagger}(\mathbf{r})c(\mathbf{r})$ thus gives zero if there is no particle in the corresponding quantum state and one if there is one particle. It thus simply counts the number of particles at the point \mathbf{r} . Quite generally the operator $c^{\dagger}_{m}c_{m}$ simply counts the number of particles in the state m. The total number of particles in the system is simply given by the expectation value of the particle number operator

$$\hat{N} = \int d\boldsymbol{r} \, c^{\dagger}(\boldsymbol{r}) c(\boldsymbol{r}) \tag{2.48}$$

The generalization to the case of particles with spins is obvious

$$\hat{\rho}(\boldsymbol{r}) = c_{\uparrow}^{\dagger}(\boldsymbol{r})c_{\uparrow}(\boldsymbol{r}) + c_{\downarrow}^{\dagger}(\boldsymbol{r})c_{\downarrow}(\boldsymbol{r})$$
(2.49)

For particles with spins we can compute the spin density along z at the point r. In that case the operator is

$$\hat{\sigma}_{z}(\boldsymbol{r}) = \sum_{\sigma\sigma'} \langle \sigma | S_{z} | \sigma' \rangle c_{\sigma}^{\dagger}(\boldsymbol{r}) c_{\sigma'}(\boldsymbol{r}) = \frac{1}{2} (c_{\uparrow}^{\dagger}(\boldsymbol{r}) c_{\uparrow}(\boldsymbol{r}) - c_{\downarrow}^{\dagger}(\boldsymbol{r}) c_{\downarrow}(\boldsymbol{r}))$$
(2.50)

In a similar way the spin density along the x and y directions gives

$$\hat{\sigma}_{x}(\boldsymbol{r}) = \frac{1}{2} (c_{\uparrow}^{\dagger}(\boldsymbol{r})c_{\downarrow}(\boldsymbol{r}) + c_{\downarrow}^{\dagger}(\boldsymbol{r})c_{\uparrow}(\boldsymbol{r}))
\hat{\sigma}_{y}(\boldsymbol{r}) = \frac{i}{2} (c_{\uparrow}^{\dagger}(\boldsymbol{r})c_{\downarrow}(\boldsymbol{r}) - c_{\downarrow}^{\dagger}(\boldsymbol{r})c_{\uparrow}(\boldsymbol{r}))$$
(2.51)

Alternatively we could have used the basis of the eigenstates of the momentum $|\mathbf{k}\rangle$ where

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{\sqrt{\Omega}} e^{i \boldsymbol{k} \boldsymbol{r}}$$
(2.52)

Since the spin and orbital part are independent in the above we will just give the expressions for the spinless case, the addition of the spin sector being exactly as above. The operator c_k thus now destroys a particle with momentum k (i.e. in a plane wave state with momentum k).

Using (2.47) one gets

$$\hat{\rho}(\boldsymbol{r}) = c^{\dagger}(\boldsymbol{r})c(\boldsymbol{r}) = \\ = \left[\sum_{\boldsymbol{k}} c_{\boldsymbol{k}}^{\dagger} \langle \boldsymbol{k} | \boldsymbol{r} \rangle\right] \left[\sum_{\boldsymbol{p}} \langle \boldsymbol{r} | \boldsymbol{p} \rangle c_{\boldsymbol{p}}\right] = \\ = \frac{1}{\Omega} \sum_{\boldsymbol{k}\boldsymbol{p}} e^{-i\boldsymbol{k}\boldsymbol{r}} e^{i\boldsymbol{p}\boldsymbol{r}} c_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{p}}$$
(2.53)

The expression (2.53) is not as simple as (2.47) since the density operator is not diagonal in the momentum basis. However both (2.53) and (2.47) represent the same operator. This gives us a direct connection between the operators creating a particle at point r and the ones creating a particle with momentum k. Comparing the expressions (2.53) and (2.47) one gets

$$c(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum e^{i\mathbf{k}\mathbf{r}} c_{\mathbf{k}}$$
(2.54)

Using the expression (2.53) we can also compute the total number of particles in the system

$$\hat{N} = \int d\mathbf{r} \frac{1}{\Omega} \sum_{\mathbf{k}\mathbf{p}} e^{-i\mathbf{k}\mathbf{r}} e^{i\mathbf{p}\mathbf{r}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{p}}$$

$$= \sum_{\mathbf{k}\mathbf{p}} \delta_{\mathbf{k},\mathbf{p}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{p}}$$

$$= \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$
(2.55)

Keeping in mind that $c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}$ simply counts the number of particles in the quantum state \mathbf{k} , one gets again that the total number of particles is the sum of all numbers of particles in all possible quantum states.

Finally one can use (2.53) to get a simple expression of the Fourier transform of the density

$$\hat{\rho}_{\boldsymbol{q}} = \int d\boldsymbol{r} e^{i\boldsymbol{q}\boldsymbol{r}} \hat{\rho}(\boldsymbol{r})$$

$$= \int d\boldsymbol{r} e^{i\boldsymbol{q}\boldsymbol{r}} \frac{1}{\Omega} \sum_{\boldsymbol{k}\boldsymbol{p}} e^{-i\boldsymbol{k}\boldsymbol{r}} e^{i\boldsymbol{p}\boldsymbol{r}} c^{\dagger}_{\boldsymbol{k}} c_{\boldsymbol{p}}$$

$$= \sum_{\boldsymbol{k}\boldsymbol{p}} \delta_{\boldsymbol{p},\boldsymbol{k}-\boldsymbol{q}} c^{\dagger}_{\boldsymbol{k}} c_{\boldsymbol{p}}$$

$$= \sum_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}/2} c_{\boldsymbol{k}-\boldsymbol{q}/2}$$
(2.56)

Another important operator is of course the kinetic energy of the particles.

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$
(2.57)

assuming that the kinetic energy does not depend on spin (no spin-orbit coupling). Note that since the total number of particles is $\hat{N} = \sum_{k} c_{k}^{\dagger} c_{k}$ adding a chemical potential $-\mu \hat{N}$ does not

change the form of the Hamiltonian

$$\hat{H} - \mu \hat{N} = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$
(2.58)

but simply replaces $\varepsilon_{\mathbf{k}}$ by $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$. At zero temperature the energy $\xi_{\mathbf{k}}$ is zero at the Fermi level, negative below and positive above.

Finally we mention the "regular" current operator, which we will need in the discussion of electrical transport and optical properties

$$\hat{\boldsymbol{j}}^{(r)} = -\frac{e}{\Omega} \sum_{\boldsymbol{k},\sigma} \boldsymbol{v}_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$
(2.59)

where $\boldsymbol{v}_{\boldsymbol{k}} = \hbar^{-1} \partial \epsilon / \partial \boldsymbol{k}$ is the group velocity.

2.4 Two body operators

Let us now look at operators that involve two particles to define their matrix elements. This is in particular the case of the interaction between two particles. Let us show some examples. The most common interaction between the electrons is one that depends on the distance between the two particles. For the Coulomb interaction it is

$$V(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0 r} \tag{2.60}$$

but other types of interactions such as a local interaction $V(\mathbf{r}) = U\delta(\mathbf{r})$ are also possible choices. We will keep V as a general function in what follows.

To express the operator, we have again the choice for the basis. Because the operator $V(\mathbf{r}_1 - \mathbf{r}_2)$ is diagonal in the position basis, let us start with this one. Since the interaction requires the presence of two particles at coordinates \mathbf{r}_1 and \mathbf{r}_2 the operator probing the interacting between those two particles is simply

$$\hat{H}^{(i)} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) c^{\dagger}(\mathbf{r}_1) c^{\dagger}(\mathbf{r}_2) c(\mathbf{r}_2) c(\mathbf{r}_1)$$
(2.61)

where the factor 1/2 corrects for double counting, since each pair of coordinates appears twice in the double integral over coordinate space. If one includes spin the complete basis becomes $m = (\mathbf{r}, \sigma)$ one gets

$$\hat{H}^{(i)} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) c^{\dagger}_{\sigma_1}(\mathbf{r}_1) c^{\dagger}_{\sigma_2}(\mathbf{r}_2) c_{\sigma_2}(\mathbf{r}_2) c_{\sigma_1}(\mathbf{r}_1)$$
(2.62)

The expression (2.62) can be cast in a more familiar form using the (anti)commutation relations. For fermions

$$\begin{aligned} c^{\dagger}_{\sigma_{1}}(\boldsymbol{r}_{1})c^{\dagger}_{\sigma_{2}}(\boldsymbol{r}_{2})c_{\sigma_{2}}(\boldsymbol{r}_{2})c_{\sigma_{1}}(\boldsymbol{r}_{1}) &= -c^{\dagger}_{\sigma_{1}}(\boldsymbol{r}_{1})c^{\dagger}_{\sigma_{2}}(\boldsymbol{r}_{2})c_{\sigma_{1}}(\boldsymbol{r}_{1})c_{\sigma_{2}}(\boldsymbol{r}_{2}) \\ &= -c^{\dagger}_{\sigma_{1}}(\boldsymbol{r}_{1})(\delta(\boldsymbol{r}_{1}-\boldsymbol{r}_{2})\delta_{\sigma_{1},\sigma_{2}}-c_{\sigma_{1}}(\boldsymbol{r}_{1})c^{\dagger}_{\sigma_{2}}(\boldsymbol{r}_{2}))c_{\sigma_{2}}(\boldsymbol{r}_{2}) \\ &= -\delta(\boldsymbol{r}_{1}-\boldsymbol{r}_{2})\delta_{\sigma_{1},\sigma_{2}}c^{\dagger}_{\sigma_{1}}(\boldsymbol{r}_{1})c_{\sigma_{2}}(\boldsymbol{r}_{2}) + c^{\dagger}_{\sigma_{1}}(\boldsymbol{r}_{1})c_{\sigma_{1}}(\boldsymbol{r}_{1})c^{\dagger}_{\sigma_{2}}(\boldsymbol{r}_{2})c_{\sigma_{2}}(\boldsymbol{r}_{2}) \\ &= -\delta(\boldsymbol{r}_{1}-\boldsymbol{r}_{2})\delta_{\sigma_{1},\sigma_{2}}\hat{\rho}_{\sigma_{1}}(\boldsymbol{r}_{1}) + \hat{\rho}_{\sigma_{1}}(\boldsymbol{r}_{1})\hat{\rho}_{\sigma_{2}}(\boldsymbol{r}_{2}) \end{aligned}$$

$$(2.63)$$

There is a similar expression for bosons with a + sign. The second term would lead to the interaction

$$\hat{H}^{(i)} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \hat{\rho}_{\sigma_1}(\mathbf{r}_1) \hat{\rho}_{\sigma_2}(\mathbf{r}_2)$$
(2.64)

This is the familiar expression of the interaction between two densities of particles (or charges) at two different points. The difference is that now the $\hat{\rho}$ are *operators* measuring the density instead of classical variables. The first term gives

$$\sum_{\sigma} \int d\boldsymbol{r}_1 V(0) \hat{\rho}_{\sigma_1}(\boldsymbol{r}_1) = V(0) \hat{N}$$
(2.65)

is simply a chemical potential term. Notice that it can be infinite for some interactions such as the Coulomb interaction. This first terms is there to correct that the expression (2.64) contrarily to (2.62) does not contain *only* the interaction between two different particles. Indeed (2.62)has two annihilation operators on the right, which means that the operators can only act on states containing two particles. One the contrary (2.64) is of the form

$$c_{\sigma_1}^{\dagger}(\boldsymbol{r}_1)c_{\sigma_1}(\boldsymbol{r}_1)c_{\sigma_2}^{\dagger}(\boldsymbol{r}_2)c_{\sigma_2}(\boldsymbol{r}_2)$$

$$(2.66)$$

and can thus act even if there is only one particle in the system. It thus contains a fake "self-interaction" of the particle with itself. It is this interaction that leads to the chemical potential (2.65) that need to be properly included together with (2.64). Note however that if one fixes the chemical potential by ensuring that the total number of particles is fixed, then this modification is irrelevant since it is simply absorbed in the redefinition of the chemical potential and one can use (2.62) or (2.64) indifferently.

It is easy to rewrite the interaction in the momentum basis using the Fourier transformation which by now have become familiar

$$\hat{H}^{(i)} = \frac{1}{2\Omega^2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4, \\ \sigma_1 \sigma_2}} \int d\mathbf{r}_1 \, d\mathbf{r}_2 e^{-i(\mathbf{k}_3 \mathbf{r}_1 + \mathbf{k}_4 \mathbf{r}_2)} V(\mathbf{r}_1 - \mathbf{r}_2) e^{i(\mathbf{k}_1 \mathbf{r}_1 + \mathbf{k}_2 \mathbf{r}_2)} c^{\dagger}_{\mathbf{k}_3 \sigma_1} c^{\dagger}_{\mathbf{k}_4 \sigma_2} c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1}$$
(2.67)

One can use the new variables of center of mass $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and relative motion $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ to reexpress $\mathbf{r}_1 = \mathbf{R} + \mathbf{r}/2$ and $\mathbf{r}_2 = \mathbf{R} - \mathbf{r}/2$, to obtain

$$\hat{H}^{(i)} = \frac{1}{2\Omega^2} \sum_{\substack{\mathbf{k}_1, \substack{\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4 \\ \sigma_1, \sigma_2}}} \int d\mathbf{R} d\mathbf{r} e^{i(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\mathbf{R}} V(\mathbf{r}) e^{i(\mathbf{k}_1 - \mathbf{k}_3 - \mathbf{k}_2 + \mathbf{k}_4)\mathbf{r}/2} c^{\dagger}_{\mathbf{k}_3 \sigma_1} c^{\dagger}_{\mathbf{k}_4 \sigma_2} c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1}$$

$$= \frac{1}{2\Omega} \sum_{\substack{\mathbf{k}_1, \substack{\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4 \\ \sigma_1, \sigma_2}}} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \int d\mathbf{r} V(\mathbf{r}) e^{i(\mathbf{k}_1 - \mathbf{k}_3)\mathbf{r}} c^{\dagger}_{\mathbf{k}_3 \sigma_1} c^{\dagger}_{\mathbf{k}_4 \sigma_2} c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1}$$

$$= \frac{1}{2\Omega} \sum_{\substack{\mathbf{k}_1, \substack{\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4 \\ \sigma_1, \sigma_2}}} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} V_{\mathbf{k}_3 - \mathbf{k}_1} c^{\dagger}_{\mathbf{k}_3 \sigma_1} c^{\dagger}_{\mathbf{k}_4 \sigma_2} c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1}$$

$$(2.68)$$

Let us comment this expression. The integration over \mathbf{R} gives the term $\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}$ which expresses the conservation of the momenta of the two particles before and after the interaction. This is the direct consequence of the fact that we have chosen an interaction term that is translationally invariant $V(\mathbf{r}_1 - \mathbf{r}_2)$ and thus the total momentum $(\mathbf{k}_1 + \mathbf{k}_2 \text{ and } \mathbf{k}_3 + \mathbf{k}_4)$ should be conserved. The integral over the relative coordinates leads directly to the Fourier transform of the interaction potential with a wavevector that corresponds to momentum transferred on


Figure 2.1: Pictorial visualization of the term (2.69). Each annihilation operator is represented by an incoming arrow, each creation one by an outgoing one. One sees that the interaction can be viewed as the scattering of one particle going from state $\mathbf{k}_1\sigma_1$ to $\mathbf{k}_1 + \mathbf{q}, \sigma_1$ by another one going from state $\mathbf{k}_2\sigma_2$ to state $\mathbf{k}_2 - \mathbf{q}, \sigma_2$. The amplitude of such matrix elements is the Fourier transform of the interaction potential $V(\mathbf{q})$. Since the potential is invariant by translation in space, the momentum is conserved across the interaction. Since the potential does not depend on the spin degrees of freedom the spin of each particle is individually conserved by the interaction. This representation is known as Feynman diagrams. It is extremely useful when constructing the perturbation theory.

one of the particles during the interaction. One can rewrite the term taking into account the $\delta_{k_1+k_2,k_3+k_4}$ constraint as

$$\hat{H}^{(i)} = \frac{1}{2\Omega} \sum_{\substack{k_1, k_2, q \\ \sigma_1, \sigma_2}} V_{q} c^{\dagger}_{k_1 + q, \sigma_1} c^{\dagger}_{k_2 - q, \sigma_2} c_{k_2 \sigma_2} c_{k_1 \sigma_1}$$
(2.69)

This term can be represented visually as shown in Fig. 2.1.

2.5 Bandstructure

If we now consider electrons moving in a periodic potential $\phi(\mathbf{r})$, the Hamiltonian describing the many-body system is the following

$$\hat{H} = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{\sigma} \int d\mathbf{r} \phi(\mathbf{r}) c_{\sigma}^{\dagger}(\mathbf{r}) c_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \hat{\rho}_{\sigma}(\mathbf{r}_1) \hat{\rho}_{\sigma'}(\mathbf{r}_2)$$
(2.70)

where $V(\mathbf{r}_1 - \mathbf{r}_2)$ is the Coulomb interaction between the electrons. The conventional Hartree approach consists of treating the interaction term as a mean-field background potential. The self-consistant solution of this then leads to the so-called band-structure, consisting of a series of bands with momentum q constrained to the first Brillouin zone of reciprocal space:

$$\hat{H} = \sum_{\substack{j,\sigma\\\mathbf{k}\in\mathrm{BZ}}} \epsilon_{\mathbf{k},j} \tilde{c}^{\dagger}_{\mathbf{k},j,\sigma} \tilde{c}_{\mathbf{k},j,\sigma} + \frac{1}{2\Omega} \sum_{\substack{i,j,m,n;\sigma,\sigma'\\\mathbf{k},\mathbf{p},\mathbf{q}\in\mathrm{BZ}}} U_{\mathbf{q}}(i,j,m,n) \tilde{c}^{\dagger}_{\mathbf{k}+\mathbf{q},i,\sigma} \tilde{c}^{\dagger}_{\mathbf{p}-\mathbf{q},j,\sigma'} \tilde{c}_{\mathbf{p},m,\sigma'} \tilde{c}_{\mathbf{k},n,\sigma}$$
(2.71)

where \tilde{c} refers to an electron accompanied by the screening clouds of all other electrons with which it interacts. $U_q(i, j, m, n)$ are the residual interactions, which remain after the bandstructure has been calculated using aforementioned mean-field approximation, and the effects caused by electron-electron interactions have been taken into account in the band-dispersion. The summations over momentum are constrained to the first Brillouin-zone, and i, j, m, n are the band indices. A rigorous canonical transformation of Eq. 2.70 can in principle lead to an expression like Eq. 2.71, but will include additional interaction terms, and the anti-commutation relations of the \tilde{c} operators are more complex than those of the electrons.

Since from the context it usually clear whether one is referring to quasi-particles in a solid or free electrons in vacuum, in practice one doesn't place wiggles on the electron creation and annihilation operators and we will cease to do so from here on. The creation and annihilation operators of the bands describe the complete set of orthogonal states in Hilbert space. It is therefor possible to relate them to plane-wave solutions by means of a transformation matrix, which we can formally express as follows:

$$c_{\boldsymbol{k}+\boldsymbol{Q},\sigma}^{\dagger} = \sum_{j} m_{\boldsymbol{Q},j}(k) c_{\boldsymbol{k},j,\sigma}^{\dagger}$$

$$c_{\boldsymbol{k},j,\sigma}^{\dagger} = \sum_{\boldsymbol{Q}} m_{j,\boldsymbol{Q}}^{inv}(k) c_{\boldsymbol{k}+\boldsymbol{Q},\sigma}^{\dagger}$$
(2.72)

where the Q are reciprocal lattice vectors. The matrix elements $m_{Q,j}$ are entirely determined by the solutions of the Hamiltonian 2.71, together with the set of eigenvalues $\epsilon_{k,j}$.

2.6 Hubbard model

One important particular case of the Hamiltonian in the previous chapter is the case of a contact interaction for a system on a lattice without orbital degeneracy. In practice situations this situation can occur due to a sufficiently strong crystal field. In La₂CuO₄ for example, the $3d_{x^2-y^2}$ is several eV above the other four states. Since the copper is divalent in this compound, it has a $3d^9$ configuration corresponding to a single hole, and this hole occupies the $3d_{x^2-y^2}$ band. Also, in this material the tight-binding model for the kinetic energy (see chapter 1 Eq. 1.59) is already quite accurate. Moreover, since the $3d_{x^2-y^2}$ band is the only relevant one for the low energy physics, the on-site Coulomb interaction becomes the dominating interaction term in Eq. 2.71, and often much of the most important physical consequences can be studied by keeping only this term in the Hamiltonian

$$\hat{H}^{(i)} = \frac{U}{2} \sum_{\sigma,\sigma'} \sum_{i} c^{\dagger}_{i\sigma} c^{\dagger}_{i,\sigma'} c_{i,\sigma'} c_{i\sigma}$$

$$= U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$
(2.73)

The physical interpretation of this term is very simple. Since the interaction is a contact interaction, the electrons of the same spin cannot feel it since they cannot be on the same sites of the lattice. Thus only the interaction between electrons of opposite spins remains. Two electrons of opposite spins only feel the interaction when they are sitting on the same site, thus when both the density of spin up $n_{i\uparrow}$ and the density of spin down $n_{i\downarrow}$ on this site verify $n_{i\uparrow} = n_{i\downarrow} = 1$, as shown in Fig. 2.2 The total Hamiltonian for such a model is thus

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$
(2.74)

This Hamiltonian, known as the Hubbard Hamiltonian, is remarkably simple and yet contains all the essential effect necessary to describe interacting electrons in a solid. It contains the band via the presence of the lattice and the tight binding Hamiltonian and thus, via the filling of the band, can describe bands insulators. The contact interaction is the simplest one can put. Thus this model plays for interacting quantum system the same role that the Ising model played to describe phase transitions. Despite its apparent simplicity this model is essentially still unsolved.

2.7 Solving with second quantization

We now have the tools to express all the operators we need, either for the Hamiltonian or other physical observables, in second quantization. We also saw how to compute averages of an arbitrary number of such creation and annihilation operators in the vacuum. However one important question that remains is how to solve practically a problem, in second quantization, when we know the Hamiltonian. In the first quantization we write the Schrödinger equation, and from that find both the eigenvalues and eigenvectors. But the very essence of the second quantization is to avoid to ever deal with wavefunction so we want to follow another route to obtain the eigenvalues and eigenvectors. How to do this is what we examine now.

Let us first look if we can find the eigenvalues or eigenvector of some simple Hamiltonian. Let us start with a general quadratic Hamiltonian

$$\hat{H} = \sum_{j} \epsilon_j c_j^{\dagger} c_j \tag{2.75}$$

where $\{j, j', ...\}$ is some complete basis, and the coefficients ϵ_j are arbitrary numbers. Several Hamiltonians are of such forms, for example the kinetic energy (2.58). For quadratic and diagonal Hamiltonians of the form (2.75) the problem is solved. Indeed each vector of the form

$$c_1^{\dagger} c_2^{\dagger} c_3^{\dagger} \dots c_p^{\dagger} \left| 0 \right\rangle \tag{2.76}$$

is an eigenvector of \hat{H} with an eigenvalue

$$E = \sum_{i=1}^{p} \epsilon_i \tag{2.77}$$

To show this let us illustrate the calculation with two terms $|\psi\rangle = c_1^{\dagger} c_2^{\dagger} |0\rangle$ (for fermions, an



Figure 2.2: (left) A contact interaction on a lattice. The Fock space on a single state has four possible states. The interaction only acts when a site is doubly occupied. (right) A cartoon of the Hubbard model, where electrons hop on a lattice via a tight binding Hamiltonian and only feel a local interaction.

analogous calculation can be performed for bosons)

$$\hat{H}c_{1}^{\dagger}c_{2}^{\dagger}|0\rangle = \left(\sum_{m} \epsilon_{m}c_{m}^{\dagger}c_{m}\right)c_{1}^{\dagger}c_{2}^{\dagger}|0\rangle$$

$$= \sum_{m} \epsilon_{m}c_{m}^{\dagger}(\delta_{1} - c_{1}^{\dagger}c_{m})c_{2}^{\dagger}|0\rangle$$

$$= \epsilon_{1}|\psi\rangle - \sum_{m} \epsilon_{m}c_{m}^{\dagger}c_{1}^{\dagger}c_{m}c_{2}^{\dagger}|0\rangle$$

$$= \epsilon_{1}|\psi\rangle - \sum_{m} \epsilon_{m}c_{m}^{\dagger}c_{1}^{\dagger}(\delta_{2,m} - c_{2}^{\dagger}c_{m})|0\rangle$$

$$= \epsilon_{1}|\psi\rangle - \epsilon_{2}c_{2}^{\dagger}c_{1}^{\dagger}|0\rangle$$

$$= \epsilon_{1}|\psi\rangle + \epsilon_{2}|\psi\rangle$$
(2.78)

The physics of this result is simple to understand. The operator $c_m^{\dagger} c_m$ counts the particles in the state m. Thus if in $|\psi\rangle$ there is a particle in such a state it will return 1 and the corresponding energy will be counted in \hat{H} .

We thus see that if we have an Hamiltonian that is in a diagonal quadratic form such as (2.75) then we can get all the eigenvalues and eigenvectors of the system. At zero temperature the ground state will simply consist (for fermions) in occupying all the states with the minimum energy according to the number of particles in the system.

$$|\mathbf{F}\rangle = \prod_{i=1}^{N} c_{i}^{\dagger} |0\rangle \tag{2.79}$$

if $\epsilon_1 \leq \epsilon_2 \leq \ldots \leq \epsilon_M$. Note that the Fermi sea is a particular case of (2.79).

At finite temperature we can also compute the averages of many operators. A reminder of the quantum statistical physics is given in the Appendix at the end of this chapter. One important case is the operator giving the number of particles in the state p for a given temperature T and chemical potential μ

$$\langle c_p^{\dagger} c_p \rangle_{T,\mu} = \frac{\operatorname{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}c_p^{\dagger}c_p]}{\operatorname{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]}$$

$$= \frac{\sum_{n_1,\dots,n_M} \langle n_1,\dots,n_M | e^{-\beta\sum_m \xi_m c_m^{\dagger} c_m} c_p^{\dagger} c_p | n_1,\dots,n_M \rangle}{\sum_{n_1,\dots,n_M} \langle n_1,\dots,n_M | e^{-\beta\sum_m \xi_m c_m^{\dagger} c_m} | n_1,\dots,n_M \rangle}$$
(2.80)

where $\xi_m = \epsilon_m - \mu$ is the energy relative to μ . Using the fact that (both for fermions and bosons) $[c_m^{\dagger}c_m, c_h] = 0$ if $m \neq n$ and a similar relation for c_h^{\dagger} , we see that the term $e^{-\beta(\hat{H}-\mu\hat{N})}$ factorizes

$$e^{-\beta(\hat{H}-\mu\hat{N})} = \prod_{n=1}^{M} e^{-\beta\xi_n c_n^{\dagger} c_n}$$
(2.81)

Since in the trace each term n_i is independent the average factorizes. The numerator becomes

$$\left(\sum_{n_p} \langle n_p | e^{-\beta \xi_p c_p^{\dagger} c_p} c_p^{\dagger} c_p | n_p \rangle \right) \prod_{m \neq p} \left(\sum_{n_m} \langle n_m | e^{-\beta \xi_m c_m^{\dagger} c_m} | n_m \rangle \right)$$
(2.82)

All the terms for $m \neq p$ are identical in the numerator and denominator and cancel each other. The trace thus reduces to

$$\langle c_p^{\dagger} c_p \rangle_{T,\mu} = \frac{\sum_{n_p} \langle n_p | e^{-\beta \xi_p c_p^{\dagger} c_p} c_p^{\dagger} c_p | n_p \rangle}{\sum_{n_p} \langle n_p | e^{-\beta \xi_p c_p^{\dagger} c_p} | n_p \rangle}$$
(2.83)

Since $c_p^{\dagger} c_p |n_p\rangle = n_p |n_p\rangle$ one simply has

$$\langle c_{p}^{\dagger}c_{p}\rangle_{T,\mu} = \frac{\sum_{n_{p}} e^{-\beta\xi_{p}n_{p}}n_{p}}{\sum_{n_{p}} e^{-\beta\xi_{p}n_{p}}}$$
 (2.84)

So far all what we did is independent on having bosons or fermions. The final result however will depend on what are the allowed values of n_p

For fermions only $n_p = 0$ and $n_p = 1$ are in the sum. Thus

$$\langle c_p^{\dagger} c_p \rangle_{T,\mu} = \frac{e^{-\beta\xi_p}}{1 + e^{-\beta\xi_p}} = \frac{1}{1 + e^{\beta(\epsilon_p - \mu)}}$$
 (2.85)

and one recovers the Fermi factor. We see that this is a totally general result (not limited to eigenstates of momentum) as soon as one has a quadratic Hamiltonian and one is in thermal equilibrium.

For bosons $n_p = 0, \ldots, +\infty$, and thus the sum becomes

$$\langle c_p^{\dagger} c_p \rangle_{T,\mu} = -\frac{1}{\xi_p} \frac{\partial}{\partial \beta} \log\left[\sum_{n_p=0}^{+\infty} e^{-\beta n_p \xi_p}\right]$$

$$= -\frac{1}{\xi_p} \frac{\partial}{\partial \beta} \log\left[\frac{1}{1-e^{-\beta \xi_p}}\right]$$

$$= \frac{e^{-\beta \xi_p}}{1-e^{-\beta \xi_p}}$$

$$= \frac{1}{e^{\beta(\epsilon_p-\mu)}-1}$$

$$(2.86)$$

and one recovers the Bose factor.

2.8 Appendix: Statistical Quantum Mechanics

In the interest of keeping the notation light, we adopt in the present chapter units for which $\hbar = 1$.

For a quantum mechanical system in a pure state $|\psi\rangle$, any observable can be measured by computing the average of the corresponding operator in the state $|\psi\rangle$

$$\mathcal{O} = \langle \psi | \hat{\mathcal{O}} | \psi \rangle \tag{2.87}$$

where here $\hat{\mathcal{O}}$ is an operator that represents the observable we want to measure and \mathcal{O} is the value (thus a number) corresponding to the result of the average of the operator. In what follows we will use the same symbol for the operators and the average value, the context making it clear whether one deals with an operator or with a number. If there is a possibility of confusion the average value will be denoted $\langle \hat{\mathcal{O}} \rangle$

A priori the function $|\psi\rangle$ can be time dependent which we will denote as $|\psi(t)\rangle$. If this is the case the average depends on time and this will be denoted by the various notations

$$\mathcal{O}(t) = \langle \hat{\mathcal{O}}_S \rangle_t = \langle \psi(t) | \hat{\mathcal{O}}_S | \psi(t) \rangle \tag{2.88}$$

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This is the standard Schrödinger representation. The operators are time independent and all the time dependence is put in the wave function that obeys the Schrödinger equation

$$i\partial_t \left| \psi \right\rangle = \hat{H} \left| \psi \right\rangle \tag{2.89}$$

For an Hamiltonian that is not explicitly dependent on time, the equation has the formal solution

$$|\psi(t)\rangle = e^{-iHt} |\psi(t=0)\rangle \tag{2.90}$$

This allows for an alternative representation of the physical observables known as the Heisenberg representation. An observable at time t reads

$$\mathcal{O}(t) = \langle \psi(t) | \hat{\mathcal{O}}_S | \psi(t) \rangle = \langle \psi_0 | e^{i\hat{H}t} \hat{\mathcal{O}}_S e^{-i\hat{H}t} | \psi_0 \rangle$$
(2.91)

where $\psi_0 = \psi(t = 0)$ One can thus consider that the wavefunctions are time independent and characterize the state of the system and that all the time dependence is due to *time dependent* operators. These operators are given by

$$\hat{\mathcal{O}}_H(t) = e^{i\hat{H}t}\hat{\mathcal{O}}_S e^{-i\hat{H}t} \tag{2.92}$$

where $O_H(t)$ and O_S denote respectively the operators in the Heisenberg and Schrödinger representation. The indices H and S are here added to emphasize the two representations. In the following, operators in the Schrödinger representation will be denoted without any special notation, and when an explicit time dependence will be noted for an operator it will mean that this is the operator in the Heisenberg representation.

The average of a physical quantity is thus given in the Heisenberg representation by

$$\mathcal{O}(t) = \langle \psi_0 | \hat{\mathcal{O}}_H(t) | \psi_0 \rangle \tag{2.93}$$

The definition of the operators in the Heisenberg representation (2.92) can be rewritten in a different form.

$$\frac{d\hat{\mathcal{O}}_{H}(t)}{dt} = (i\hat{H})e^{i\hat{H}t}\hat{\mathcal{O}}e^{-i\hat{H}t} - e^{i\hat{H}t}\hat{\mathcal{O}}e^{-i\hat{H}t}(i\hat{H})$$

$$= i[\hat{H},\hat{\mathcal{O}}_{H}(t)]$$
(2.94)

Note that the Hamiltonian is time independent both in the Schrödinger and Heisenberg representation $\hat{H}_H = \hat{H}_S$. This representation is particularly useful when we are dealing the second quantization chapter.

For systems which are not in pure states the average is a superposition of the averages in pure states with the corresponding probabilities. Thus if p_i are the probabilities of finding the system in the state $|\psi_i\rangle$, a physical observable is given by

$$\langle \hat{\mathcal{O}} \rangle = \sum_{i} p_i \langle \psi_i | \hat{\mathcal{O}} | \psi_i \rangle \tag{2.95}$$

It is more convenient to introduce a density matrix that describes the system. The density matrix for the above average is given by

$$\hat{\rho} = \sum_{i} p_{i} |\psi_{i}\rangle \langle\psi_{i}|$$
(2.96)

and the average of the observable is now given generally by

$$\langle \hat{\mathcal{O}} \rangle = \text{Tr}[\hat{\rho} \ \hat{\mathcal{O}}]$$
(2.97)

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where $\operatorname{Tr}[\hat{\mathcal{O}}]$ denotes the trace of the operator $\hat{\mathcal{O}}$. Note that the density matrix can of course be time dependent if for example the functions $|\psi_i(t)\rangle$ are time dependent.

For a quantum system, with a time independent Hamiltonian \hat{H} in equilibrium with a bath at temperature T, a very natural density matrix corresponds to a superposition state where each level $|n\rangle$ of energy E_n corresponding to the eigenstates of the Hamiltonian is occupied with a probability given by the Boltzmann factor $p_n(T) = e^{-\beta E_n}/Z$

$$\hat{\rho}(T) = \sum_{n} p_n(T) |n\rangle \langle n|$$
(2.98)

where $Z = \sum_{n} e^{-\beta E_n}$ ensures that the probabilities are normalized, and $\beta = 1/(k_{\rm B}T)$ is the inverse temperature. It is easy to check that the density matrix (2.98) can be simply rewritten as

$$\hat{\rho}(T) = \frac{e^{-\beta H}}{Z} \tag{2.99}$$

with

$$Z = \text{Tr}[e^{-\beta H}] \tag{2.100}$$

being the partition function of the system. All averages at finite temperature can thus be computed as

$$\langle \hat{\mathcal{O}} \rangle_T = \text{Tr}[\hat{\rho}(T)\hat{\mathcal{O}}]$$
 (2.101)

We also recall the statistical definition of the entropy

$$S = -k_B \sum_{n} p_n \ln(p_n) \tag{2.102}$$

which, upon substituting the particular choice of the Boltzmann factor $p_n(T) = e^{-\beta E_n}/Z$, and after some standard manipulations which we recommend the students to work out as an exercise, results in the following expression for the Helmholtz free energy $F(T) = \text{Tr}[\hat{\rho}(T)\hat{H}] - ST$

$$F(T) = -k_B T \ln(Z) \tag{2.103}$$

CHAPTER 3

Single particle Green's function

In the interest of keeping the notation light, we adopt in the present chapter units for which $\hbar = 1$.

3.1 Free electron excitations

In order to understand the differences between interacting systems and free electrons, let us recall first the salient properties of the free electron system (or any free quantum fermionic system). We mostly focuss here on the T = 0 properties, that fully characterize the quantum state of the system.

The ground state of a free fermionic system is a "Fermi sea", where the lowest band energy states are fully occupied

$$|\mathbf{F}\rangle = \prod_{k,\varepsilon(k) \le E_{\mathbf{F}}} c_{k,\uparrow}^{\dagger} c_{k\downarrow}^{\dagger} |\varnothing\rangle$$
(3.1)



Figure 3.1: The standard way to describe a metal is to represent it as electrons occupying states up to ϵ_F , as indicated in the left panel. The corresponding single particle *excitations* are either *particle*-like obtained by adding an electron (charge $-e \operatorname{spin} \pm 1/2$), or *antiparticle*-like ("holes") obtained by removing an electron (charge $e \operatorname{spin} \pm 1/2$) as indicated on the righthand side. The energy of an *excited* state is by definition always positive.

There is (at T = 0) a sharp separation between the occupied and non-occupied states in the ground state and in particular n(k) the probability that a state k is occupied has a sharp discontinuity at $k = k_{\rm F}$. The amplitude of this discontinuity is 1.

The excitations of the system above the ground state consist either in creating particles in a given state k above the Fermi level

$$|\psi_{k_1,k_2,\ldots}\rangle = c_{k_1}^{\dagger} c_{k_2}^{\dagger} \dots |\mathbf{F}\rangle \tag{3.2}$$

or annihilating particles (creating holes) among the states that are in the Fermi sea

$$\left|\psi_{k_{1},k_{2},\ldots}^{\prime}\right\rangle = c_{k_{1}^{\prime}}c_{k_{2}^{\prime}}\ldots\left|\mathbf{F}\right\rangle \tag{3.3}$$

The individual excitations are thus particles with all the quantum numbers of the electrons (or holes), in particular with a well defined momentum k and energy $\xi(k)$. The also carry the other quantum numbers of the electrons (or hole), i.e. a charge $\pm e$, and a spin 1/2. The wavefunction of such excitations corresponds to Bloch waves with the momentum k.

3.2 Excitations of interacting electrons

In the interacting system one can expect the nature of such excitations to change. We would thus like to have a correlation function that tells us how much such excitations look like independent particles.

One way to realize this is to construct the correlation function that would correspond to the gedanken experiment described in Fig. 3.2. We consider a material described by a hamiltonian H, which at a given time t = 0 is in a state $|\psi_N\rangle$ with N particles. To remain fully general, we do not assume that this is necessarily an eigenstate, so the state evolves as a function of time. According to the Schroedinger equation the evolution is given by $e^{-iHt} |\psi\rangle_N$. At time t_1 one injects a particle at coordinate r_1 . The wavefunction of the system becomes

$$|\psi_{N+1}(t_1)\rangle = c^{\dagger}(r_1)e^{-iHt_1} |\psi_N\rangle \tag{3.4}$$

One then let this wavefunction, with one additional particle, evolve until a later time t_2

$$|\psi_{N+1}(t_2)\rangle = e^{-iH(t_2-t_1)}c^{\dagger}(r_1)e^{-iHt_1}|\psi_N\rangle$$
(3.5)

The question is how much this state resembles the one if one would have added the particle at time t_2 and, and some other coordinate r_2 .

$$\left|\psi_{N+1}'(t_2)\right\rangle = c^{\dagger}(r_2)e^{-iHt_2}\left|\psi_N\right\rangle \tag{3.6}$$

The overlap between $|\psi_{N+1}(t_2)\rangle$ and $|\psi'_{N+1}(t_2)\rangle$ will thus tell how much the particle that has been injected in the system at point r_1 and time t_1 has evolved freely and still resembles a free particle at point r_2 and time t_2 . This overlap is

$$\langle \psi_{N+1}'(t_2) | \psi_{N+1}(t_2) \rangle = \langle \psi_N | e^{iHt_2} c(r_2) e^{-iHt_2} e^{iHt_1} c^{\dagger}(r_1) e^{-iHt_1} | \psi_N \rangle$$
(3.7)

Using the Heisenberg representation for the operators, this correlation can also be viewed as

$$\langle \psi'_{N+1}(t_2) | \psi_{N+1}(t_2) \rangle = \langle \psi_N | c(r_2, t_2) c^{\dagger}(r_1, t_1) | \psi_N \rangle$$
(3.8)

It consists of the process described in Fig. 3.2 where one creates a particle at point (r_1, t_1) and annihilates it at point (r_2, t_2) to leave the system in the same state it started from.



Figure 3.2: One way to understand the nature of the excitations in an interacting system is to inject a particle at point r_1 and time t = 0. One lets the resulting system evolves, and then one annihilates a particle at time t and point r_2 . The amplitude of such a process indicates how much the propagation of the excitation between the two points and times is similar to the case of non interacting electrons or not.

One can also start by removing a particle at point r_2 at time t_2 , and measure the overlap with the state that we obtain by injecting at time t_1 a particle at point r_1 . The corresponding correlation can be viewed as

$$\langle \psi_{N-1}'(t_2) | \psi_{N-1}(t_2) \rangle = \langle \psi_N | c^{\dagger}(r_1, t_1) c(r_2, t_2) | \psi_N \rangle$$
(3.9)

This type of correlation functions is called a Green's function. We will see in the following section how to relate it to well defined experimental quantities.

The one-electron addition Green's function (Eq. 3.8) refers to excitations where an electron is added, which for non-interacting electrons at T = 0 is only possible for the empty states above E_F . In contrast the one-electron removal (or one-hole) Green's function (Eq. 3.9) refers to excitations where an electron is removed, which for non-interacting electrons at T = 0is only possible for the occupied states below E_F . These two Green's functions are therefor complementary. To describe simultaneously all (occupied and unoccupied) states with a single Green's function, it is therefore necessary to take the sum of the Green's functions of Eqs. 3.8 and 3.9. Following this procedure we arrive at the generalized single-particle Green's function (where "particle" = electron or hole)

$$G(r_1, r_2; t_2 - t_1) = -i\,\theta(t_2 - t_1)\frac{1}{\Omega}\sum_{k,p} e^{-ikr_1}e^{ipr_2}\langle c_k(t_2)c_p^{\dagger}(t_1) + c_p^{\dagger}(t_1)c_k(t_2)\rangle_T$$
(3.10)

In the subsequent chapter we will obtain spectral representation of the Greens function by Fourier transformation of this expression. Taken together with the step-function in time in the definition, the particular way in which the electron and hole Green's functions are combined in the above expression, ensures that negative energies in the spectral representation correspond to the occupied states below the Fermi energy, and positive energies to the empty states above the Fermi energy. The correlation $\langle c_k(t_2)c_p^{\dagger}(t_1) + c_p^{\dagger}(t_1)c_k(t_2)\rangle_T$ corresponds to the creation of a particle with momentum p and the annihilation of a particle with momentum k. The righthand summation is, apart from factors, just the Fourier transform of the Green's function in momentum space, $G(k, p; t_2 - t_1)$. If the system is invariant by translation over time (in other words, there are no time-dependent perturbations acting on the system) then the state vector only depends on $t_2 - t_1$. Without loss of generality one can than choose $t_1 = 0$ and write the momentum space representation of the Green's function as

$$G(k,p;t) = -i\,\theta(t)\langle \left\{ c_k(t), c_p^{\dagger} \right\} \rangle_T$$
(3.11)

3.3 Properties and spectral function

Let us first compute the Green's function for independent electrons. We consider the Hamiltonian

$$\hat{H} = \sum_{k} \xi_k c_k^{\dagger} c_k \tag{3.12}$$

One can easily compute

$$c_k(t) = e^{i\hat{H}t}c_k e^{-i\hat{H}t} \tag{3.13}$$

by looking at the action of the operator on the two states $|0_k\rangle$ and $|1_k\rangle$ with zero and one particle in the state k. These two states are the complete Hilbert space for fermions.

$$c_{k}(t) |0_{k}\rangle = 0$$

$$c_{k}(t) |1_{k}\rangle = e^{iHt}c_{k}e^{-i\xi_{k}t} |1_{k}\rangle = e^{-i\xi_{k}t} |0_{k}\rangle$$
(3.14)

which immediately leads to

$$c_k(t) = e^{-i\xi_k t} c_k \tag{3.15}$$

The Green's function (3.11) thus becomes

$$G^{0}(k, p, t) = -i \theta(t) \langle \left\{ c_{k}(t) c_{p}^{\dagger} \right\} \rangle$$

$$= -i \theta(t) e^{-i\xi_{k}t} \langle \left\{ c_{k}, c_{p}^{\dagger} \right\} \rangle$$

$$= -i \theta(t) e^{-i\xi_{k}t} \delta_{k, p} \qquad (3.16)$$

The Fourier transform is thus

$$G^{0}(k, p, \omega) = \int dt e^{i(\omega+i\delta)t} G^{0}(k, p, t)$$

$$= -i \int_{0}^{+\infty} dt e^{i(\omega+i\delta)t} e^{-i\xi_{k}t} \delta_{k,p}$$

$$= \frac{1}{\omega - \xi_{k} + i\delta} \delta_{k,p}$$
(3.17)

This correlation creates a particle in a well defined momentum state k at time 0, let it propagate and then annihilates a particle in a well defined momentum state p at time t. It thus measures how well in the interacting system the single particle excitations still resemble Bloch waves, i.e. independent particles.

The general case, including disorder and interactions might be described by a Hamiltonian like

$$\hat{H} = \sum_{i,j} t(r_i, r_j) c^{\dagger}(r_i) c(r_j) + \sum_{i,j,m,n} U(r_i, r_j, r_m, r_n) c^{\dagger}(r_i) c^{\dagger}(r_j) c(r_m) c(r_n)$$
(3.18)

Even though the eigenstates of this Hamiltonian are in general difficult to calculate, it is relatively easy to work out the expression for the frequency and momentum dependent Green's function starting from Eq. 3.11

$$\begin{aligned} G(k,p,\omega) &= \int_{-\infty}^{\infty} dt e^{i(\omega+i\delta)t} G(k,p,t) \\ &= -i \int_{0}^{\infty} dt e^{i(\omega+i\delta)t} \langle c_{k}(t) c_{p}^{\dagger} + c_{p}^{\dagger} c_{k}(t) \rangle_{T} \\ &= -i \int_{0}^{\infty} dt e^{i(\omega+i\delta)t} \langle e^{i\hat{H}t} c_{k} e^{-i\hat{H}t} c_{p}^{\dagger} + c_{p}^{\dagger} e^{i\hat{H}t} c_{k} e^{-i\hat{H}t} \rangle_{T} \\ &= -i \sum_{n} p_{n}(T) \int_{0}^{\infty} dt e^{i(\omega+i\delta)t} \left[\langle n|e^{i\hat{H}t} c_{k} e^{-i\hat{H}t} c_{p}^{\dagger} | n \rangle + \langle n|c_{p}^{\dagger} e^{i\hat{H}t} c_{k} e^{-i\hat{H}t} | n \rangle \right] \\ &= -i \sum_{n} p_{n}(T) \left[\langle n|c_{k} \int_{0}^{\infty} dt e^{i(\omega+i\delta+E_{n}-\hat{H})t} c_{p}^{\dagger} | n \rangle + \langle n|c_{p}^{\dagger} \int_{0}^{\infty} dt e^{i(\omega+i\delta-E_{n}+\hat{H})t} c_{k} | n \rangle \right] \\ &= \sum_{n} \frac{e^{-\beta E_{n}}}{Z} \left[\langle n|c_{k} \frac{1}{\omega+i\delta+E_{n}-\hat{H}} c_{p}^{\dagger} | n \rangle + \langle n|c_{p}^{\dagger} \frac{1}{\omega+i\delta-E_{n}+\hat{H}} c_{k} | n \rangle \right] \end{aligned}$$
(3.19)

The imaginary part of the Green's function takes a specially simple form. For a translationally invariant system momentum is conserved, hence the only non-zero $G(k, p, \omega)$ are for k = p. For the imaginary part this implies

$$-\operatorname{Im} G(k,k,\omega) = \pi A(k,\omega) \tag{3.20}$$

where $A(k, \omega)$ is called *spectral function* because it corresponds to the single particle spectrum that can be measured with tunneling or photo-emission spectroscopy. For the general case we obtain

$$A(k,\omega) = \sum_{m,n} \frac{e^{-\beta E_n}}{Z} \left[\langle n | c_k^{\dagger} | m \rangle \langle m | c_k | n \rangle \,\delta(\omega + E_m - E_n) + \langle n | c_k | m \rangle \,\langle m | c_k^{\dagger} | n \rangle \,\delta(\omega + E_n - E_m) \right]$$
$$= \sum_{m,n} \frac{e^{-\beta E_n} + e^{-\beta E_m}}{Z} |\langle m | c_k^{\dagger} | n \rangle |^2 \delta(\omega + E_m - E_n)$$
(3.21)

One can express the full Green's function (real and imaginary part) as a function of $A(k, \omega)$ using the Kramers-Kronig relation. The two terms in the first line correspond to a physically different process. In the second term, reading from right to left, first an electron with momentum k is created on top of the N electrons already present in the ground state. The N + 1 particle state propagates following the time-dependent Schroedinger equation and finally returns to the N particle state by annihilation of an electron with momentum k. The first term on the other hand creates a hole with momentum k. The resulting N - 1 particle state propagates, and finally, by creation of an electron with momentum k the system returns to the ground state. So we see that the two terms represent the density of states of the N - 1 and N + 1 electron spectrum. This is equivalent to representing the occupied and unoccupied states, but formulated in a way which remains valid for a system of interacting electrons.

Let us look at the special case of non-interacting electrons described by Eq. 3.12. For this part of the discussion we integrate the spectral function over all values of k. In a photo-electron spectroscopy experiment this is achieved by studying a polycrystalline sample, and/or measuring in a non-angular resolved mode. We then obtain after application of standard manipulations of statistical physics (exercise !)

$$\sum_{k} A(k,\omega) = \sum_{k} \delta(\omega - \xi_k) = \rho(\omega)$$
(3.22)

which is exactly the density of states (occupied and unoccupied parts combined).

3.4 Connection with photoemission

Photoemission spectroscopy is a technique where one can use photons to kick out electrons out of a system. One measures the energy and momenta of the outgoing electron. Let us now show that the photoemission technique is (in an idealized world) a direct measure of the spectral function $A(k, \omega)$.

In the experiment one starts with the system in the state $|n\rangle$. If one is at T = 0 $|n\rangle$ is the ground state, at finite temperature $|n\rangle$ is as usual distributed with the probability $e^{-\beta E_n}$. The photon removes one particle with momentum k (directly measured) from the system, and thus induces a transition to the state $|m\rangle$ (which contains N - 1 electrons). Using the Fermi Golden rule the probability of transition from state $|n\rangle$ to $|m\rangle$ is thus

$$P_{n \to m} = \sum_{m} |\langle m | c_k | n \rangle|^2 \delta(\omega - E_n + E_m)$$
(3.23)

where ω is the energy of the outgoing particle. If one considers all possible transitions from all possible initial states, the total probability of transition is thus

$$P(k,\omega) = \sum_{m,n} \frac{e^{-\beta E_n}}{Z} |\langle m|c_k|n \rangle|^2 \delta(\omega - E_n + E_m)$$
(3.24)

This probability of transition is the one measured in photoemission since it will directly give the number of outgoing electrons with a momentum k and the energy ω for a fixed influx of photons.

This expression is to be compared with Eq. 3.21. Using the δ function this equation can be rewritten as

$$A(k,\omega) = \frac{e^{\beta\omega} + 1}{Z} \sum_{m,n} e^{-\beta E_n} |\langle m | c_k | n \rangle |^2 \delta(\omega - E_n + E_m)$$

$$= \frac{1}{f(\omega)} \sum_{m,n} \frac{e^{-\beta E_n}}{Z} |\langle m | c_k | n \rangle |^2 \delta(\omega - E_n + E_m)$$
(3.25)

So we see, that

$$P(k,\omega) = f(\omega)A(k,\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle m|c_k |n\rangle|^2 \delta(\omega - E_n + E_m)$$
(3.26)

Thus, up to a factor $f(\omega)$, that can be easily taken into account since one works at fixed energy ω , the photoemission experiment directly measures the spectral function $A(k, \omega)$. It is therefore invaluable tool to analyze the nature of the single particle excitations. Integrating over ω gives

$$\int d\omega P(k,\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle m | c_k | n \rangle|^2 = \sum_n \frac{e^{-\beta E_n}}{Z} \langle n | c_k^{\dagger} c_k | n \rangle = \langle c_k^{\dagger} c_k \rangle$$
(3.27)

which directly relates the spectral function to the occupation factor. For non-interacting electrons $A(k, \omega) = \delta(\omega - \xi_k)$ and one recovers

$$\int d\omega P(k,\omega) = f(\xi_k) \tag{3.28}$$

3.5 Dyson equation

To further develop the notion of a Green's function in quantum many body theory, we return to Eq. 3.19, and reformulate it in the following compact form

$$G_e(k, p, \omega) = \sum_n p_n(T) \langle n | c_k \hat{G}(\omega + E_n) c_p^{\dagger} | n \rangle \quad G_h(k, p, \omega) = \sum_n p_n(T) \langle n | c_k^{\dagger} \hat{G}^*(\omega - E_n) c_p | n \rangle$$
(3.29)

where

$$\hat{G}(E) \equiv \frac{1}{E + i\delta - \hat{H}} \qquad (\delta > 0) \qquad (3.30)$$

is the generalized Green's matrix. This is an operator in the Fockspace of all many-electron states with different particle numbers.

If we now look at the two terms in Eq. 3.29 we notice that the first one describes N + 1 states, and the second N - 1 states where N is the number of electrons in $|n\rangle$.

As to the Greens-function operator itself, we first pout out an extremely useful relation when a system is described by an unperturbed Hamiltonian and perturbation V, as follows

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{3.31}$$

and that the eigenstates of Hamiltonian \hat{H}_0 are known, so that we also know the corresponding unperturbed green's function operator in Fock space

$$\hat{g} = \frac{1}{\omega + i\delta - \hat{H}_0} \tag{3.32}$$

The green's function operator of the full Hamiltonion (Eq. 3.30) and the unperturbed one than are related through the so-called Dyson equation

$$\hat{G}(\omega) = \hat{g}(\omega) + \hat{g}(\omega)\hat{V}\hat{G}(\omega)$$
(3.33)

The validity of Eq. 3.33 can be proven as follows. We start by noticing that the denominator of Eq. 3.30 can be replaced by

$$\omega + i\delta - \hat{H} = \omega + i\delta - \hat{H}_0 - \hat{V} = \hat{g}(\omega)^{-1} - \hat{V}$$

Consequently:

$$\hat{G}(\omega) = \frac{1}{\hat{g}(\omega)^{-1} - \hat{V}}$$

We multiply both sides from the left by $[\hat{g}(\omega)^{-1} - \hat{V}]$, so that

$$[\hat{g}(\omega)^{-1} - \hat{V}]\hat{G}(\omega) = 1$$

We multiply both sides from the left by $\hat{g}(\omega)$, providing

$$\hat{G}(\omega) - \hat{g}(\omega)\hat{V}\hat{G}(\omega) = \hat{g}(\omega)$$

which, with a slight re-arrangement of terms, is just Eq.3.33. The Dyson equation suggests a simple iterative procedure whereby the expression is inserted in itself resulting in the series

$$\hat{G}(\omega) = \hat{g}(\omega) + \hat{g}(\omega)\hat{V}\hat{g}(\omega) + \hat{g}(\omega)\hat{V}\hat{g}(\omega)\hat{V}\hat{g}(\omega) + \dots$$
(3.34)

However, care should be taken that this series doesn't converge for all values of ω , even if \hat{V} represents a small perturbation. Having said that, cases exist where the solution of this expression is particularly simple.

We illustrated this with the density of states of Ag and a $\operatorname{Ag}_{1-x}\operatorname{Pd}_x$ alloy. The occupied DOS can be measured by photoemission spectroscopy. As we saw in the previous section the photoemission spectrum gives $f(\omega)A(k,\omega)$, or, of we integrate of all angles (i.e. all values of k) $f(\omega)\sum_k A(k,\omega)$. An example is given in Fig. 3.3, where the bottom graph is that of pure silver. The strong density of states between 4 and 8 eV binding energy corresponds to the silver 4d band. As indicated in the inset of 3.3, palladium is next left to silver. Consequently the nucleus contains one proton less than that of silver. Compared to silver, the outer electrons are in a less shallow potential. In the experiment shown a small fraction of the silver atoms has been replaced by palladium atoms. This results in a narrow peak at an energy closer to the Fermi energy. Also we see that the density of states between 4 and 8 eV appears rounded. What has happened ? In order to describe this in some detail, we can take advantage of what we have learned about Green's functions.

If we substitute one of the silver atoms with a Pd atom, we can model this by adding locally a potential $\Delta_0 > 0$ to a silver atom. When we choose here $\Delta_0 = 3.4$ eV, we effectively transform the silver atom into Pd. In a tightbinding description of the 4d bands we choose a Hamiltionian of the form

$$\langle i|\hat{V}|j\rangle = \Delta_0 \delta_{i,0} \delta_{j,0} \tag{3.35}$$

corresponding to a perturbation on a particular site $|0\rangle$ in a crystal lattice. The Dyson equation in matrix form is now

$$G_i^j(\omega) = g_i^j(\omega) + g_i^0(\omega)\Delta_0 G_0^j(\omega)$$
(3.36)

which for the special case i = j = 0 has the simple solution

$$G_0^0(\omega) = \frac{g_0^0(\omega)}{1 - \Delta_0 g_0^0(\omega)}$$
(3.37)



Figure 3.3: Photon emission spectra of pure silver (bottom), and silver with 3 percent of the atoms replaced by palladium atoms. Adopted from Physical Review B 32, 6331 (1985).

and all the other matrix elements $G_i^j(\omega)$ follow in a relatively straightforward way. This model is known as the Clogston-Wolff model. Considering that $|i\rangle$ refers to a particular site in a perfect lattice of some pure crystal (for example the copper 3d band) described by the tight-binding model, than

$$g_h^j(\omega) = \sum_{k,p} e^{i(kah - paj)} g(k,\omega) \delta_{k,p} = \sum_k e^{ika(h-j)} \frac{1}{\omega - \xi_k}$$
(3.38)

Here a is the lattice parameter and k and p refer to momentum quantum numbers. For each so-called local Green's function at site h = j we obtain for the imaginary part

$$-\frac{1}{\pi} \operatorname{Im} g_h^h(\omega) = \sum_k \delta(\omega - \xi_k)$$
(3.39)

in which we recognize the expression for the density of states. As a model function for the DOS we select for the purpose of this discussion the model function of a semi-spherical density of states, $Img_0^0(\omega) = -B^{-2}\sqrt{B^2 - \omega^2}$, which is described by the Green's function

$$g_0^0(\omega) = \frac{\omega - \sqrt{\omega^2 - B^2}}{B^2}$$
(3.40)

with the help of which we obtain the solution for $G_0^0(\omega)$

$$G_0^0(\omega) = \frac{\omega - \sqrt{\omega^2 - B^2}}{B^2 - \Delta_0 \left(\omega - \sqrt{\omega^2 - B^2}\right)}$$
(3.41)

In Fig. 3.4 we display the solution for different values of V_0 . We see, that the effect of the local potential Δ_0 is to create a bound state above the semi-spherical band, provided that Δ_0 exceeds a certain critical value. This kind of situation can for example be created by substituting a Pd atom for Ag in an otherwise clean silver crystal. The resulting split-off state is localized in space at the site $|0\rangle$. For Δ_0 smaller than this critical value no bound state is formed, but the local density of states at site $|0\rangle$ is still different from the surrounding atoms.

If, instead of Pd, we take nickel, cobalt or iron, which are magnetic elements, the many-body aspects become very important and we get all kinds of interesting magnetic phenomena related to the local electron-electron correlations on the nickel-atom, in particular the Kondo-effect.

3.6 Spectral function of interacting electrons

We now have to analyze the single particle Green's function (as well as other physical properties) for the interacting problem. This is clearly a very difficult question. The time evolution of the operators such as in (3.15) becomes highly non trivial since there is no simple commutator of H and the operators c_k anymore. In the same vein since in general the interaction Hamiltonian is non quadratic, there is no simple transformation that can bring is to a diagonal form.

We thus have to rely to different approximate techniques to tackle this problem. Indeed even if one takes an Hamiltonian as simple as the Hubbard model there is despite about 50 years of research no exact solution except in dimension d = 1 and $d = \infty$. Contrarily to other models such as the Ising model, there is still no agreement on what the physics of the model is for intermediate dimensions, specially for d = 2.

One method that could be used to tackle the interacting problem is to perform perturbation in the interaction term H_{int} . Indeed we know how to compute the free Green's function and other observable so this is a quite logical approach. Even if in real solids, as we saw the interaction is not effectively small, one can still expect the perturbation theory to give us information on



Figure 3.4: Left panel: Real part of $g_0^0(\omega)$ together with $1/\Delta$ for different choices of Δ . The frequencies where $g_0^0(\omega) = 1/\Delta$ represent poles of the total Green's function $G_0^0(\omega)$ and therefor represent bound states provided that ω is outside the band. These conditions are met for the case $\Delta = 2$ at $\omega = 1.26$. Right panel: Imaginary part of $G_0^0(\omega)$ for 4 different choices of the local potential Δ . The conditions for a split-off bound state are met for the case $\Delta = 2$ at $\omega = 1.26$. All energies are indicated in units of B.

the qualitative effects of the interactions. However performing such a perturbation is in itself a formidable task. Indeed the perturbation must be made at two places: both in the time evolution e^{iHt} and in the Bolzmann factor $e^{-\beta H}$. There are two difficulties. One is purely technical and linked to the fact that $H_{\rm kin}$ and $H_{\rm int}$ are operators and that these operators do not commute (in general). So performing the expansion of the exponentials is clearly more complicated than for simple numbers. The second difficulty is much more profound in nature. In the time evolution, we are in principle interested in computing the value of the operators at all times, thus in principle one can have $t \to \infty$. It is thus unclear whether one can perform an expansion of the exponentials

$$e^{-i(H_0+H_1)t} \simeq e^{-iH_0t} [1-iH_1t+\cdots]$$
(3.42)

Fortunately these problems can be solved and one can construct a perturbation method for quantum problems at finite temperature. This is the method known as Feynmann diagrams generalized to finite temperature. We will not pursue more in this direction and refer the reader to "Many particle physics" by G.D. Mahan for more details on this technique.

Instead of following a systematic route we will play with the single particle Green's function and determine which parameters can control its shape. It will thus give us, in a phenomenological way, the properties of interacting systems.

3.7 Self energy: lifetime and effective mass

Let us first consider the single particle Green's function for an interacting problem. One can always write it as

$$G(k,\omega) = \frac{1}{\omega - \xi_k - \Sigma(k,\omega)}$$
(3.43)

where $\Sigma(k,\omega)$ called the self energy is a certain function of momenta and frequency. The relation (3.43) in fact defines the function Σ . Given the form (3.43) and the expressions (3.17) one sees that Σ must go to zero in the absence of interactions. To make connection with the perturbation method $\Sigma(k,\omega)$ is thus an object that is expected to have a well behaved



Figure 3.5: A finite imaginary part in the self energy gives a Lorentzian peak. The width of the Lorentzian is $\text{Im}\Sigma$ and the height $1/\text{Im}\Sigma$. The smaller the imaginary part, the sharper the peaks. The imaginary part of the self energy has thus the meaning of an inverse lifetime for a particle with momentum k.

perturbation expansion in powers of the interactions. However we will not attempt here to compute the self energy Σ but simply to examine how it controls the spectral function. We will absorb the small imaginary part $i\delta$ in Σ for simplicity, since one can expect in general Σ to have a finite imaginary part as well. The spectral function is

$$A(k,\omega) = -\mathrm{Im}G(k,\omega) = \frac{1}{\pi} \frac{\mathrm{Im}\,\Sigma(k,\omega)}{(\omega - \xi_k - \mathrm{Re}\,\Sigma(k,\omega))^2 + (\mathrm{Im}\,\Sigma(k,\omega))^2}$$
(3.44)

and we thus see that Im Σ and Re Σ have very different actions on the spectral function. We also see that quite generally (3.44) imposes that Im $\Sigma(k, \omega) < 0$ to get a positive spectral function.

Imaginary part of the self energy: inverse lifetime

Let us fist assume that the real part of the spectral function $\operatorname{Re} \Sigma(k, \omega)$ is zero to investigate the consequences of the existence of an imaginary part. Note that doing this kind of crude approximation might violate some relations between the real and imaginary part of the self energy, which in general should be related by the Kramers-Kronig relations. There is thus a chance that we will get some absurd, or incorrect results, due to that, but we will face this problem if or when it occurs. Moreover let us assume that the imaginary part is a constant.

With these approximations the spectral function would simply be

$$A(k,\omega) = -\frac{1}{\pi} \frac{\operatorname{Im}\Sigma}{(\omega - \xi_k)^2 + (\operatorname{Im}\Sigma)^2}$$
(3.45)

As shown in Fig. 3.5 a finite imaginary part in the self energy thus gives a Lorentzian shape for the peaks. The peaks are still centered at $\omega = \xi_k$ but have now a finite width and height instead of being δ functions. The width is given by the imaginary part of the self energy and the height in $1/\text{Im}\Sigma$. As usual with a Lorentzian the total spectral weight in the peak is a constant, hence the height inversely proportional to the width. As we see the peaks are sharper We thus see that the imaginary part of the self energy controls the spread of the energies of the particles. One can see the spectral function as a particle which has an average energy $\omega = \xi_k$, related to its momentum, but with a certain spread Im Σ in energy. To understand the physics of this spread let us consider the Green's function of a free particle in real time (3.16). This function when Fourier transform would give the perfect δ function. However if one modifies it by

$$G(k,t) = -i\theta(t)e^{-i\xi_k t}e^{-t/\tau}$$
(3.46)

the Fourier transform becomes

$$G(k,\omega) = \frac{1}{\omega - \xi_k + i/\tau}$$
(3.47)

and the spectral function is

$$A(k,\omega) = \frac{1/\tau}{(\omega - \xi_k)^2 + (1/\tau)^2}$$
(3.48)

which is exactly the one we are considering with the identification

$$\frac{1}{\tau} = \operatorname{Im} \Sigma \tag{3.49}$$

We thus see from (3.46) that a Lorentzian spectral function corresponds to a particle with a well defined energy ξ_k which defines the center of the peak, but also with a finite *lifetime* τ . Of course this does not mean that the electron physically disappears, but simply that it does not exist as an excitation with the given quantum number k. This is indeed an expected effect of the interaction since the particle will exchange momenta with the others particles and thus is able to change its quantum state.

To go back to the more general form of the self energy, which depends on k and ω we see that we can keep this interpretation in terms of a lifetime, if the peak is narrow enough. Indeed in that case what will matter is the self energy at the position of the peak Im $\Sigma(k, \omega = \xi_k)$ if one assumes that the self energy varies slowly enough with ω compared to $\omega - \xi_k$.

Real part of the self energy: effective mass and quasiparticle weight

Let us now turn to the real part. Now that we understand that the imaginary part provides a lifetime for the particle let us turn the imaginary part to zero to focuss on the effects of the real part of the self energy. Of course in doing so we strongly violated the Kramers-Kronig relation since the real part should have been zero as well. But this simplification is only to replace the Lorentzian peaks by sharp δ functions for simplicity so we do not expect it to drastically affect the physics driven by the real part.

If we only consider the real part the spectral function becomes

$$A(k,\omega) = \delta(\omega - \xi_k - \operatorname{Re}\Sigma(k,\omega))$$
(3.50)

The role of the real part of the self energy is thus to modify the position of the peak. Instead of having the peak at $\omega = \xi_k$, one has now a new dispersion relation E_k which is defined by the self-consistent solution for $\omega = E_k$

$$E_k = \xi_k + \operatorname{Re}\Sigma(k, E_k) \tag{3.51}$$

The relation (3.51) defines the new dispersion relation. The interactions, via the real part of the self-energy are thus leading to a modification of the energy of single particle excitations. Although we can in principle compute the whole dispersion relation E_k , in practice we do not need it to characterize the system. Indeed we are only interested in low energy excitations close to the Fermi level. Close to the Fermi level the energy, with a suitable subtraction of the chemical potential is zero. One can thus expand it in powers of k. For free electrons with $\xi_k = \frac{k^2}{2m} - \frac{k_F^2}{2m}$ the corresponding expansion would give

$$\xi_k = \frac{k_{\rm F}}{m} (k - k_F) \tag{3.52}$$

A similar expansion for the new dispersion E_k gives

$$E_k = 0 + \frac{k_{\rm F}}{m^*} (k - k_{\rm F}) \tag{3.53}$$

which defines the coefficient m^* . Comparing with (3.52) we see that m^* has the meaning of a mass. This is an effective mass which traduces the fact that the dispersion relation has been changed by the interactions. We thus see that close to the Fermi level we only need to compute the effective mass m^* to fully determine (at least for a spherical Fermi surface) the effects of the interactions on the energy of single particle excitations. To relate the effective mass to the self energy we differentiate the right of Eq. 3.51 in parts

$$\frac{dE_k}{dk} = \frac{d\xi_k}{dk} + \frac{\partial \operatorname{Re}\Sigma(k, E_k)}{\partial k} + \frac{\partial \operatorname{Re}\Sigma(k, \omega)}{\partial \omega} \bigg|_{\omega = E_k} \times \frac{dE_k}{dk}$$
(3.54)

which can be solved to give

$$\frac{d\xi_k}{dk} \left[1 + \frac{1}{d\xi_k/dk} \frac{\partial \operatorname{Re} \Sigma(k, E_k)}{\partial k} \right] = \frac{dE_k}{dk} \left[1 - \frac{\partial \operatorname{Re} \Sigma(k, \omega)}{\partial \omega} \Big|_{\omega = E_k} \right]$$
(3.55)

so that, using $d\xi_k/dk = k_F/m$,

$$\frac{m^*}{m} = \frac{d\xi_k/dk}{dE_k/dk} = \frac{1 - \frac{\partial \operatorname{Re}\Sigma(k,\omega)}{\partial\omega}\Big|_{\omega=E_k}}{1 + \frac{m}{k_{\rm F}} \left.\frac{\partial \operatorname{Re}\Sigma(k,\omega)}{\partial k}\right|_{\omega=E_k}}$$
(3.56)

To determine the effective mass these relations should be computed on the Fermi surface $E(k_{\rm F}) = 0$. The equation (3.56) indicates how the self energy changes the effective mass of the particles. We thus see that although one can keep single particle excitations they will have in general, due to interactions, a different mass than the one of independent electrons. This renormalization of the mass by interaction is well consistent with the experimental findings of Section 1.12 where we saw that in the specific heat one had something that was resembling the behavior of free electrons but with a different mass m^* .

However the interactions have another effects. Indeed if we try to write the relation (3.50) in the canonical form $\delta(\omega - E_k)$ that we would naively expect for a free particle with the dispersion E_k we see that we cannot do it. Instead, using (3.50) we obtain

$$A(k,\omega) = Z_k \delta(\omega - E_k) \tag{3.57}$$

with

$$Z_{k} = \left[\frac{\partial}{\partial \omega} (\omega - \xi_{k} - \operatorname{Re} \Sigma(k, \omega)) \Big|_{\omega = E_{k}} \right]^{-1}$$

$$= \frac{1}{1 - \frac{\partial \operatorname{Re} \Sigma(k, \omega)}{\partial \omega} \Big|_{\omega = E_{k}}}$$
(3.58)

Because of the frequency dependence of the real part of the self energy, we see that the total spectral weight in the peak is not one any more but the total weight is now Z_k , which is in general a number smaller than one. It is thus as if not the whole electron (or rather the total spectral weight of an electron) was converted into something that looks like a free particle with a new dispersion relation, but only a faction Z_k of it. With our crude approximation the rest of the spectral function has totally vanished and the spectral weight no longer integrates to 1. This is the consequence of our crude approximation for the self energy that violates the Kramers-Kronig relation. However the effect that we found is quite real, and what becomes of the remaining spectral weight will be described in the next section.

To conclude we see that the real part of the self energy controls the dispersion relation and the total weight of excitations which in the spectral function would produce peaks exactly like free particles. The frequency and momentum dependence of the real part of the self energy lead to the two independent quantities m^* the effective mass of the excitations and Z_k the weight. In the particular case when the momentum dependence of the self energy is small on can see from (3.58) and (3.56)

$$\frac{m}{m^*} = Z_{k_{\rm F}} \tag{3.59}$$

CHAPTER 4

Linear response

Let us now see how we can compute observables for a quantum problem. Such observables correspond always to the average of some operator. In quantum mechanics the averages are taken in the ground state of the system. In solid state we always work at finite temperature so one has to generalize this concept to finite temperatures, and we will see how later.

Forgetting this question for the moment computing averages is easy if we know well enough the Hamiltonian to diagonalize it or at least if the system is in thermodynamic equilibrium. However this is often not the case: to probe a system one exert on it small perturbations such as the application of a small magnetic field to see how it magnetizes, a small voltage to see whether it conducts, etc. . One is thus very often faced with the situation of trying to study a problem which is described by an equilibrium (time independent) Hamiltonian H to which one will add in general a time dependent perturbation, $\hat{H}^{(p)}(t)$. Computing the full properties of the time dependent Hamiltonian would be a formidable task. However if the perturbation is small (in a sense to be defined) then one can hope to compute the observable in a development in the perturbing Hamiltonian.

This is what is called the linear response theory, and we will examine how one can make such a calculation for a quantum system.

4.1 Linear response

Let us start with a system described by an Hamiltonian $\hat{H}^{(0)}$ which is time independent and add to the Hamiltonian of the system a perturbation, a priori time and space dependent

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(p)}(t)$$
$$\hat{H}^{(p)}(t) = \int d\mathbf{r}_1 \mathbf{F}(\mathbf{r}_1, t) \cdot \hat{\mathbf{x}}(\mathbf{r}_1)$$
(4.1)

where $\mathbf{F}(\mathbf{r}, t)$ is some external field (magnetic field, electric field, pressure, etc.), and $\hat{\mathbf{x}}(\mathbf{r})$ the operator to which it couples (magnetization, current, density, etc.). We consider that this operator can depend on space. We choose $\hat{\mathbf{x}}$ such that in the absence of perturbation its average is zero $\langle \hat{\mathbf{x}}(\mathbf{r}) \rangle = 0$, since one can always subtract this average value. For the remaining part of the chapter we will assume fields oscillating periodically in space, i.e.

$$\boldsymbol{F}(\boldsymbol{r}_{1},t) = \boldsymbol{F}_{q}(t)\cos(\boldsymbol{q}\cdot\boldsymbol{r}_{1})$$
$$\hat{\boldsymbol{x}}_{q} = \int d\boldsymbol{r}_{1}\cos(\boldsymbol{q}\cdot\boldsymbol{r}_{1})\hat{\boldsymbol{x}}(\boldsymbol{r}_{1})$$
$$\widehat{\boldsymbol{H}}^{(p)}(t) = \boldsymbol{F}_{q}(t)\cdot\hat{\boldsymbol{x}}_{q} \qquad (4.2)$$

so that

In addition we will assume, that the Hamiltonian $\hat{H}^{(0)}$ is invariant by translation, so that the perturbation and the induced fields oscillate with the same wavevector q. For the remainder of this chapter we are going to drop the indices q in order to keep the notation as general as possible. These indices can always be reintroduced if needed. The goal of this chapter is to calculate the response of a parameter $\boldsymbol{u}(t)$ at time t to the field $\boldsymbol{F}(t_1)$ where $t_1 < t$. If the applied field $\boldsymbol{F}(t)$ is not too big, it makes sense to expand \boldsymbol{u} in powers of $\boldsymbol{F}(t)$. We restrict this introduction to the *linear* response, expressed by the *susceptibility* $\chi_{ux}(\omega)$

$$\boxed{\boldsymbol{u} = \boldsymbol{\chi}_{ux}(\omega) \cdot \boldsymbol{F}}$$
(4.3)

Since the Schrödinger equation gives the time evolution of the quantum system, we are in a position to compute the response to a *time dependent* perturbation. Let us emphasize that here $\hat{H}^{(0)}$ does designate a totally general (interacting etc.) Hamiltonian, as long as this Hamiltonian does not contain an explicit time dependence. Typically $\hat{H}^{(0)}$ is the full Hamiltonian of the system whose properties one is trying to probe by the perturbation.

Let us consider an observable described by an operator $\hat{\boldsymbol{u}}$. As we have already done for $\hat{\boldsymbol{x}}$, we choose the operator $\hat{\boldsymbol{u}}$ such that its average in the unperturbed system vanishes. We want to compute this observable at given time t. As can be readily guessed computing the full response for the complete Hamiltonian $\hat{H}^{(0)} + \hat{H}^{(p)}(t)$ is hopeless. However if the perturbation $\boldsymbol{F}(t)$ is small we can compute the average of $\hat{\boldsymbol{u}}$ in a perturbation expansion in \boldsymbol{F} . By definition of $\hat{\boldsymbol{u}}$ the term of order zero vanishes. The term of order one (linear response)

$$\boldsymbol{u}(t) = \int_{-\infty}^{t} \boldsymbol{\chi}_{u,x}(t-t_1) \cdot \boldsymbol{F}(t_1) dt_1 + O\left(\boldsymbol{F}^2\right)$$
(4.4)

 $\chi_{ux}(t-t_1)$ is the susceptibility measuring at time t the linear response of the observable $\boldsymbol{u}(t)$ to a perturbation $\boldsymbol{F}(t_1)$ at an earlier time t_1 , which is coupled to a degree of freedom $\hat{\boldsymbol{x}}$ of the system. Because we have performed an expansion in powers of \boldsymbol{F} and confined the expansion to the linear term, χ_{ux} depends only on the unperturbed Hamiltonian $\hat{H}^{(0)}$. One can thus exploit the existing symmetries of $\hat{H}^{(0)}$ to simplify the expression for χ_{ux} . First $\hat{H}^{(0)}$ does not explicitly depend on time, thus the susceptibility that measures the response between a perturbation at time t_1 and a response at time t_2 can only depend on the difference between the two times. Since earlier on we assumed that the Hamiltonian $\hat{H}^{(0)}$ has translational symmetry, a perturbation of wavevector q gives rise to a response with exactly the same q. This last point depends on the precise Hamiltonian $\hat{H}^{(0)}$, and can be easily generalized to a disordered system. On the other hand, the first point about the time-invariance is totally general.

We want now to explicitly compute the susceptibility χ_{ux} . To do so we first need to know how to compute the average for a system which is time dependent since the full Hamiltonian $\hat{H}(t) = \hat{H}^{(0)} + \hat{H}^{(p)}(t)$ contains an *explicit* time dependence. Clearly we need to define what is the density matrix of the system at time t, to be able to use (2.97).

$$\boldsymbol{u}(t) = \operatorname{Tr}\{\hat{\rho}(t)\hat{\boldsymbol{u}}\} = \sum_{n} p_{n}(t)\langle n(t)|\hat{\boldsymbol{u}}|n(t)\rangle$$
(4.5)

Let us look at the time evolution of the density matrix. Let us assume that the perturbation was switched on at a certain time $-\tau$, so for times $t < -\tau$ the perturbation vanishes, $\mathbf{F}(\mathbf{r}, t < -\tau) =$ 0. Since for $t < -\tau$ the system is fully determined by the time independent Hamiltonian $\hat{H}^{(0)}$, we know that the density matrix is simply given by $\hat{\rho}_0 = e^{-\beta \hat{H}^{(0)}}/Z_0$ or the expression (2.98). If now we switch on the perturbation at $t = -\tau$, from that moment on the time evolution of the state-vectors $|n(t)\rangle$ are easy (formally) to compute since they simply obey the Schrödinger equation.

We have to make an assumption here about the time evolution of the *probabilities* p_n that the system can be found in the state $|n\rangle$. In fact, we will assume that the coefficients p_n are not

changing as the system is evolving with time, and thus the populations of the levels are constant as a function of time. The time evolution is thus solely given by the evolution of the state vectors. According to the definition of the entropy, Eq. 2.102, fixing the probabilities p_n implies that the *entropy* is also independent of time (but note that consequently other thermodynamic variables, in particular temperature, will evolve with time). From a thermodynamical perspective this implies that the system evolves without any exchange of heat with the environment. The time evolution is thus supposed to be **adiabatic**. The energy of the system does change, by virtue of the time-evolution of the functions $|n(t)\rangle$, a process that we should interpret as work being effected by $\mathbf{F}(t)$.

In other words the thermal bath is introduced at a given time $t \leq -\tau$ when the perturbation does not exist, and the levels are populated according to the (time independent) distribution $p_n = e^{-\beta E_n}/Z$. The thermal bath is then removed and the perturbation switched on, so that the wavefunction starts to evolve as a function of time. The time-independence of the probabilities p_n allows us to express the expectation value of the operator $\hat{\boldsymbol{u}}$ in the following way

$$\boldsymbol{u}(t) = \sum_{n} p_n \langle n(t) | \hat{\boldsymbol{u}} | n(t) \rangle \tag{4.6}$$

Interlude on time varying external fields

Before continuing with the evaluation of Eq. 4.6, we first need to develop the theoretical method by which we can evaluate the time dependence of the state vectors $|n(t)\rangle$ under the influence of the full Hamiltonian, including the time varying external field. The time-evolution of the state vectors is determined by the time dependent Schrödinger equation

$$i\partial_t |n(t)\rangle = \left[\hat{H}^{(0)} + \hat{H}^{(p)}(t)\right] |n(t)\rangle$$
(4.7)

For a Hamiltonian that is not explicitly depending on time, this equation has the formal solution, Eq. 2.90. To take into account the time-dependence of $\hat{H}^{(p)}(t)$ we try the following

$$|n(t)\rangle = e^{-i\hat{H}^{(0)}t}\hat{A}(t)|n\rangle \tag{4.8}$$

where $\hat{A}(t)$ is an operator yet to be defined, which describes the effect of the time-dependent perturbation on the time-evolution of the state-vector $|n(t)\rangle$, starting from $|n(-\tau)\rangle = e^{i\hat{H}^{(0)}\tau} |n\rangle$ at the time at which the perturbation was switched on. To obtain an explicit expression for $\hat{A}(t)$ we substitute the righthand-side of Eq. 4.8 for $|n(t)\rangle$ on both sides of the time dependent Schrödinger equation, Eq.4.7, and work out the time derivatives on the left-hand side by differentiating $e^{-i\hat{H}^{(0)}t}\hat{A}(t)$ in parts

$$\left[\hat{H}^{(0)}e^{-i\hat{H}^{(0)}t}\hat{A}(t) + e^{-i\hat{H}^{(0)}t}i\partial_t\hat{A}(t)\right]|n\rangle = \left[\hat{H}^{(0)} + \hat{H}^{(p)}(t)\right]e^{-i\hat{H}^{(0)}t}\hat{A}(t)|n\rangle$$
(4.9)

Since this equation is valid for the entire Fock space spanned by the time-independent vectors $|n\rangle$, we are allowed to write it as a general relation for the operators appearing in the equation. The first term is the same on each side of the equation and cancels. We multiply the remaining term on both sides by the operator $-ie^{i\hat{H}^{(0)}t}$, so that

$$\partial_t \hat{A}(t) = -ie^{i\hat{H}^{(0)}t} F(t) \cdot \hat{x} e^{-i\hat{H}^{(0)}t} \hat{A}(t)$$
(4.10)

where we have substituted the definition of $\hat{H}^{(p)}(t)$, given in Eq. 4.2. At this point it is useful to introduce the Heisenberg representation describing the time-evolution of an operator $\hat{\mathcal{O}}$ in the absence of the perturbation $\hat{H}^{(p)}(t)$

$$\hat{\mathcal{O}}^{(0)}(t) = e^{i\hat{H}^{(0)}t}\hat{\mathcal{O}}e^{-i\hat{H}^{(0)}t}$$
(4.11)

With the help of this definition Eq. 4.10 becomes

$$\partial_t \hat{A}(t) = -i\boldsymbol{F}(t) \cdot \hat{\boldsymbol{x}}^{(0)}(t)\hat{A}(t) \tag{4.12}$$

We wish to solve this differential equation, and as a first step we integrate both sides of the expression from $-\infty$ to t. Keeping in mind that $\mathbf{F}(t \leq -\tau) = 0$ and $\hat{A}(-\tau) = 1$, we obtain for $t > -\tau$

$$\hat{A}(t) = 1 - i \int_{-\tau}^{t} dt_1 \boldsymbol{F}(t_1) \cdot \hat{\boldsymbol{x}}^{(0)}(t_1) \hat{A}(t_1)$$
(4.13)

To obtain an expansion in powers of \mathbf{F} we proceed by iteration of this expression. This is done by re-substituting the entire expression for $\hat{A}(t_1)$ in the integral on the righthand side, and so we obtain

$$\hat{A}(t) = 1 - i \int_{-\tau}^{t} dt_1 \boldsymbol{F}(t_1) \cdot \hat{\boldsymbol{x}}^{(0)}(t_1) - \int_{-\tau}^{t} dt_1 \boldsymbol{F}(t_1) \cdot \hat{\boldsymbol{x}}^{(0)}(t_1) \int_{-\tau}^{t_1} dt_2 \boldsymbol{F}(t_2) \cdot \hat{\boldsymbol{x}}^{(0)}(t_2) \hat{A}(t_2)$$
(4.14)

This can be repeated as often as necessary to arrive at the required order of F. Here we just need the first two terms on the righthand side of the expression. Interlude on time varying external fields ends here

We now return to Eq. 4.6. With the help of the time evolution operator we express this relation as

$$\boldsymbol{u}(t) = \sum_{n} p_{n} \langle n | \hat{A}^{\dagger}(t) e^{i \hat{H}^{(0)} t} \hat{\boldsymbol{u}} e^{-i \hat{H}^{(0)} t} \hat{A}(t) | n \rangle = \left\langle \hat{A}^{\dagger}(t) \hat{\boldsymbol{u}}^{(0)}(t) \hat{A}(t) \right\rangle$$
(4.15)

We like to expand the expression for \boldsymbol{u} in orders of \boldsymbol{F} , and we will concentrate on the linear response. Since the definition of $\hat{\boldsymbol{u}}^{(0)}(\boldsymbol{r},t)$ contains $\hat{H}^{(0)}$, it does not depend on \boldsymbol{F} . The only term that needs to be expanded is therefore $\hat{A}(t)$. Substitution in Eq. 4.15 of the first two terms of the expansion, Eq.4.14, yields

$$\boldsymbol{u}(t) = \left\langle \left(1 + i \int_{-\tau}^{t} dt_1 \boldsymbol{F}(t_1) \cdot \hat{\boldsymbol{x}}^{(0)}(t_1) \right) \hat{\boldsymbol{u}}^{(0)}(t) \left(1 - i \int_{-\tau}^{t} dt_2 \boldsymbol{F}(t_2) \cdot \hat{\boldsymbol{x}}^{(0)}(t_2) \right) \right\rangle$$
(4.16)

The matrix element $\langle \hat{\boldsymbol{u}}^0(t) \rangle = 0$ for a system in equilibrium. Furthermore the term proportional to $\boldsymbol{F}(t_1)\boldsymbol{F}(t_2)$ can be neglected since it doesn't contribute to the linear response. The remaining two terms give

$$\boldsymbol{u}(t) = -i \int_{-\tau}^{\infty} dt_1 \,\theta(t-t_1) \left\langle \left[\hat{\boldsymbol{u}}^{(0)}(t), \boldsymbol{F}(t_1) \cdot \hat{\boldsymbol{x}}^{(0)}(t_1) \right] \right\rangle$$
(4.17)

where the step function $\theta(t - t_1)$ limits the time integral to $t_1 < t$. Until this point we have assumed that F(t) and $\mathbf{x}(t)$ are real numbers. For this reason we have used $F(t_1) = F^*(t_1)$ in the expression for $\hat{A}^{\dagger}(t)$ on the lefthand side of Eqs 4.15 and 4.16. On the other hand, the real-valuedness implies that the time-dependence of F(t) in the commutator above is described by $\sin(\omega t - \phi)$ (rather than $e^{-i\omega t}$). The perturbation should than be defined as a superposition of two components $e^{-i\omega t}$ and $e^{i\omega t}$ having frequencies of opposite sign. While the susceptibility can be worked out in a straightforward way with this definition, the equations become lengthy. In the end one obtains the same result by substituting the following time dependence

$$F(t) = Fe^{-i\omega t}$$

$$u(t) = ue^{-i\omega t}$$
(4.18)

and we will use this until the end of this section in the interest of compactness of the expressions. In the last section we will come back to this point, and replace the perturbation by a field with real expectation values. We proceed by removing the explicit time-dependence from the left-hand side by multiplying both sides of the expression by the factor $e^{i\omega t}$. The quantity in brackets is the unequal time correlation function, where we note, that due to time-invariance of the unperturbed system described by $\hat{H}^{(0)}$, the commutator depends only on the time difference $t - t_1$. We can therefore set $t_1 = 0$ and obtain

$$\boldsymbol{\chi}_{ux}(t) = -i\,\theta(t)\left\langle \left[\hat{\boldsymbol{u}}^{(0)}(t), \hat{\boldsymbol{x}}^{(0)}(0) \right] \right\rangle$$
(4.19)

Comparing with the definition of the susceptibility, Eq. 4.3, we find

$$\boldsymbol{\chi}_{ux}(\omega) = \int_{-\infty}^{\infty} \boldsymbol{\chi}_{ux}(t) e^{i\omega t} dt$$
(4.20)

4.2 Spectral representation, Kramers-Kronig relations

The result (4.20) is very general. Let us now examine some of the properties of the retarded correlation function. To do so it is very convenient to introduce a formal decomposition known as the spectral representation. Let us again introduce a complete basis $|n\rangle$ constituted of the eigenstates of the Hamiltonian H

$$\hat{H}^{(0)}|n\rangle = E_n|n\rangle \tag{4.21}$$

It is important to realize that -except for very simple Hamiltonians- determining the eigenstates $|n\rangle$ and eigenvalues E_n is a formidable problem. In general we are not able to compute those explicitly, but in what follows we will simply use these quantities to derive formally a series of relations, and it is simply sufficient to know that such a basis exists without having to know it explicitly.

Let us first rewrite the retarded correlation function inside the integral of Eq. ??

$$\boldsymbol{\chi}_{ux}(t) = -i\,\theta(t)\sum_{n} p_n \langle n | \left[\hat{\boldsymbol{u}}^{(0)}(t)\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}^{(0)}\hat{\boldsymbol{u}}(t) \right] | n \rangle$$
(4.22)

We now insert the closure relation $1 = \sum_{m} |m\rangle \langle m|$ inbetween \hat{x} and $\hat{u}^{(0)}(t)$ in both terms of the above expression. Using the definition of the Heisenberg operators of the unperturbed system (4.11) and the fact that $|n\rangle$ and $|m\rangle$ are eigenstates of the Hamiltonian $\hat{H}^{(0)}$, one gets

$$\boldsymbol{\chi}_{ux}(t) = -i\,\theta(t)\sum_{n,m} p_n e^{i(E_n - E_m)t} \langle n|\hat{\boldsymbol{u}}|m\rangle \,\langle m|\hat{\boldsymbol{x}}|n\rangle \tag{4.23}$$

$$+ i \theta(t) \sum_{n,m} p_n e^{i(E_m - E_n)t} \langle n | \hat{\boldsymbol{x}} | m \rangle \langle m | \hat{\boldsymbol{u}} | n \rangle$$
(4.24)

It is convenient to relabel $n \to m$ and $m \to n$ in the second term, to get

$$\boldsymbol{\chi}_{ux}(t) = -i\,\theta(t)\sum_{n,m} (p_n - p_m)e^{i(E_n - E_m)t} \langle n|\hat{\boldsymbol{u}}|m\rangle \,\langle m|\hat{\boldsymbol{x}}|n\rangle \tag{4.25}$$

This allows to directly write the Fourier transform as

$$\chi_{ux}(\omega) = \int dt e^{i(\omega+i\delta)t} \chi_{ux}(t) =$$
$$= -i \sum_{n,m} (p_n - p_m) \langle n | \hat{\boldsymbol{u}} | m \rangle \langle m | \hat{\boldsymbol{x}} | n \rangle \int_0^{+\infty} dt e^{i(\omega + E_n - E_m + i\delta)t}$$

LINEAR RESPONSE

Integration is straightforward, so that

$$\chi_{ux}(\omega) = \sum_{n,m} (p_n - p_m) \frac{\langle n | \hat{\boldsymbol{u}} | m \rangle \langle m | \hat{\boldsymbol{x}} | n \rangle}{\omega + E_n - E_m + i\delta}$$
(4.26)

We see that the frequency dependence consists in a series of poles, when the frequency is in resonance with an energy difference between two energy levels.

Often the response is measured of the same observable \hat{x} to which the external force couples. In the following chapter we will for example encounter the current response to an electric field. The susceptibility is then labeled $\chi_{jj}(\omega)$. The real and imaginary parts of the response function are in these cases given by

$$\boldsymbol{\chi}'(\omega) = \sum_{n,m} (p_n - p_m) \frac{|\langle n | \hat{\boldsymbol{x}} | m \rangle |^2}{\omega + E_n - E_m}$$
$$\boldsymbol{\chi}''(\omega) = -\sum_{n,m} (p_n - p_m) |\langle n | \hat{\boldsymbol{x}} | m \rangle |^2 \pi \delta(\omega + E_n - E_m)$$
(4.27)

From which it is easy to verify that

$$\chi'(\omega) = \chi'(-\omega)$$

$$\chi''(\omega) = -\chi''(-\omega)$$

$$\chi''(\omega) \le 0 \qquad (\omega > 0)$$
(4.28)

The last property of the sign of the imaginary susceptibility is mandatory, since in the following section we will see, that $-\omega \chi''(\omega)$ is proportional to the energy absorbed by the system in an oscillatory field. We also see directly that for $\omega = 0$ one has $\chi''(0) = 0$ and thus in particular no absorption or dissipation of energy is possible with a static field.

The decomposition in poles allows to immediately show the very general and remarkable relation

$$\boldsymbol{\chi}'(\omega) = \frac{-1}{\pi} \mathcal{P} \int \frac{\boldsymbol{\chi}''(\omega_1)}{\omega - \omega_1} d\omega_1$$
(4.29)

This relation that related the real and imaginary parts of the response function is known as the Kramers-Kronig relation. As we saw it is fully general , and is the direct consequence of causality of the response function.

4.3 Fluctuation dissipation theorem

In the previous section we have discussed the average response to an applied field, and derived an expression for the susceptibility. Since the susceptibility describes the ratio of an observable to an external field, both of which are in principle real quantities, one might naively expect that the susceptibility is purely real. However, there is also an imaginary part, which has the meaning of the rate of energy dissipation of the external force, i.e. the rate at which energy is transferred into heat inside the material. One of the deep consequences of the linear response theory is the **fluctuation-dissipation theorem**, which expresses the relation between the mean square fluctuations of an observable in the absence of a perturbing potential and the imaginary part of the susceptibility of this observable. The fluctuating field and the corresponding susceptibilities can for example be fluctuations of charge $(\hat{x} = \hat{\rho})$, current $(\hat{x} = \hat{j})$ or spin $(\hat{x} = \hat{s})$ density. The average fluctuations of a fluctuating field \hat{x}_q with wavenumber q are described by the *static* form factor

$$\langle \hat{x}_{-q} \hat{x}_{q} \rangle = \lim_{t \to 0} \int_{-\infty}^{\infty} e^{i\omega t} S(q,\omega) d\omega$$
(4.30)

$$S(q,\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \langle n | \hat{x}_{-q} | m \rangle \langle m | \hat{x}_q | n \rangle \, \delta(\omega + E_n - E_m) \tag{4.31}$$

Taking advantage of the properties of the δ -function it is easy to show that for negative frequencies:

$$S(q, -\omega) = e^{-\beta\omega} S(q, \omega) \tag{4.32}$$

Comparing Eq. 4.31 and Eq. 4.27 we see, that

$$S(q,\omega) - S(q,-\omega) = -\pi^{-1}\chi''(q,\omega)$$
 (4.33)

inserting Eq. 4.33 in Eq. 4.30 we obtain

$$\langle \hat{x}_{-\boldsymbol{q}} \hat{x}_{\boldsymbol{q}} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \chi_{xx}^{\prime\prime}(\boldsymbol{q},\omega) \frac{1}{1 - e^{-\beta\omega}} d\omega$$
(4.34)

With the help of the symmetry property that $\chi''_{xx}(q,\omega) = -\chi''_{xx}(q,-\omega)$, and some standard manipulations, the expression can be recast in one of the most standard forms of the fluctuation-dissipation theorem,

$$\left\langle \hat{x}_{-\boldsymbol{q}}\hat{x}_{\boldsymbol{q}} \right\rangle = -\frac{1}{\pi} \int_{0}^{\infty} \chi_{xx}^{\prime\prime}(\boldsymbol{q},\omega) \coth\left(\frac{\beta\omega}{2}\right) d\omega$$
(4.35)

where $1/\beta = k_B T$. For further reading on this theorem we refer to the book of Nozières and Pines. The fluctuation-dissipation theorem relies *only* on two very general assumptions: (i) that we restrict to linear response; (ii) that the system is in thermodynamic equilibrium. The fluctuation dissipation theorem is a very powerful tool since it quantifies the fact that by slightly perturbing the system (as expressed by the susceptibility on the r.h.s.) we can probe the various correlations and physical properties of the unperturbed system (l.h.s). In the opposite direction it provides a very practical and powerful way to compute the response of a system to an arbitrary time and space dependent perturbation (r.h.s) as soon as we are able to compute the correlations of the system in equilibrium (l.h.s).

4.4 Summary

It is useful for later reference to summarize the main ingredients and outcome of this chapter. Suppose that we drive the system with an external field F(t) (magnetic field, electric field, pressure, etc.) which is coupled to the observable $\hat{x}(r)$ (e.g. magnetization, current, density, etc.):

$$\hat{H}^{(p)}(t) = \mathbf{F}(t) \cdot \hat{\mathbf{x}}$$
(4.36)

The susceptibility $\chi_{ux}(\omega)$, defined as

$$\boldsymbol{u} = \boldsymbol{\chi}_{ux}(\omega)\boldsymbol{F}$$
(4.37)

follows from the microscopic relation

$$\boldsymbol{\chi}_{ux}(t) = -i\,\theta(t)\left\langle \left[\hat{\boldsymbol{u}}^{(0)}(t), \hat{\boldsymbol{x}}^{(0)}(0) \right] \right\rangle$$
(4.38)

$$\boldsymbol{\chi}_{ux}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} \boldsymbol{\chi}_{ux}(t) dt$$
(4.39)

A completely equivalent expression for the susceptibility in many-body physics is

$$\boldsymbol{\chi}_{ux}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \frac{\langle n | \hat{\boldsymbol{u}} | m \rangle \langle m | \hat{\boldsymbol{x}} | n \rangle}{\omega + E_n - E_m + i\delta}$$
(4.40)

The fluctuation-dissipation theorem relates the mean square thermal fluctuations of the observable \hat{x} (l.h.s) to the imaginary part of the susceptibility (r.h.s.)

$$\langle \hat{x}_{-\boldsymbol{q}} \hat{x}_{\boldsymbol{q}} \rangle = -\frac{1}{\pi} \int_0^\infty \chi_{xx}''(\boldsymbol{q}, \omega) \coth\left(\frac{\beta\omega}{2}\right) d\omega$$
(4.41)

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CHAPTER 5

Optical conductivity

5.1 Coupling of interacting electrons in solids to an electromagnetic field

We start with a short reminder of some basic notions, and establish the notations that will be used throughout this chapter. In the interest of compactness of notation we will use Planck units: $\hbar = 1$ and c = 1. In these units the electron charge is equal to the square root of the fine structure constant, *i.e.* $q_e = -\sqrt{\alpha} \approx -0.085$. The optical conductivity expresses the current response to an electric field

$$q_e \boldsymbol{v}(\boldsymbol{r}, t) = \int d^3 \boldsymbol{r}' \int_{-\infty}^t dt' \sigma(\boldsymbol{r}, \boldsymbol{r}', t - t') \boldsymbol{E}(\boldsymbol{r}', t')$$
(5.1)

We consider the situation where the electric field is described by a plane wave with a wavevector q and a frequency ω , hence $\mathbf{E}(r,t) = \mathbf{E}_q e^{i(q \cdot \mathbf{r} - \omega t)}$, with a similar definition, $q_e \boldsymbol{v}_q$, for the current. We will assume here, that the fields are sufficiently small, so that we may consider only induced electrical currents which are linearly proportional to the electric fields at each coordinate \mathbf{r} of the matter. Consequently the currents oscillate at the same frequency and wavelength as the electric field. Written in frequency and momentum representation the relation between \mathbf{E}_q and $q_e \boldsymbol{v}_q$ is

$$q_e \boldsymbol{v}_q = \sigma(q, \omega) \boldsymbol{E}_q \tag{5.2}$$

The electric field of a plane electromagnetic wave is transverse to the photon momentum. The tensor elements of the optical conductivity which can be measured in an optical experiment, are therefore transverse to the direction of propagation of the electromagnetic wave. We consider the effect of a time-varying electric field, which is the time derivative of the vector potential, i.e. the relation between $A = A_q e^{-i\omega t}$ and $E = E_q e^{-i\omega t}$ is

$$\boldsymbol{E}(t) = -\frac{\partial \boldsymbol{A}(t)}{\partial t} = i\omega \boldsymbol{A}(t).$$
(5.3)

The optical conductivity defined in Eq. 5.2 can be calculated using the formalism of the linear response theory outlined in chapter 4. For further reading we recommend "Many-Particle Physics" Gerald D. Mahan (2d edition, Plenum 1990 (p 207-223), and 'The theory of quantum liquids' part I by Nozières and Pines (p 252-255).

The coupling between the electromagnetic field and the electrons is introduced through the "minimal substitution" of the momentum \boldsymbol{p} of the particle by $\boldsymbol{p} - q_e \boldsymbol{A}$ where q_e is it's charge, and \boldsymbol{A} is the vector potential. For a single electron the corresponding Hamiltonian is

$$H = \frac{1}{2m} \left| \boldsymbol{p} - q_e \boldsymbol{A}(\boldsymbol{r}, t) \right|^2 + q_e \phi(\boldsymbol{r})$$

where $\mathbf{A}(\mathbf{r}, t)$ is the electromagnetic field at the position of the electron with coordinate \mathbf{r} respectively. The term $e\phi(\mathbf{r})$ describes the periodic potential of the solid in which the electrons move. We can express it as a Hilbert space operator on the complete basis of coordinate eigenstates $|\mathbf{r}\rangle$ in the following way:

$$\hat{\phi} = \sum_{r} \phi(\boldsymbol{r}) \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) = \sum_{r} \phi(\boldsymbol{r}) \hat{\rho}(\boldsymbol{r})$$

Without loss of generality the vector potential can be expanded in Fourier components as $\mathbf{A}(\mathbf{r},t) = \sum_{q} e^{iq\cdot\mathbf{r}} \mathbf{A}_{q}(t)$, with the understanding that $\mathbf{A}_{-q}(t) = \mathbf{A}_{q}^{*}(t)$ such as to have real values for $\mathbf{A}(\mathbf{r},t)$. We can furthermore use without loss of generality the Coulomb gauge $\nabla \cdot \mathbf{A}(r) = 0$, implying for the Fourier transform of the vector potential that $\mathbf{q} \cdot \mathbf{A}_{q} = 0$. For compactness of notation we will substitute $\mathbf{A}_{q}(t) = \mathbf{A}_{q}$ in the remainder of this chapter. The most convenient basis for the kinetic energy is provided by the set of momentum eigenstates $|\mathbf{k}\rangle$. The field-operator for the momentum of a many-body system is then:

$$\hat{oldsymbol{p}} = \sum_k \hbar oldsymbol{k} \hat{c}_k^\dagger \hat{c}_k$$

In a similar way the contribution of the vector potential $A(r_i)$ to the canonical momentum is

$$\begin{split} \hat{\boldsymbol{A}} &= \sum_{r} \sum_{q} \boldsymbol{A}_{q} e^{iqr} \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) = \\ &= \frac{1}{N^{2}} \sum_{r} \sum_{q} \sum_{k} \sum_{p} \boldsymbol{A}_{q} e^{iqr} e^{ikr} e^{-ipr} \hat{c}_{k}^{\dagger} \hat{c}_{p} = \\ &= \sum_{k,q} \boldsymbol{A}_{q} \hat{c}_{k}^{\dagger} \hat{c}_{k+q} \end{split}$$

The full Hamiltonian of interacting particles in the presence of a vector potential and Coulomb potential is

$$\begin{aligned}
\hat{H} &= \hat{H}^{(0)} + \hat{H}^{(p)} + \hat{H}^{(p')} \\
\hat{H}^{(0)} &= \sum_{k} \frac{\hbar^{2}k^{2}}{2m} \hat{c}_{k}^{\dagger} \hat{c}_{k} + q_{e} \int d\mathbf{r} \phi(\mathbf{r}) \hat{\rho}(\mathbf{r}) + \frac{1}{2} \sum_{i,j} V^{(i)} (\mathbf{r}_{i} - \mathbf{r}_{j}) \hat{\psi}^{\dagger}(\mathbf{r}_{i}) \hat{\psi}^{\dagger}(\mathbf{r}_{j}) \hat{\psi}(\mathbf{r}_{j}) \hat{\psi}(\mathbf{r}_{i}) \\
\hat{H}^{(p)} &= -\frac{\hbar q_{e}}{m} \sum_{k,q} \mathbf{k} \cdot \mathbf{A}_{q} \hat{c}_{k}^{\dagger} \hat{c}_{k+q} \\
\hat{H}^{(p')} &= \frac{q_{e}^{2}}{2m} \sum_{k,q,q'} \mathbf{A}_{q} \cdot \mathbf{A}_{q'} \hat{c}_{k}^{\dagger} \hat{c}_{k+q+q'}
\end{aligned}$$
(5.4)

In obtaining this expression we have chosen the Coulomb gauge, $\mathbf{q} \cdot \mathbf{A}_q = 0$. In the present expression the \sum_k runs over the entire momentum space, *i.e.* it is not restricted to the first Brillouin-zone. It is also important to note that additional terms appear when relativistic effects such as spin-orbit coupling are taken into account.

5.2 General considerations about the calculation of the linear response to an electromagnetic field

We are going to calculate the linear response of the charge current $q_e \boldsymbol{v}(r,t) = q_e \boldsymbol{v}_q e^{i(qr-\omega t)}$ to the vector potential $\boldsymbol{A}(r,t) = \boldsymbol{A}_q e^{i(qr-\omega t)}$. In general terms our task is to compute the timedependent expectation value of the current operator in the presence of the vector potential. The vector potential enters the problem on two levels: First, the time-independent current operator in the presence of the vector potential is already different from the current operator without vector potential. Secondly the time evolution of the current operator is described by the Hamiltionian Eq. 5.4, which also contains the vector potential. Taken together

$$\left| \vec{\sigma} \left(\omega \right) = \frac{q_e \boldsymbol{v}_q}{i \omega \boldsymbol{A}_q} \quad (\lim \, \boldsymbol{A}_q \to 0) \right| \tag{5.5}$$

Both \hat{H} and $q_e \boldsymbol{v}_q$ are implicit functions of the vector potential. We will proceed by making a Taylor series expansion, and collect at the end the terms linear in A_q . The current $q_e \boldsymbol{v}_q$ is an observable which, as always in quantum mechanics, is described by an operator, in this case the current operator $q_e \hat{\boldsymbol{v}}_q$. In a measurement, the current follows from the appropriate average

$$\boldsymbol{v}_q = \langle \hat{\boldsymbol{v}}_q \rangle = \operatorname{Tr}\left[\hat{\rho}\hat{\boldsymbol{v}}_q\right] \tag{5.6}$$

The theory of quantum electrodynamics of coupled electron and photon fields describes the connection between current, vector potential, and Hamiltonian. In most textbooks it is described for case of individual (non-interacting) particles in the way it was presented in the previous section. For the purpose of the present chapter it will be useful to relate the current-operator in second quantization to the Hamiltonian operator operator in second quantization and the vector potential treated as a classical field.

The current operator $\hat{\boldsymbol{v}}(\boldsymbol{r})$ (which is the Fourier-transform of $\hat{\boldsymbol{v}}_q$) is defined by the fact that, together with the density operator ($\hat{\rho}(\boldsymbol{r})$ which we have introduced before) it satisfies the continuity equation, which can be phrased as follows: For any eigen state $|m\rangle$ of the manybody system

$$\nabla \cdot \langle m | \hat{\boldsymbol{v}}(\boldsymbol{r}, t) | m \rangle = -\partial / \partial t \langle m | \hat{\rho}(\boldsymbol{r}, t) | m \rangle$$
(5.7)

This property is satisfied when we define $\hat{\boldsymbol{v}}_q$ as follows:

$$q_e \hat{\boldsymbol{v}}_q \equiv -\partial \hat{H} / \partial \boldsymbol{A}_{-q} \tag{5.8}$$

Application to the Hamiltonian, Eq. 5.4, this implies

$$\hat{\boldsymbol{v}}_{q} = \hat{\boldsymbol{v}}_{q}^{(r)} + \hat{\boldsymbol{v}}_{q}^{(d)}$$

$$\hat{\boldsymbol{v}}_{q}^{(r)} = \frac{1}{m} \sum_{k} \boldsymbol{k} c_{k+q/2}^{\dagger} c_{k-q/2}$$

$$\hat{\boldsymbol{v}}_{q}^{(d)} = -\frac{q_{e}}{m} \sum_{k,p} \boldsymbol{A}_{-p} c_{k+(q+p)/2}^{\dagger} c_{k-(q+p)/2}$$
(5.9)

We leave it as an exercise to check that the continuity equation, Eq. 5.7, is indeed satisfied (hint: Fourier transform to $\hat{\boldsymbol{v}}_q$ and $\hat{\rho}_q$ and use the Heisenberg equation of motion for the timederivative). The first term in Eq. 5.9 is the so-called "regular" part of the current operator, since it is independent of the vector potential. It is important to realize, that the regular part represents in fact the time derivative of the position operator: If $\hat{\boldsymbol{r}}_i = \boldsymbol{r}_i \hat{\psi}^{\dagger}(\boldsymbol{r}_i) \hat{\psi}(\boldsymbol{r}_i)$ represents the position operator of an individual site, than the global position operator of the system with N_s sites is

$$\hat{\boldsymbol{r}} = \sum_{i=1}^{N_s} \boldsymbol{r}_i \hat{\psi}^{\dagger}(\boldsymbol{r}_i) \hat{\psi}(\boldsymbol{r}_i)$$
(5.10)

The corresponding current operator follows from the Heisenberg equation of motion

$$\hat{\boldsymbol{v}}^{(r)} = i \left[\hat{H}^{(0)}, \hat{\boldsymbol{r}} \right]$$
(5.11)

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It can be easily verified that for free electrons this corresponds to the expression in Eq. 5.9. However, it is important to notice that Eq. 5.11 is valid for any energy-momentum dispersion of the electrons; we will therefore use this expression in further discussion of the optical conductivity.

The second term is the "diamagnetic part". The expectation value has finite contributions only from p = -q in the above expression, hence, with the help of the equality $\sum_k \left\langle c_k^{\dagger} c_k \right\rangle = n$ we obtain

$$\vec{\sigma}(q,\omega) = \frac{q_e \boldsymbol{v}_q}{i\omega \boldsymbol{A}_q} = \frac{i}{\omega} \frac{nq_e^2}{m} + \frac{q_e \boldsymbol{v}_q^{(r)}}{i\omega \boldsymbol{A}_q}$$
(5.12)

where the first term is the diamagnetic contribution, and the second term represents the "regular" contribution due to the combined effect of the crystal potential in which the electrons move, and their mutual interactions. The linear relation between $q_e \boldsymbol{v}_q^{(r)}$ and \boldsymbol{A}_q follows from linear response theory. Combining the terms linear in \boldsymbol{A} of Eq. 5.4 and Eq. 5.9 we obtain

$$\hat{H}^{(p)} = -q_e \sum_q \boldsymbol{A}_q \cdot \hat{\boldsymbol{v}}_{-q}^{(r)}$$
(5.13)

and comparing Eq. 5.13 with Eqs. 4.36 and 4.37, we see that we can associate

$$\begin{split} F_q &= -\boldsymbol{A}_q \\ \hat{x} &= q_e \hat{\boldsymbol{v}}_{-q}^{(r)} \\ \chi_{jj}(q,\omega) &= -q_e \boldsymbol{v}_{-q}^{(r)} / \boldsymbol{A}_q \end{split}$$

We can use the general result for susceptibility functions in Eq. 4.20, and this way obtain the relation between the optical conductivity and the current-current susceptibility

$$\begin{aligned} \vec{\sigma}(q,\omega) &= \frac{i}{\omega} \frac{nq_e^2}{m} + i \frac{\vec{\chi}_{jj}(q,\omega)}{\omega} \\ \vec{\chi}_{jj}(q,\omega) &= \int_{-\infty}^{\infty} e^{i\omega t} \vec{\chi}_{jj}(q,t) dt \\ \vec{\chi}_{jj}(q,t) &= -i \theta(t) \left\langle \left[\hat{\boldsymbol{j}}_q^{(0)}(t), \hat{\boldsymbol{j}}_{-q}^{(0)}(0) \right] \right\rangle \end{aligned}$$
(5.14)

Due to the high velocity of light compared to electron velocities in a solid, absorption of light involves photons for which $qa \ll 1$, where a is a lattice constant. Therefore, q = 0 is usually a very good approximation for optical absorption in solids. With the help of the results of linear response theory of the previous section, in particular Eq. 4.40, we find the expression for the current-current susceptibility

$$\vec{\chi}_{jj}(\omega) = \sum_{n,m} \left(p_n - p_m \right) \frac{q_e^2 |\langle n | \hat{\boldsymbol{v}} | m \rangle |^2}{\omega + E_n - E_m + i\delta}$$
(5.15)

where $p_n = e^{-\beta E_n}/Z$ is the statistical probability of occurrence of the many-body quantum state $|n\rangle$. Note that, in the interest of compactness, we have suppressed the label (r) of the "regular" velocity operator and will continue to do so in the remainder of this section.

A curious aspect of Eq. 5.15, not obviously visible in its actual form, is that the regular term *also* contains a pole at the origin, of opposite sign of the diamagnetic term. In normal metals and insulators the two poles in the origin precisely compensate each other, leaving for the case of an insulator only poles at finite frequency. For a normal metal there *is* however a Drude peak at the origin, corresponding to a pole away from the origin along the imaginary frequency

axis. In the case of a superconductor there is a pole at the origin with pole strength limited by nq_e^2/m , but usually much smaller. It is in fact possible to combine the two terms in Eq. 5.15 in a single one with the same sign for all poles including the one in the origin. This requires a bit of algebra, which we will detail in the following page. We are in fact talking about free electrons here, so in principle we could rely on Eq. 5.11 for the current. On the other hand, Eq. 5.11 is valid regardless of the energy-momentum dispersion, and it is useful as a pedagogical tool to work out the expressions for a general dispersion relation. For the matrix elements in $\tilde{\chi}(\omega)$ this implies:

$$\begin{split} \sum_{\beta} \frac{\langle \alpha | \hat{\boldsymbol{v}} | \beta \rangle \langle \beta | \hat{\boldsymbol{v}} | \alpha \rangle}{E_{\beta} - E_{\alpha}} &= -\left\langle \alpha \left| \left[\hat{H}, \hat{\boldsymbol{r}} \right] \frac{1}{\hat{H} - E_{\alpha}} \left[\hat{H}, \hat{\boldsymbol{r}} \right] \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \left(\hat{H} \hat{\boldsymbol{r}} - \hat{\boldsymbol{r}} \hat{H} \right) \frac{1}{\hat{H} - E_{\alpha}} \left(\hat{H} \hat{\boldsymbol{r}} - \hat{\boldsymbol{r}} \hat{H} \right) \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \hat{\boldsymbol{r}} \left(E_{\alpha} - \hat{H} \right) \frac{1}{\hat{H} - E_{\alpha}} \left(\hat{H} - E_{\alpha} \right) \hat{\boldsymbol{r}} \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \hat{\boldsymbol{r}} \left(E_{\alpha} - \hat{H} \right) \hat{\boldsymbol{r}} \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \left(E_{\alpha} \hat{\boldsymbol{r}} \hat{\boldsymbol{r}} - \hat{\boldsymbol{r}} \hat{H} \hat{\boldsymbol{r}} \right) \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \left(\hat{H} \hat{\boldsymbol{r}} \hat{\boldsymbol{r}} - \hat{\boldsymbol{r}} \hat{H} \hat{\boldsymbol{r}} \right) \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \left(\hat{H} \hat{\boldsymbol{r}} \hat{\boldsymbol{r}} - \hat{\boldsymbol{r}} \hat{H} \hat{\boldsymbol{r}} \right) \right| \alpha \right\rangle = \\ &= -\left\langle \alpha \right| \left[\hat{H}, \hat{\boldsymbol{r}} \right] \hat{\boldsymbol{r}} \right| \alpha \right\rangle = \\ &= -\frac{1}{2} \left\langle \alpha \right| \left[\left[\hat{H}, \hat{\boldsymbol{r}} \right], \hat{\boldsymbol{r}} \right] \right| \alpha \right\rangle = \\ &= -\frac{1}{2} \left\langle \alpha \right| \left[\hat{\boldsymbol{v}}, \hat{\boldsymbol{r}} \right] \right| \alpha \right\rangle$$

where $|\alpha\rangle$ are many-body eigenstates of the system. To address the commutator in the last line we can use the result of the following section, Eqs. 5.36 and 5.37. At this point the electrons are still treated as having a free electron dispersion, and all band effects are incorporated in the periodic potential that is stated explicitly in the Hamiltonian. In this limit the commutator is:

$$i\left[\hat{\boldsymbol{v}},\hat{\boldsymbol{r}}\right] = \sum_{k} \frac{1}{m_e} \hat{n}_k \tag{5.16}$$

so that:

$$\sum_{\beta} \frac{\langle \alpha \, | \hat{\boldsymbol{v}} | \, \beta \rangle \, \langle \beta \, | \hat{\boldsymbol{v}} | \, \alpha \rangle}{E_{\beta} - E_{\alpha}} = \frac{N_e}{2m_e} \tag{5.17}$$

We multiply both sides by $2p_{\alpha}$, sum over α , use $\sum_{\alpha} p_{\alpha} = 1$, split $\sum_{\alpha,\beta}$ at the l.h.s. in two terms, rearrange, and obtain:

$$\frac{n_e}{m_e} = \frac{N_e}{m_e \Omega} = \frac{1}{\Omega} \sum_{\alpha,\beta} \left(p_\alpha - p_\beta \right) \frac{\langle \alpha \, | \, \hat{\boldsymbol{v}} | \, \beta \rangle \, \langle \beta \, | \, \hat{\boldsymbol{v}} | \, \alpha \rangle}{E_\beta - E_\alpha} \tag{5.18}$$

This substitution allows us to merge the diamagnetic and regular terms of the optical conduc-

tivity (Eq. 5.15) in a single term, as shown in the following few steps:

$$\begin{split} \vec{\sigma}\left(\omega\right) &= i\frac{q_e^2}{\omega\Omega}\sum_{\alpha,\beta}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle\left(p_{\alpha}-p_{\beta}\right)\left(\frac{1}{\omega+E_{\alpha}-E_{\beta}}+\frac{1}{E_{\beta}-E_{\alpha}}\right)=\\ &= i\frac{q_e^2}{\omega\Omega}\sum_{\alpha,\beta}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle\left(p_{\alpha}-p_{\beta}\right)\frac{\omega}{(\omega+E_{\alpha}-E_{\beta})(E_{\beta}-E_{\alpha})}=\\ &= i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{E_{\beta}-E_{\alpha}}\left(p_{\alpha}-p_{\beta}\right)\frac{1}{\omega+E_{\alpha}-E_{\beta}}=\\ &= i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{p_{\alpha}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{E_{\beta}-E_{\alpha}}\frac{1}{\omega+E_{\alpha}-E_{\beta}}-i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{p_{\beta}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{\omega+E_{\alpha}-E_{\beta}}=\\ &= i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{p_{\alpha}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{E_{\beta}-E_{\alpha}}\frac{1}{\omega+E_{\alpha}-E_{\beta}}-i\frac{q_e^2}{\Omega}\frac{p_{\alpha}\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle}{\omega+E_{\beta}-E_{\alpha}}=\\ &= i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{p_{\alpha}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{E_{\beta}-E_{\alpha}}\left[\frac{1}{\omega+E_{\alpha}-E_{\beta}}+\frac{1}{\omega+E_{\beta}-E_{\alpha}}\right]=\\ &= i\frac{q_e^2}{\Omega}\sum_{\alpha,\beta}\frac{p_{\alpha}\left\langle\alpha\left|\hat{\boldsymbol{v}}\right|\beta\right\rangle\left\langle\beta\left|\hat{\boldsymbol{v}}\right|\alpha\right\rangle}{E_{\beta}-E_{\alpha}}\frac{\omega}{\omega^2-(E_{\beta}-E_{\alpha})^2} \end{split}$$

The conductivity up to this point is a purely imaginary quantity. To describe dissipation processes we need to extend it with a real part. According to the fluctuation dissipation theorem outlined in the previous chapter, this is achieved by adding a $i\delta$ term in the denominator, providing the following expression for the complex optical conductivity tensor:

$$\vec{\sigma}(\omega) = \frac{2q_e^2}{\Omega} \sum_{\alpha,\beta} \frac{p_\alpha \langle \alpha | \hat{\boldsymbol{v}} | \beta \rangle \langle \beta | \hat{\boldsymbol{v}} | \alpha \rangle}{E_\beta - E_\alpha} \frac{i\omega}{\omega (\omega + i\delta) - (E_\beta - E_\alpha)^2}$$
(5.19)

5.3 Current operator of the electrons in a periodic lattice

To describe the optical properties of a solid one could start with the Hamiltonian of Eq. 5.4, where $\phi(\mathbf{r})$ describes the periodic potential of the atomic lattice, diagonalize it with a powerful computer, and plug the outcome in Eq. 5.19. Obtaining the full set of many-body eigenstates will be time consuming, and calculating the current matrix elements cumbersome. It is not a particularly insightful approach. Instead we will take as a starting point the bandstructure that is obtained by solving the single-particle Schroedinger equation of an electron in the background of all other electrons. The electrons in the b^{th} band are characterized the energy-momentum dispersion $\varepsilon_{k,b}$ (including spin-index, if any). The corresponding expression for the Hamiltonian is

$$\hat{H} = \sum_{k,b}^{1^t BZ} \varepsilon_{k;b} \hat{c}^{\dagger}_{k;b} \hat{c}_{k;b} + \hat{H}^{int}$$
(5.20)

The expression is sufficiently general to include spin-orbit interaction. The "translation" of the electron-electron Coulomb interaction into \hat{H}^{int} results in a rather complicated looking 4-operator expression which we will not discuss here. In this chapter we will only look into slimmed down models of the interaction.

A very important consequence of the bandstructure for the optical properties is, that interband excitations occur in addition to conduction by electrons in a metal, where the valence band is partially occupied. We will see in the following section that, to calculate the optical transition, requires knowledge of the interband matrix elements of the current operator. In the present section we derive the expression for the current operator. Since in many cases we will need it to describe multi-electron processes, and processes such as excitons where the many-body aspects really matter, we continue to use the field-theoretical approach, i.e. of second quantization.
The single-electron eigen states are characterized by their band index b and the momentum quantum number k. The band index is also used to label the spin state (or any other quantum number, e.g. as appropriate in the presence of spin-orbit coupling). Due to the lattice periodicity the eigenstates are Bloch waves. Fourier transformation of these band states defines the Wannier wavefunctions, forming a complete set of orthonormal states centered at the lattice sites. The number of Wannier states associated to each lattice site, is the same as the number of bands, hence this number is in principle infinite although in practical computations one can, and has to, truncate the set. One can for example take a (limited) set of atomic orbitals at each site as the starting point, and do some patchwork to orthoganalize the states centered at different cites. We reserve the symbol $\psi_{i;\mu}^{\dagger}$ for the creation operator of these states, where i is the site index corresponding to position vector \mathbf{r}_i , and μ refers to the orbital quantum numbers (e.g. $1s, 1p_x, 1p_y, 1p_z, 2p_x, 2p_y, 2p_z, 3d_{xy}, 3d_{yz}, 3d_{zx}$, etc.). In the simplest examples that one usually treats in textbooks the Bloch-states have a one-to-one relation to these Wannier orbitals, e.g. $\hat{c}_k^{\dagger} = \sum_i e^{ikr_j} \hat{\psi}_{j,1s}$. In particular for k = 0 the character of the Bloch states has a one-to-one correspondence to the eigenstates of an isolated site of the same point group. However, for general k, and/or in the presence of spin-orbit coupling, the mapping from Bloch to Wannier states and vice-versa involves a momentum dependent mixing of character, described by the coefficients $u_{\mu,b}(\mathbf{k})$, corresponding to the amplitude of Wannier state ψ_{μ} in a given Bloch state corresponding to the b'th band. For some of the considerations later in this section, it is crucial to note that these amplitudes can in principle depend on the momentum k. This momentum dependence can occur for a variety of reasons, and is typically the result of a competition between kinetic energy (which is typically strongly momentum dependent) and, e.g., spin-orbit coupling (which typically isn't). The relation between the Bloch and the Wannier basis is described by:

$$\hat{c}_{k;b}^{\dagger} = \sum_{i;\mu} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i)} u_{\mu,b}(\boldsymbol{k}) \hat{\psi}_{i;\mu}^{\dagger} \qquad \& \qquad \hat{c}_{k;b} = \sum_{i;\mu} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_i)} u_{\mu,b}^*(\boldsymbol{k}) \hat{\psi}_{i;\mu}$$
(5.21)

The reverse transformation is as follows:

$$\hat{\psi}_{i;\mu}^{\dagger} = \sum_{k;b}^{1^{t}BZ} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_{i})} u_{\mu,b}^{*}(\boldsymbol{k}) \hat{c}_{k;b}^{\dagger} \qquad \& \qquad \hat{\psi}_{i;\mu} = \sum_{k;b}^{1^{t}BZ} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{i})} u_{\mu,b}(\boldsymbol{k}) \hat{c}_{k;b}$$
(5.22)

This transformation allows us to obtain an alternative expression of the Hamiltonian on the basis of Wannier states in coordinate space. To do so we substitute Eq. 5.21 in the Hamiltonian Eq. 5.20

$$\hat{H} = \sum_{i,j;\mu,\mu'} \sum_{k,b}^{1^t BZ} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \varepsilon_{k;b} u_{\mu,b}(\boldsymbol{k}) u_{\mu',b}^*(\boldsymbol{k}) \hat{\psi}_{i;\mu}^{\dagger} \hat{\psi}_{j;\mu'}$$
(5.23)

We now define

$$t_{i,j;\eta,\mu} = \sum_{k,b}^{1^t BZ} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} u_{\mu,b}^*(\boldsymbol{k}) \varepsilon_{k;b} u_{\eta,b}(\boldsymbol{k})$$
(5.24)

with the help of which

$$\hat{H} = \sum_{i,j;\eta,\mu} t_{i,j;\eta,\mu} \hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu} = \sum_{i,j;\eta,\mu} \hat{H}_{i,j;\eta,\mu}$$
(5.25)

In the first step diagonalizing the lattice periodicity the inverse transformation of Eq. 5.23 yields:

$$\sum_{m} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}} t_{0,m;\eta,\mu} = H_{\eta,\mu}(\boldsymbol{k})$$
(5.26)

and the second step diagonalizing the Wannier basis for a given k gives:

$$\sum_{\mu,\eta} u_{\mu,a}^*(\boldsymbol{k}) H_{\eta,\mu}(\boldsymbol{k}) u_{\eta,b}(\boldsymbol{k}) = \varepsilon_{k;b} \delta_{a,b}$$
(5.27)

We are interested in obtaining an expression for the current operator.

First of all we note that computation of the current operator connecting different Wannier orbitals sharing the same center coordinate requires knowledge of the wavefunctions. Note also, that in many cases of interest this refers to transitions on the order of a Rydberg. In any case, we will not dwell on this in detail, but simply state that these matrix elements exist and can be written as

$$\langle i, \mu | \hat{\boldsymbol{v}} | j, \eta \rangle = \boldsymbol{v}_{\mu,\eta}^{(at)} \delta_{i,j}$$
(5.28)

In addition to these on-site terms, there exist current matrix elements for $i \neq j$. The latter matrix elements provide the spectral weight of the Drude peak in the optical conductivity, but they also contribute to the intensity of the inter-band transitions, and for transitions in bands of the same atomic shell it is the dominant contribution to the intensity. We will now describe these contributions: The position operator is just the sum of all position operators of the different Wannier states at site j, $\mathbf{r}_m + \mathbf{d}_\rho$, where \mathbf{d}_ρ is at the center of weight of Wannier orbital ρ relative to the center of the unit cell.

$$\hat{\boldsymbol{r}} = \sum_{m,\rho} (\boldsymbol{r}_m + \boldsymbol{d}_\rho) \hat{\psi}^{\dagger}_{m,\rho} \hat{\psi}_{m,\rho} = \sum_{m,\rho} \hat{\boldsymbol{r}}_{m,\rho}$$
(5.29)

We calculate the current operator with the help of the Heisenberg equation of motion:

$$\hat{\boldsymbol{v}} = \frac{d\hat{\boldsymbol{r}}}{dt} = i \left[\hat{H}, \hat{\boldsymbol{r}} \right] \tag{5.30}$$

We decompose this as: $\hat{\bm v} = \sum_{i,j,m;\mu,\eta,\rho} \hat{\bm v}_{i,j,m;\mu,\eta,\rho}$, where each separate term satisfies

$$\hat{\boldsymbol{v}}_{i,j,m;\eta,\mu,\rho} = i \left[\hat{H}_{i,j;\eta,\mu}, \hat{\boldsymbol{r}}_{m,\rho} \right] = i t_{i,j;\eta,\mu} \boldsymbol{r}_m \left[\hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu}, \hat{\psi}_{m,\rho}^{\dagger} \hat{\psi}_{m,\rho} \right]$$
(5.31)

It is easy to verify that the commutator on the right hand side of Eq. 5.31 has the following properties:

$$\begin{bmatrix} \hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu}, \hat{\psi}_{m,\rho}^{\dagger} \hat{\psi}_{m,\rho} \end{bmatrix} = \begin{cases} 0 & (\{i;\eta\} \neq \{m;\mu\} \& \{j;\mu\} \neq \{m;\rho\}) \\ -\hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu} & (\{i;\eta\} = \{m;\mu\} \& \{j;\mu\} \neq \{m;\rho\}) \\ \hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu} & (\{i;\eta\} \neq \{m;\mu\} \& \{j;\mu\} = \{m;\rho\}) \\ 0 & (\{i;\eta\} = \{m;\mu\} \& \{j;\mu\} = \{m;\rho\}) \end{cases}$$
(5.32)

with the help of which we obtain for the current operator

$$\hat{\boldsymbol{v}} = i \sum_{i,j;\mu,\eta} t_{i,j;\eta,\mu} \left(\boldsymbol{r}_j - \boldsymbol{r}_i + \boldsymbol{d}_\mu - \boldsymbol{d}_\eta \right) \hat{\psi}_{i;\eta}^{\dagger} \hat{\psi}_{j;\mu}$$
(5.33)

Translational invariance of the lattice implies that $t_{i,j;\eta,\mu} = t_{0,j-i;\eta,\mu}$. We insert the transformation to the momentum field operators (Eq. 5.22), so that:

$$\hat{\boldsymbol{v}} = i \sum_{k,p;a,b}^{1^{t}BZ} \sum_{i,j;\mu,\eta} e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_{j}-\boldsymbol{p}\cdot\boldsymbol{r}_{i})} u_{\eta,a}^{*} t_{0,j-i;\eta,\mu} u_{\mu,b}(\boldsymbol{r}_{j}-\boldsymbol{r}_{i}+\boldsymbol{d}_{\mu}-\boldsymbol{d}_{\eta}) \hat{c}_{k;a}^{\dagger} \hat{c}_{p;b}$$
(5.34)

We relabel j = i + m and work out the expression for the current operator in a handful of steps:

$$\hat{\boldsymbol{v}} = i \sum_{\substack{k,p;a,b \ i,m;\mu,\eta}}^{1^{*}BZ} \sum_{\substack{k,p;a,b \ i,m;\mu,\eta}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}+i(\boldsymbol{k}-\boldsymbol{p})\cdot\boldsymbol{r}_{i}} u_{\eta,a}^{*}(\boldsymbol{k}) t_{0,m;\eta,\mu} u_{\mu,b}(\boldsymbol{k}) (\boldsymbol{r}_{m}+\boldsymbol{d}_{\mu}-\boldsymbol{d}_{\eta}) \hat{c}_{k;a}^{\dagger} \hat{c}_{p;b} = \\
= i \sum_{\substack{k,p;a,b \ m;\mu,\eta}}^{1^{*}BZ} \sum_{\substack{m;\mu,\eta}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}} \delta_{\boldsymbol{k},\boldsymbol{p}} u_{\eta,a}^{*}(\boldsymbol{k}) t_{0,m;\eta,\mu} u_{\mu,b}(\boldsymbol{k}) (\boldsymbol{r}_{m}+\boldsymbol{d}_{\mu}-\boldsymbol{d}_{\eta}) \hat{c}_{k;a}^{\dagger} \hat{c}_{p;b} = \\
= \sum_{\substack{k;a,b \ m;\mu,\eta}}^{1^{*}BZ} \sum_{\substack{m;\mu,\eta}} i(\boldsymbol{r}_{m}+\boldsymbol{d}_{\mu}-\boldsymbol{d}_{\eta}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}} u_{\eta,a}^{*}(\boldsymbol{k}) t_{0,m;\eta,\mu} u_{\mu,b}(\boldsymbol{k}) \hat{c}_{k;a}^{\dagger} \hat{c}_{k;b} = (5.35) \\
= \sum_{\substack{k;a,b \ m;\mu,\eta}}^{1^{*}BZ} u_{\eta,a}^{*}(\boldsymbol{k}) \left[\frac{d}{dk'} \sum_{\substack{m;\mu,\eta}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}} u_{0,m;\eta,\mu} \right]_{k'=k} u_{\mu,b}(\boldsymbol{k}) \hat{c}_{k;a}^{\dagger} \hat{c}_{k;b} + \\
+ i \sum_{\substack{k;a,b \ m;\mu,\eta}}^{1^{*}BZ} \sum_{\substack{m;\mu,\eta}} (\boldsymbol{d}_{\mu}-\boldsymbol{d}_{\eta}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m}} u_{\eta,a}^{*}(\boldsymbol{k}) t_{0,m;\eta,\mu} u_{\mu,b}(\boldsymbol{k}) \hat{c}_{k;a}^{\dagger} \hat{c}_{k;b}$$

We insert the transformation of Eq. 5.26 and obtain:

$$\hat{\boldsymbol{v}} = \sum_{k;a,b}^{1^t BZ} \upsilon_{a,b}(\boldsymbol{k}) \hat{c}_{k;a}^{\dagger} \hat{c}_{k;b}$$
(5.36)

where with the help of the above expressions and Eq. 5.28

$$v_{a,b}(\boldsymbol{k}) = \sum_{\eta,\mu} u_{\eta,a}^{*}(\boldsymbol{k}) u_{\mu,b}(\boldsymbol{k}) \left[\boldsymbol{v}_{\eta,\mu}^{(at)} + \frac{dH_{\eta,\mu}(\boldsymbol{k})}{d\boldsymbol{k}} + i(\boldsymbol{d}_{\mu} - \boldsymbol{d}_{\eta})H_{\eta,\mu}(\boldsymbol{k}) \right]$$
(5.37)

Note that for intra-shell transitions such as d-d transitions the first term in the square brackets, $v_{\mu,\eta}^{(at)}$, is manifestly zero due to the dipole selection rule.

We close this section with two peculiarities of the expressions for the current density. We start by recalling that diagonalisation of the Hamiltonian is achieved by the following unitary transformation:

$$\epsilon_{a,b}(\boldsymbol{k}) = \sum_{\eta,\mu} u_{\eta,a}^*(\boldsymbol{k}) H_{\eta,\mu}(\boldsymbol{k}) u_{\mu,b}(\boldsymbol{k})$$
(5.38)

As an alternative to Eq. 5.37, the current operator for the intraband-transitions can be obtained in a straightforward way by differentiating the energy-eigenvalues

$$v_{a,a}(\mathbf{k}) = \partial \epsilon_{a,a}(\mathbf{k}) / \partial \mathbf{k}$$
 (bandproperty i) (5.39)

Since the Hamiltonian is diagonalized by the transformation $u_{\eta,a}(\mathbf{k})$, the off-diagonal matrix elements satisfy:

$$\epsilon_{a,b}(\mathbf{k}) = 0 \quad (a \neq b)$$
 (bandproperty ii) (5.40)

Combining Eqs. 5.37 and 5.38 we arrive at the following consequence of bandproperty (i) :

$$\sum_{\eta,\mu} \frac{d \left[u_{\eta,a}^*(\boldsymbol{k}) u_{\mu,b}(\boldsymbol{k}) \right]}{d\boldsymbol{k}} H_{\eta,\mu}(\boldsymbol{k}) = 0 \qquad (a=b)$$
(5.41)

Using Eq. 5.37 we arrive at the following consequence of bandproperty (ii) :

$$\sum_{\eta,\mu} \frac{d \left[u_{\eta,a}^*(\boldsymbol{k}) u_{\mu,b}(\boldsymbol{k}) \right]}{d\boldsymbol{k}} H_{\eta,\mu}(\boldsymbol{k}) = -\sum_{\eta,\mu} u_{\eta,a}^*(\boldsymbol{k}) u_{\mu,b}(\boldsymbol{k}) \frac{d H_{\eta,\mu}(\boldsymbol{k})}{d\boldsymbol{k}} \qquad (a \neq b) \tag{5.42}$$

These two properties can be easily checked numerically. An example for a model of coupled ladders is given in Fig. 5.1.



Figure 5.1:

5.4 Interband transitions

Equation 5.19 is the most general form of the optical conductivity. It correctly accounts for all effects of the potential in which the electrons move, and their mutual interactions. However, this comes at a cost: The (ground and excited) states $|n\rangle$ and are many-body states, which are difficult to compute. Yet, for the purpose of describing the optical properties of a single atom this expression can be adequate. However, for samples of macroscopic dimensions one has to face the problem of the huge density of excited many-body states, and the way to label them. For this reason Eq. 5.19 is rarely applied to solids in this form. According to the type of material and the part of the optical spectrum that one wants to describe, various different approximations are used.

To gain some insight in this we first consider the optical spectrum of an insulating material. We neglect for the moment the Coulomb interaction between the electrons in Eq. 5.4. At T = 0 the Fermi energy lies inside a gap in the density of states, and the lowest possible excitations are those where an electron is excited across the gap. In terms of the many body states in we have to reformulate this as: The absorption of a photon results in the excitation of an electron-hole pair, where the hole is in the j'th band just below the gap, and the electron in the j + 1th band just above the gap. In a standard semiconducting material such as GaAs the optical absorption is understood to arise from the optical excitation of individual electrons across the band gap, resulting in optical spectra such as displayed in Fig. 5.2 In the special case of a system of



Figure 5.2: Optical conductivity of the semiconductors GaAs, Si and GaP (after D. E. Aspnes and A. A. Studna, Phys. Rev. B **27**, 985 (1983).)

non-interacting electrons, the groundstate is

$$|g\rangle = \prod_{k,j}^{\varepsilon_{k,j} < \varepsilon_F} c_{k,j}^{\dagger} |0\rangle$$
(5.43)

For an optical transition to occur between $|\mathbf{k}, j\rangle$ and $|\mathbf{k}', m\rangle$ ($\delta \mathbf{k} = \mathbf{k}' - \mathbf{k} = \mathbf{q}_{photon}$) requires that the former is occupied and the latter empty. The statistical probability of such a state $c_{k',m}c_{k,j}^{\dagger}|g\rangle$ is: $p_{k,j} = f_{k,j} (1 - f_{k',m})$. The transition in this case takes place from the initial state $c_{k,m}c_{k,j}^{\dagger}|g\rangle$ to the final state $|g\rangle$, leaving out all states that are not involved in the optical transition. Since we are now considering non-interacting electrons, it is not necessary to employ the full artillery of many-body field theory. In the remainder we will therefor switch notation for the matrix elements, and write

$$\left\langle g \left| \hat{\boldsymbol{v}} c_{k',m}^{\dagger} c_{k,j} \right| g \right\rangle = \left\langle k', m \left| \hat{\boldsymbol{v}} \right| k, j \right\rangle$$
(5.44)

where the right hand side refers to single particle states and the current operator is a single particle operator.

Summing over all combinations provides the optical conductivity of non-interacting electrons in a multi-band system:

$$\vec{\sigma}\left(\omega\right) = \frac{2q_e^2}{\Omega} \sum_{\boldsymbol{k},j,m}^{1^*BZ} \lim_{\boldsymbol{k}' \to \boldsymbol{k}} \frac{f_{\boldsymbol{k},j}(1 - f_{\boldsymbol{k}',m}) \langle \boldsymbol{k}, j \, | \, \hat{\boldsymbol{v}} | \, \boldsymbol{k}', m \rangle \langle \boldsymbol{k}', m \, | \, \hat{\boldsymbol{v}} | \, \boldsymbol{k}, j \rangle}{\varepsilon_{\boldsymbol{k}',m} - \varepsilon_{\boldsymbol{k},j}} \frac{i\omega}{\omega \left(\omega + i\delta\right) - \left(\varepsilon_{\boldsymbol{k}',m} - \varepsilon_{\boldsymbol{k},j}\right)^2} \tag{5.45}$$

Each state $c_{k',m}c_{k,j}^{\mathsf{T}}|g\rangle$ is encountered twice in the summation, with opposite sign for $\varepsilon_{k,m} - \varepsilon_{k,j}$ and the same value of $\langle k, j | \hat{\boldsymbol{v}} | k', m \rangle \langle k', m | \hat{\boldsymbol{v}} | k, j \rangle$. Inside the summation we can therefor make the substitution

$$f_{k,j}\left(1 - f_{k',m}\right) \to f_{k,j}\left(1 - f_{k',m}\right)/2 - f_{k',m}\left(1 - f_{k,j}\right)/2 = \left(f_{k,j} - f_{k',m}\right)/2 \tag{5.46}$$

We furthermore define

$$\vec{W}_{j,m}(\boldsymbol{k},\boldsymbol{k}') \equiv \langle \boldsymbol{k}, j | \hat{\boldsymbol{v}} | \boldsymbol{k}', m \rangle \langle \boldsymbol{k}', m | \hat{\boldsymbol{v}} | \boldsymbol{k}, j \rangle \frac{f_{\boldsymbol{k},j} - f_{\boldsymbol{k}',m}}{\varepsilon_{\boldsymbol{k}',m} - \varepsilon_{\boldsymbol{k},j}}$$
(5.47)

so that

$$\vec{\sigma}(\omega) = \frac{q_e^2}{\Omega} \sum_{\boldsymbol{k},j,m}^{1^t BZ} \lim_{\boldsymbol{k}' \to \boldsymbol{k}} \vec{W}_{j,m}(\boldsymbol{k}, \boldsymbol{k}') \frac{i\omega}{\omega(\omega + i\delta) - (\varepsilon_{\boldsymbol{k}',m} - \varepsilon_{\boldsymbol{k},j})^2}$$
(5.48)

5.5 Drude term

Special consideration is needed for the Drude optical conductivity where now the transition takes place within the same band. Taking m = j and the limit $\mathbf{k}' \to \mathbf{k}$ in the expression for he optical conductivity gives:

$$\lim_{\mathbf{k}'\to\mathbf{k}} \vec{W}_{j,j}(\mathbf{k},\mathbf{k}') = \mathbf{v}_{j,j}(\mathbf{k}) \, \mathbf{v}_{j,j}(\mathbf{k}) \left[-\frac{df(\varepsilon)}{d\varepsilon} \right]_{\varepsilon_{\mathbf{k},j}}$$
(5.49)

Note that $\text{Im}\boldsymbol{v}_{j,j} = 0$. The Drude term becomes:

$$\vec{\sigma}_D(\omega) = \frac{iq_e^2 \vec{K}_D}{\omega + i\gamma}$$
(5.50)

where

$$\vec{K}_{D} = \frac{1}{\Omega} \sum_{\boldsymbol{k}}^{1^{t}BZ} \sum_{j} \boldsymbol{v}_{j,j}(\boldsymbol{k}) \boldsymbol{v}_{j,j}(\boldsymbol{k}) \left[-\frac{df(\varepsilon)}{d\varepsilon} \right]_{\varepsilon_{\boldsymbol{k},j}}$$
(5.51)

This expression is essentially a Fermi surface integral of the square of the velocity operator. The Drude current operator describes the current response from the conduction electrons, which is entirely an intraband response.

5.6 Spectral weight sum rules

The optical spectral weight sum rule in its most general incarnation is provided by the following formula:

$$\operatorname{Re}\int_{-\infty}^{\infty} \overleftarrow{\sigma}(\omega) d\omega = \frac{\pi q_e^2}{\Omega} \sum_{\boldsymbol{k},a} \frac{\partial^2 \epsilon_{a,a}(\boldsymbol{k})}{\partial \boldsymbol{k}^2} \left\langle \hat{c}_{k;a}^{\dagger} \hat{c}_{k;a} \right\rangle$$
(5.52)

Examples. Two cases of the spectral weight sumrule, Eq. 5.52, are of particular importance:

f-Sum rule

The free electron dispersion $\epsilon_k = k^2/(2m)$ gives

$$\operatorname{Re}\int_{-\infty}^{\infty} \overleftarrow{\sigma}(\omega) d\omega = \frac{\pi n q_e^2}{m}$$
(5.53)

This is the f-sum rule, or Thomas-Reich-Kuhn rule. It is a cornerstone for optical studies of materials, since it relates the integrated optical conductivity directly to the density of charged objects, and the absolute value of their charge and mass. It reflects the fundamental property that also in strongly correlated matter the number of electrons is conserved.

The f-sum rule, or Thomas Reich Kuhn (TRK) rule, is one of the most powerful tools in optical studies of materials. It relates the integrated optical conductivity directly to the density of



Figure 5.3: Illustration of the *f*-sum rule for the case of aluminum (after E. Shiles, Taizo Sasaki, Mitio Inokuti, and D. Y. Smith, Phys. Ref. B 22, 1612 (1980).

charged objects, and the absolute value of their charge and mass. In Fig. 5.3 the f-sum rule is illustrated by the earlier example of the aluminum: The right hand panel shows the partial integral

$$n_{eff}(\omega) = \frac{2m_e \Omega_u}{\pi q_e^2} \int_0^\omega \operatorname{Re}\sigma(\omega') d\omega'$$
(5.54)

First of all it demonstrates that in the limit $\omega \to \infty$ the number n_{eff} approaches 13, which is exactly the number of electrons (core and valence together) per aluminum atom. Moreover, the function $n_{eff}(\omega)$ rises in a number of steps: The first step from 0 to 2 eV gives approximately 2 electrons, from 2 to 100 eV yields an additional one, from 100 to 1000 eV adds 8 more, and above 1000 eV a final pair of electrons is added. We see, that the number of electrons in a given shell is recovered in the optical transitions from the corresponding shell to the empty states above the Fermi energy, revealing in the present example the configuration $1s^22s^22p^63s^13p^2$ (where the labels 3s and 3p are not to be taken literally in view of the lattice surrounding each Al atom). The plot gives also an impression of the scale over which one has to integrate in order to detect the spectral weight of the valence electrons: The full spectral weight corresponding to the 3 valence electrons is retrieved only at $\hbar\omega \approx 50$ eV.

Kinetic energy sum rule

The nearest-neighbour tight-binding model has a dispersion relation $\epsilon_k = -2t \cos(ka)$, where a is the lattice constant. The implication for the spectral weight is

$$\operatorname{Re}\int_{-\infty}^{\infty} \overleftarrow{\sigma}(\omega) d\omega = \frac{\pi q_e^2 a^2}{\Omega} \sum_k 2t \cos(ka) \langle \hat{c}_k^{\dagger} \hat{c}_k \rangle = -\frac{\pi q_e^2 a^2}{\Omega} \langle \hat{H}^{kin} \rangle$$
(5.55)

This is also known as the "kinetic energy sum rule", since the spectral weight is proportional to the minus the average kinetic energy of the electrons. This sum rule is instrumental in studies of high T_c superconductors (see e.g. *Science* **295**, p 2239 (2002))

5.7 Optical conductivity of dressed band electrons

We return to Eq. 5.19, and rearrange the terms

$$\vec{\sigma}\left(\omega\right) = \frac{q_e^2}{\Omega} \sum_{\alpha} p_\alpha \left\langle \alpha \left| \hat{\boldsymbol{v}} \frac{1}{\hat{H} - E_\alpha} \left[\frac{i}{\omega + i\delta + E_\alpha - \hat{H}} + \frac{i}{\omega + i\delta + \hat{H} - E_\alpha} \right] \hat{\boldsymbol{v}} \right| \alpha \right\rangle \tag{5.56}$$

We substitute Eq. 5.36 for the current operators and obtain for the ground state (T = 0)

$$\vec{\sigma} \left(\omega \right) = \frac{q_e^2}{\Omega} \sum_{\boldsymbol{k}, \boldsymbol{p}; a, b, c, d} \boldsymbol{v}_{a, b}(\boldsymbol{k}) \boldsymbol{v}_{c, d}(\boldsymbol{p}) \left\langle g \left| \hat{c}^{\dagger}_{\boldsymbol{k}; a} \hat{c}_{\boldsymbol{k}; b} \frac{1}{\hat{H} - E_0} \left[\frac{i}{\omega + i\delta + E_0 - \hat{H}} + \frac{i}{\omega + i\delta + \hat{H} - E_0} \right] \hat{c}^{\dagger}_{\boldsymbol{p}; c} \hat{c}_{\boldsymbol{p}; d} \right| g \right\rangle$$

$$(5.57)$$

The left term in square brackets refers to positive ω . Limiting to positive frequencies and $\text{Re}\sigma(\omega)$ for the remainder of this section we obtain

$$\operatorname{Re}\vec{\sigma}\left(\omega^{+}\right) = \frac{q_{e}^{2}}{\Omega} \sum_{\boldsymbol{k},\boldsymbol{p};a,b,c,d} \boldsymbol{v}_{a,b}(\boldsymbol{k}) \boldsymbol{v}_{c,d}(\boldsymbol{p}) \operatorname{Im}\left\langle g \left| \hat{c}_{\boldsymbol{k};a}^{\dagger} \hat{c}_{\boldsymbol{k};b} \frac{1}{\hat{H} - E_{0}} \frac{1}{\omega + E_{0} - \hat{H} - i\delta} \hat{c}_{\boldsymbol{p};c}^{\dagger} \hat{c}_{\boldsymbol{p};d} \right| g \right\rangle$$

$$(5.58)$$

Since the second term in the bracket is δ -function, we can substitute $\hat{H} - E_0$ in the denominator by ω , which in turn can be taken out of the bracket, so that

$$\operatorname{Re}\vec{\sigma}\left(\omega^{+}\right) = \frac{q_{e}^{2}}{\omega\Omega} \sum_{\boldsymbol{k},\boldsymbol{p};a,b,c,d} \boldsymbol{v}_{a,b}(\boldsymbol{k})\boldsymbol{v}_{c,d}(\boldsymbol{p})\operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};a}^{\dagger}\hat{c}_{\boldsymbol{k};b}\hat{G}_{e,h}(\omega)\hat{c}_{\boldsymbol{p};c}^{\dagger}\hat{c}_{\boldsymbol{p};d}\right|g\right\rangle$$
(5.59)

$$\hat{G}_{e,h}(\omega) \equiv \frac{1}{\omega + E_0 - \hat{H} - i\delta}$$
(5.60)

The is an insightfull expression: The operator part within the brackets describes the propagator that transforms an electron hole pair with momentum (p, -p) into an electron-hole par with momentum (k, -k). To proceed one has to make some assumptions about the states created by $\hat{c}^{\dagger}_{k;a}\hat{c}_{k;b}$, about momentum conservation, whether or not the resulting propagator has a (real and imaginary) self energy term, and the important question of the electron-hole pair vertex.

The strategy which we wish to follow is, to factorize the e-h propagator of the expression for the optical conductivity in an a product of an electron and a hole propagator. In fact the factorization that we seek is not possible in general. However, in the absence of electron-hole interactions one can define:

$$\hat{G}_h(\omega) \equiv \frac{1}{E_0 - \hat{H}_- - \omega - i\delta}$$
(5.61)

$$\hat{G}_e(\omega) \equiv \frac{1}{E_0 - \hat{H}_+ + \omega - i\delta}$$
(5.62)

where -(+) refers to the occupied (empty) states. By virtue of the properties of delta-functions the e-h propagator factorizes as

$$\operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};a}^{\dagger}\hat{c}_{\boldsymbol{k};b}\hat{G}_{e,h}(\omega)\hat{c}_{\boldsymbol{p};c}^{\dagger}\hat{c}_{\boldsymbol{p};d}\right|g\right\rangle = \int d\omega' \operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};b}\hat{G}_{e}(\omega+\omega')\hat{c}_{\boldsymbol{p};c}^{\dagger}\right|g\right\rangle \operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};a}^{\dagger}\hat{G}_{h}(\omega')\hat{c}_{\boldsymbol{p};d}\right|g\right\rangle$$

$$(5.63)$$

The two brackets on the rhs are in fact the single-electron and single-hole spectral functions

$$\operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};a}^{\dagger}\hat{G}_{h}(\omega)\hat{c}_{\boldsymbol{p};d}\right|g\right\rangle = \pi A_{h}(\boldsymbol{k};a;\omega)\delta_{\boldsymbol{k},\boldsymbol{p}}\delta_{a,d}$$
(5.64)

$$\operatorname{Im}\left\langle g\left|\hat{c}_{\boldsymbol{k};b}\hat{G}_{e}(\omega)\hat{c}_{\boldsymbol{p};c}^{\dagger}\right|g\right\rangle = \pi A_{e}(\boldsymbol{k},b;\omega)\delta_{\boldsymbol{k},\boldsymbol{p}}\delta_{b,c}$$
(5.65)

where the Kronecker δ -functions at the rhs apply, provided the material satisfies some basic symmetry requires such as translational invariance. The expression for finite temperature is obtained with the same statistical method as in the previous sections. The restriction of the Green's functions to occupied and empty states is in fact taken care of by the Fermi occupation factors, leading thus to the final expression for the optical conductivity *without* vertex corrections between the electron and hole created in the photon absorption process:

$$\frac{\operatorname{Re}\overset{\leftrightarrow}{\sigma}(\omega) = \pi^2 q_e^2 \int d\omega' \frac{1}{\Omega} \sum_{\boldsymbol{k};a,b} \frac{f(\omega') - f(\omega' + \omega)}{\omega} \boldsymbol{v}_{a,b}^*(\boldsymbol{k}) \boldsymbol{v}_{a,b}(\boldsymbol{k}) A(\boldsymbol{k},b;\omega + \omega') A(\boldsymbol{k},a;\omega')}{(5.66)}$$

where

$$A(\mathbf{k}, a; \omega) = A_h(\mathbf{k}, a; \omega) + A_e(\mathbf{k}, a; \omega) = \frac{1}{\pi} \operatorname{Im} \frac{1}{\omega - \epsilon_{\mathbf{k}, a} + \mu - \Sigma(\mathbf{k}, a; \omega) - i\delta}$$
(5.67)

represents the total (electron + hole) spectral function, and $\Sigma(\mathbf{k}, a; \omega)$ is the self energy.

CHAPTER 6

Collective modes

As we discussed in the previous sections, the eigenstates of a system of *non-interacting* fermions are entirely described by the excitations of one or several particles and/or holes. As discussed in section 1.10, the same density of states would enter in the expression for the specific heat, the susceptibility and the compressibility. However, as we saw from the example of liquid ³He (see Fig. 1.9), the susceptibility and the compressibility do *not* appear to correspond to the same value of the density of states and differ also from the one one would get from the single particles excitations. The reason is that all known fermions, (*e.g.* electrons, neutrons, quarks, ³He atoms) *do* interact with each other. In fact we will see in this chapter, that for interacting fermions the properties of the material not only depend on the single particle excitations (*i.e.* the quasiparticles), but also on additional modes. These so-called "collective modes", while absent for the non interacting system, are prominent in interacting fermion systems.

6.1 Excitons

Consider an insulating material. The electronic states of the system are described by a set of bands, some of which are fully occupied, and the other ones empty. When photons interact with the material they can be absorbed, and in this process an electron is excited to a higher lying band leaving behind a hole. In this way we excite electron-hole pairs as described in the chapter on optical conductivity. In Fig. 6.1 we show the optical conductivity of the semiconductor Cu₂O. The value of the bandgap between the occupied oxygen 2p states, and the empty Cu 4s states is 2.17 eV. In the optical spectra this shows up as a weak absorption continuum above 2.17 eV. Since this transition involves the transfer of an electron from the oxygen to a neighboring copper atom this is called a charge transfer excitation. In addition, and in fact much more prominently, there are several sharp peaks in the spectrum below 2.17 eV. However, on the basis of the band structure there is nothing at these energies to which the photons can transfer their energy ! So what are these peaks ? In the discussion at the end of the chapter on optical conductivity we have neglected the fact that the hole and the electron attract each other due to their opposite charge. If we take this into account, we will find that due to this interaction bound states exist with an energy smaller than the band gap of 2.17 eV. These bound states are called excitons. Excitons have the following properties:

(i) The charge of an exciton is zero.

(ii) The spin of an exciton is either S=0 or S=1.

(iii) In view of point (ii) their behaviour in statistical physics is that of bosons.

(iv) Excitons can have finite momentum, which corresponds to the center-of-mass motion of the bound electron-hole pair.

(v) The excitons that one observes in an optical spectrum have zero momentum. Note however,



Figure 6.1: Lefthand panel: single crystal of the semiconductor Cu_2O . Righthand panel (reproduced from Uhlein et al, Phys. Rev. B 23, 2734 (1981)): Optical absorption spectra showing the presence of excitons within the optical band gap of of Cu_2O . The gap value is 2.17 eV.

that the momentum of the individual electron and hole are not zero.

(vi) A frequently made mistake consists of drawing the energy level of an exciton in a diagram of the bands (an example of this practice is given in the left hand panel of Fig. 6.4). However, if one thinks about this for a moment, one discovers that there exists no unambiguous way of doing so. The latter figure indicates the states of electrons, which have a Fermi energy. Since excitons are bosons, they have no Fermi energy, and can not be directly compared with the energies of the electronic bands.

For the present discussion of the optical absorption by excitons we need to work out the optical conductivity using Eq. 5.19, since this expression takes the interactions fully into account. We consider the zero-temperature limit. We can then replace the weighted thermodynamic average over states by a single state $|n\rangle = |\psi_0\rangle$ with the valence band full and the conduction band empty. We furthermore note that $|m\rangle$ is an eigenstate of \hat{H} . We are allowed to make the substitution $\langle m|F(E_m)|m\rangle = \langle m|F(\hat{H})|m\rangle$ for any function F(E). For the expression (5.19) for the optical conductivity this implies

$$\begin{aligned} \vec{\sigma}_{1}(q,\omega) &= q_{e}^{2} \mathrm{Im} \langle \psi_{0} | \hat{\boldsymbol{v}}_{-q}^{(r)} \frac{1}{\hat{H} - E_{0}} \frac{1}{\omega + E_{0} - \hat{H} - i\delta} \hat{\boldsymbol{v}}_{q}^{(r)} | \psi_{0} \rangle \\ &= \frac{q_{e}^{2}}{\Omega} \mathrm{Im} \sum_{k,p} \vec{\Phi}_{c,v}(k,p) \langle \psi_{0} | \hat{c}_{p-q/2,v}^{\dagger} c_{p+q/2,c} \frac{1}{\omega(\omega + E_{0} - \hat{H} - i\delta)} \hat{c}_{k+q/2,c}^{\dagger} \hat{c}_{k-q/2,v} | \psi_{0} \rangle \\ &= \frac{q_{e}^{2}}{\Omega \omega} \mathrm{Im} \sum_{k,p} \vec{\Phi}_{c,v}(k,p) G_{k}^{p}(q,\omega) \\ &\text{where} \quad \vec{\Phi}_{c,v}(k,p) \equiv \langle k, c | \hat{\boldsymbol{v}} | k, v \rangle \langle p, v | \hat{\boldsymbol{v}} | p, c \rangle \left(\theta_{k,c} - \theta_{k,v} \right) (\theta_{p,c} - \theta_{p,v}) \end{aligned}$$
(6.1)

where v refers to the occupied valence band and c to the empty conduction band, and $\theta_{p,v}$ are Heavyside step-functions. The Green's function describes the propagation of an interacting electron-hole pair with center of mass momentum q. If we set the interaction in \hat{H} to zero, than we can just replace $E_0 - \hat{H}$ in the denominator of the above expression by $\epsilon_{k,v} - \epsilon_{k,c}$, and we find back the expression for interband transitions, Eq. 5.56. On the other hand, \hat{H} contains the Coulomb interaction term, which is attractive for an electron-hole pair. The task of calculating $G(\omega)$ then involves the solution of this interacting two-body problem. In cases where the electron and the hole have a free particle-like dispersion, the problem becomes equivalent to that of the electron and the proton in the hydrogen atom. The main differences are, that the masses describing center-of-mass and relative motion of the electron-hole pair are $M = m_e + m_h$ and $\mu = (1/m_e + 1/m_h)^{-1}$ respectively, where m_e and m_h are the effective mass of the electron and the hole. Furthermore the Coulomb interaction is screened by the bound charge in the crystal. This last aspect can be taken into account by introducing a screened charge $e/\sqrt{\epsilon}$ where ϵ is the dielectric permeability. The solutions of this problem are the same as those of a hydrogen atom, but with scaled parameters:

(i) the continuum states of unbound electron-hole pairs with center of mass momentum q and relative momentum κ with corresponding energies

$$E(q, \kappa) = E_{gap} + q^2/(2M) + \kappa^2/(2\mu)$$
(6.2)

The states with q = 0 give rise to the optical absorption about 2.17 eV in Cu₂O (Fig. 6.1).

(ii) an effective Rydberg series of bound states with energies

$$E_n = E_{gap} + q^2 / (2M) - Ry^{eff} / n^2$$
(6.3)

where $Ry^{eff} = \mu e^4/(2\epsilon^2)$ is the effective Rydberg. In the optical spectrum this shows up as a series of peaks for $\omega = E_n$. The sharp peaks in Cu₂O (Fig. 6.1) are a striking example. Note that the binding energy of the most strongly bound state (labeled 1*S*) is only 0.14 eV, which is about 100 times smaller than the binding energy of an electron in the ground state of a hydrogen atom.

The optical spectrum of CuGeO₃ is another beautiful example, partly -but not exclusivelybecause of the material's color (see Fig. 6.2). In this compound a prominent onset is seen in the optical conductivity around 3.1 eV. This onset is due to the transfer of an electron from the occupied band related to the O-ions to the unoccupied band which has mostly Cu-3d character. Another important feature in Fig. 6.2 is the absorption peak at $\omega = 1.8$ eV, which is due to a strongly bound exciton, with binding energy $E_b = 3.1 - 1.8 = 1.3$ eV. For reasons having to do with nature of the bands, the electron-hole interaction is in this case essentially a Hubbard-type on-site interaction between an electron and a hole occupying the same unit-cell; interactions at further distances can be neglected. As we will see below, such a local interaction gives rise to at most one excitonic bound state for any value of the center-of-mass momentum q.

We illustrate this with a model. Instead of a regular Coulomb interaction, we assume that the electrons in the conduction and valence band interact through an on-site local repulsion. In coordinate space, we write this as $\hat{H}^{(i)} = U \sum_{j} \hat{c}_{c}^{\dagger}(r_{j}) \hat{c}_{v}(r_{j}) \hat{c}_{c}(r_{j})$. The Hamiltonian describing the subspace of the two bands (conduction and valence) is

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(i)} = \sum_{k} \left\{ \epsilon_{k,v} \hat{c}^{\dagger}_{k,v} \hat{c}_{k,v} + \epsilon_{k,c} \hat{c}^{\dagger}_{k,c} \hat{c}_{k,c} \right\} + U \sum_{k,p,q} \hat{c}^{\dagger}_{p-q/2,c} \hat{c}^{\dagger}_{k+q/2,v} \hat{c}_{k-q/2,v} \hat{c}_{p+q/2,c}$$

$$\tag{6.4}$$

We furthermore define the green's functions q and G, respectively without and with interaction:

$$g_{k}^{p}(\boldsymbol{q},\omega) = \delta_{k,p} \langle \psi_{0} | \hat{c}_{p-q/2,v}^{\dagger} \hat{c}_{p+q/2,c} \frac{1}{\omega + E_{0} - \hat{H}^{(0)} - i\delta} \hat{c}_{k+q/2,c}^{\dagger} \hat{c}_{k-q/2,v} | \psi_{0} \rangle = = \frac{\delta_{k,p}}{\omega + \epsilon_{k-q/2,v} - \epsilon_{k+q/2,c} - i\delta}$$

$$G_{k}^{p}(\boldsymbol{q},\omega) = \langle \psi_{0} | \hat{c}_{p-q/2,v}^{\dagger} \hat{c}_{p+q/2,c} \frac{1}{\omega + E_{0} - \hat{H}^{(0)} - \hat{H}^{(i)} - i\delta} \hat{c}_{k+q/2,c}^{\dagger} \hat{c}_{k-q/2,v} | \psi_{0} \rangle$$
(6.5)

The first Green's function (without the e-h interaction) has the property that it is diagonal in



Figure 6.2: Lefthand panel: single crystals of CuGeO₃. Righthand panel: Optical absorption in CuGeO₃ for polarizations of the electric field along two different crystallographic axis (reproduced from Bassi et al., Phys. Rev. B 54, R11030 (1996)). The absorption edge at 3.1 eV corresponds to the onset of optical transitions across the band gap. The peak at 1.8 eV is due to absorption by an exciton. This material owes its beautiful color to the exciton absorption.

k,p, i.e. $g_k^p({\bm q},\omega)=g_k^k({\bm q},\omega)\delta_{k,p}.$ The Dyson equation reads therefore

$$G_k^p(\boldsymbol{q},\omega) = g_k^k(\boldsymbol{q},\omega)\delta_{k,p} - g_k^k(\omega)UG^p(\boldsymbol{q},\omega)$$
(6.6)

where the notation G^p with only one index implies that the sum has been taken over the other index: $G^p(\boldsymbol{q},\omega) \equiv \sum_k G^p_k(\boldsymbol{q},\omega)$. On the right-hand side we have such a term. If we sum the entire expression over k, we obtain a selfconsistent relation for G^p :

$$G^{p}(\boldsymbol{q},\omega) = g_{p}^{p}(\boldsymbol{q},\omega) - g(\boldsymbol{q},\omega)UG^{p}(\boldsymbol{q},\omega)$$
$$g(\boldsymbol{q},\omega) \equiv \sum_{k,p} g_{k}^{p}(\boldsymbol{q},\omega) = \sum_{k} g_{k}^{k}(\boldsymbol{q},\omega)$$
(6.7)

from which G^p is easily solved

$$G^{p}(\boldsymbol{q},\omega) = \frac{g_{p}^{p}(\boldsymbol{q},\omega)}{1 + Ug(\boldsymbol{q},\omega)}$$
(6.8)

We reinsert this in (6.6) and obtain

$$G_{k}^{p}(\boldsymbol{q},\omega) = g_{k}^{p}(\boldsymbol{q},\omega) - \frac{U}{1 + Ug(\boldsymbol{q},\omega)}g_{k}^{k}(\boldsymbol{q},\omega)g_{p}^{p}(\boldsymbol{q},\omega)$$

$$\vec{\sigma}_{1}(\boldsymbol{q},\omega) = \frac{q_{e}^{2}}{\Omega\omega}\operatorname{Im}\left[\sum_{k}\overset{\leftrightarrow}{\Phi}_{c,v}(k,k)g_{k}^{k}(\boldsymbol{q},\omega) - \frac{U}{1 + Ug(\boldsymbol{q},\omega)}\sum_{k,p}\overset{\leftrightarrow}{\Phi}_{c,v}(k,p)g_{k}^{k}(\boldsymbol{q},\omega)g_{p}^{p}(\boldsymbol{q},\omega)\right]$$
(6.9)

where the second equation is obtained by substituting the Green's function expression in the one for the optical conductivity, Eq.6.1. As in the previous section, since for the optical spectrum the wavelength is much longer than a lattice spacing, we can we work in the approximation q = 0. The first term in the optical conductivity is exactly the same result as we already found without interactions. It therefore corresponds to the transitions toward states of unbound electron-hole pairs across the gap. The second term is absent for U = 0, and describes the bound-state part of the spectrum. An exitonic bound state corresponds to a zero of the denominator of Eq. 6.9. This occurs when $1 + Ug(\mathbf{q}, \omega) = 0$ for frequencies below the gap, i.e. for frequencies where $\mathrm{Im}g(\mathbf{q}, \omega) = 0$. The dispersion for the relative motion of the electron and the hole, Eq. 6.2, is



Figure 6.3: Calculation of the optical spectrum of a semiconductor without (orange curves) and with (dark blue curve in the top panel) interaction using equation 6.10. Bottom panel: the crossing $W/U = -g(\omega)$ corresponds to the pole in the denominator of this expression, and represents the frequency ω where the exciton shows up in $\sigma_1(\omega)$.

free-particle like. The corresponding density of states in 3 dimensions is therefor proportional to $\sqrt{\omega - E_g(q)}$, where $E_g(q) = E_g + q^2/(2M)$. Contrary to free electrons, a band in a crystal lattice with lattice parameter a has a finite band width. This is also true for the relative motion of an electron-hole pair. We will indicate this width with the symbol W, and keep in mind that W is roughly proportional to the inverse mass, $W \sim a^{-2}/(2\mu)$. The free electron behaviour still exists for small energy compared to W, *i.e.* for $|\omega - E_g(q)| \ll W$. These features are captured by the "semi-spherical" model-Green's function¹

$$g(q,\omega) = \frac{\omega - E_g(q) - W}{W^2} \left[1 - \sqrt{1 - \frac{W^2}{(\omega - E_g(q) - W)^2}} \right]$$
(6.10)

This analytically closed expression is purely real for energies outside the band $(|\omega - E_g(q)| \ge W)$, and it has both a real and imaginary part for $|\omega - E_g(q)| < W$. The imaginary part is the density of states (DOS) of the relative motion of the electron-hole pair. The DOS has the desired properties that close to the two band-edges it is the square-root of relative energy, and (ii) the integrated DOS is normalized. Comparing with the second member of Eq. 6.9 we solve the expression $1 + Ug(\mathbf{q}, \omega) = 0$ straightforwardly and obtain a critical value for U for the formation of an exciton $(U_c = W)$, as well as the photon energy for which absorption by the exciton occurs

no exciton
$$(U < W)$$

 $\omega = E_g + q^2/(2M) - \frac{(U - W)^2}{2U} \quad (U > W)$
(6.11)

¹This model does not have a simple one-to-one correspondence to an $\epsilon(k)$ dispersion relation in 3 dimensions. It nonetheless captures many of the essential features of a band-structure in 3D, and is often used for illustrating physical principles.

The exciton will show up in the optical spectrum as a sharp line in the optical spectrum below the gap edge. The numerical example shown in Fig. 6.3 is indeed quite similar to the spectrum of CuGeO₃ shown in Fig. 6.2. Note that, while the photon absorption occurs for $qa \ll 1$ where *a* is the lattice constant, the exciton itself has a center-of-mass dispersion given by the second term on the righthand side of the expression.



Figure 6.4: Left: incorrect way to plot the energy of an exciton. Middle panel: Sketch of the single electron dispersion curves of a direct gap insulator. Righthand panel: Electron-hole excitation continuum corresponding to the bandstructure of the middle panel (shaded) and sketch over several "flavours" of excitons in the gap. The red and blue blobs in the middle panel indicate roughly the envelope of momentum-values involved in creating an exciton-bound state with finite momentum of the collective center-of-mass coordinate.

Quite frequently excitons are plotted in the band structure, in the way shown in the left-hand panel of Fig. 6.4. The difficulty is, that excitons are neutral excitatons, they are bosonic, carry spin S = 0 or S = 1. Since the band-structure graph shows the energies and momenta of single-electron states, there is no unambiguous way to draw an exciton in such a diagram, and if one thinks a bit longer about the problem one realizes that by doing so one misses some important aspects of the excitonic states related to the many-body nature of these excitations having far-reaching consequences.

This brings us back to the question as to how to relate the excitons to a plot of the electron energy dispersion. One has to start by making a plot of the *combined* energies of electronhole pairs, as a function of their center-of-mass momentum. Hence electron-hole energy = $\epsilon_c(k+q/2) - \epsilon_v(k-q/2)$, and center-of-mass momentum = q. An example of what this looks like is indicated by the shaded area in Fig. 6.4. The middle and righthand graphs illustrate how, as a first step, one associates electron-hole continua with a given momentum-transfer (note that only one dimension of momentum space is shown, the additional dimensions extend the number of electron-hole states for a given value of their collective momentum q shown in the right-hand panel). The electron-hole attractive Coulomb interaction can pull one or several excitonic bound states out of the continuum for any given value of q. In this example the minimum of energy is indicated for q = 0. This happens when the insulator has a "direct" gap². For each given value of q the lower edge of the continuum is given by $E_g(q)$, and the shaded area is obtained by sweeping the relative momentum κ from 0 to ∞ in $E_g(q) + \kappa^2/(2\mu)$. The exciton, described by Eq. 6.11, lies below the gap, and outside the continuum. The fact that the exciton is situated outside the continuum implies, that cinematically it is impossible³

²Note that if the gap is indirect, the minimum of electron-hole energy will occur at non-zero value of the center-of-mass momentum q.

³For large enough q the exciton has an energy higher than the absolute minimum of the shaded area. Decay into electron-hole pair is possible for such high energy excitons, but the momentum change needs to dumped in

for it to decay by splitting into an electron-hole pair. Therefore these bound states are stable, and the one for for $q \approx 0$ shows up as a sharp resonance in the optical spectrum.

Excitons are one out of various different types of "collective modes" of an interacting electron system. These modes have no equivalent in terms of single particle excitations. Often, but not always, collective modes are bosons. In the case of the excitons this implies, that it is possible to do experiments with them in similar ways as with ⁴He or cold atoms. Among other things, it is possible to generate sufficiently high densities of excitons, to create a Bose-Einstein condensate of them. Other properties are the transfer of energy over certain distances, for example in photo-voltaic devices. One can imagine that by appropriate manipulation it is possible to generate an electron-hole pair at some particular space coordinate in the device, and then allow it to make an internal conversion to a "dark" exciton with spin S = 1. The high spin prohibits recombination under photon-emission, so now it is possible to store this energy in the form of the exciton as long as one likes, or transport it elsewhere by moving the exciton around using appropriate gap-engineering tricks. After a while, when the energy needs to be released, one can feed it into a region where the electron and hole separate and produce a photo-current.

6.2 General definition of the susceptibility

As discussed in Section 4.1, we would like to compute the response of the full interacting Hamiltonian to an external perturbation, for example coupling to the charge or spin density. One can of course use the general linear response formula (4.39) to obtain the charge and spin susceptibilities. Let us take for example a perturbation potential $\phi^{ext}(\mathbf{r},t)$ coupling to the charge density $\rho(\mathbf{r})$:

$$\hat{H}^{p} = \int d\boldsymbol{r} \phi^{ext}(\boldsymbol{r}, t) \hat{\rho}(\boldsymbol{r})$$
(6.12)

where $\hat{\rho}(\mathbf{r})$ is the density operator. The charge susceptibility $\chi_{\rho\rho}$ is defined by the relation

$$\rho^{ind}(\mathbf{r},t) = \int d\mathbf{r}_1 dt_1 \chi_{\rho\rho}(\mathbf{r} - \mathbf{r}_1, t - t_1) \phi^{ext}(\mathbf{r}_1, t_1)$$
(6.13)

between the charge fluctuation $\rho^{ind}(\mathbf{r},t)$ at time t induced by the external field $\phi^{ext}(\mathbf{r}_1,t_1)$ at an earlier time t_1 . In frequency-momentum representation the integral relation simplifies to a simple product

$$\rho^{ind}(\boldsymbol{q},\omega) = \chi_{\rho\rho}(\boldsymbol{q},\omega)\phi^{ext}(\boldsymbol{q},\omega)$$
(6.14)

One can use the standard linear response formula to relate the charge susceptibility to the charge-charge correlation function

$$\chi_{\rho\rho}(\boldsymbol{r},t) = -i\,\theta(t)\langle [\hat{\rho}(\boldsymbol{r},t),\hat{\rho}(0,0)]\rangle \tag{6.15}$$

This expression is exact, but we should keep in mind that, when \hat{H} is a fully interacting Hamiltonian, no general recipe is known to compute the susceptibility (6.15). However, if the influence of interactions is small, we can obtain an approximate expression of (6.13) which we will explore now.

The charge susceptibility is obtained by substituting $\hat{x} = \hat{u} = \hat{\rho}_q = \sum_{k,\sigma} c^{\dagger}_{k+q,\sigma} c_{k,\sigma}$ in the general response expression, Eq. 4.40,

$$\boldsymbol{\chi}_{\rho\rho}(q,\omega) = \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \frac{\langle n | \hat{\rho}_q^{\dagger} | m \rangle \langle m | \hat{\rho}_q | n \rangle}{\hbar\omega + E_n - E_m + i\delta}$$
(6.16)

the crystal, for example by impurity scattering.



Figure 6.5:

The first step of the approximation consists of working out this expression for an ensemble of non-interacting fermions using the standard method of quantum statistical physics. We leave this as an exercise for the reader, and directly state the result, which is the so-called *bare* susceptibility

$$\chi_0(\boldsymbol{q},\omega) = \frac{1}{\Omega} \sum_{\boldsymbol{k},\sigma} \frac{f_k - f_{k+q}}{\hbar\omega + \xi_k - \xi_{k+q} + i\delta}$$
(6.17)

where $f_k = f(\xi_k)$ is the Fermi-Dirac distribution.

6.3 Mean field approximation

In the presence of an external perturbation the operator representing the density (or any other observable) will acquire a certain average value $\rho(\mathbf{r}, t)$. The interaction term gives thus rise to an effective potential corresponding to the average action at point \mathbf{r}_1 of the other sites \mathbf{r}_2 mediated by the interaction (see Fig. Fig. 6.5). The idea is to find an approximate expression for the interaction part of the Hamiltonian

$$\hat{H}^{\text{int}} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \hat{\rho}(\mathbf{r}_1) \hat{\rho}(\mathbf{r}_2)$$
(6.18)

We now split the density term in a scalar and an operator part

$$\hat{\rho}(\mathbf{r}) = \rho(\mathbf{r}, t) + \delta \hat{\rho}(\mathbf{r}) \tag{6.19}$$

where the operator

$$\delta\hat{\rho}(\boldsymbol{r}) = \hat{\rho}(\boldsymbol{r}) - \rho(\boldsymbol{r}, t) \tag{6.20}$$

describes the quantum fluctuations around the average

$$\rho(\mathbf{r},t) = \langle \psi(t) | \hat{\rho}(\mathbf{r}) | | \psi(t) \rangle \tag{6.21}$$

Note that, although the operator itself does not depend on time, its average in the presence of a time dependent external perturbation does depend on time. The interaction will contain terms coming from the average value, from the quantum fluctuations, and cross-terms between these two. Using (a + b)(c + d) = (a + b)c + a(c + d) - ac + bd we can rewrite the operator product in Eq. 6.18, so that

$$\hat{H}^{\text{int}} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \left\{ \hat{\rho}(\mathbf{r}_1) \rho(\mathbf{r}_2, t) + \rho(\mathbf{r}_1, t) \hat{\rho}(\mathbf{r}_2) - \rho(\mathbf{r}_1, t) \rho(\mathbf{r}_2, t) + \delta \hat{\rho}(\mathbf{r}_1) \delta \hat{\rho}(\mathbf{r}_2) \right\}$$
(6.22)

The mean field approximation consists in assuming that the quantum fluctuations around the average value are small, or fast, or uncorrelated enough so that one can neglect the last term on the right, since it is of second order in the quantum fluctuations. The third term in the above equation is a simple constant in the energy. Although it is important if one wants to compute the energy of the ground state or some similar quantity it simply disappears when one wants to compute averages of any operators. One can thus forget about this term. The first and second term give identical contributions, and they contribute to zero'th and first order in the fluctuations. Keeping them is essential since otherwise the interaction Hamiltonian would just become a constant in the energy and would not affect the average of the operators. We thus see that in the mean field approximation the real interaction between the electrons is replaced by

$$\hat{H}^{\rm MF} = \int d\boldsymbol{r} \hat{\rho}(\boldsymbol{r}) \int d\boldsymbol{r}_2 V(\boldsymbol{r} - \boldsymbol{r}_2) \rho(\boldsymbol{r}_2, t)$$
(6.23)

For the purpose of the linear response to an external field $\phi^{ext}(\mathbf{r},t)$ we can concentrate on the density in Eq. 6.23 which is induced by the external potential, *i.e.* we can leave out the density before the external perturbation was switched on, $\rho(\mathbf{r}_2, -\infty)$ and retain only $\rho^{ind}(\mathbf{r}_2, t) = \rho(\mathbf{r}_2, t) - \rho(\mathbf{r}_2, -\infty)$. The result is a *single body* Hamiltonian of electrons subjected to the potential

$$\phi^{ind}(\boldsymbol{r},t) = \int d\boldsymbol{r}_2 V(\boldsymbol{r}-\boldsymbol{r}_2,t)\rho^{ind}(\boldsymbol{r}_2,t)$$
(6.24)

Note that we aren't ready yet, since we still need to determine $\rho^{ind}(\mathbf{r}_2, t)$. However we have now replaced the full interacting Hamiltonian by a Hamiltonian of electrons subjected to an induced potential $\phi^{ind}(\mathbf{r}, t)$. Moreover this potential is small if the external perturbation $\phi^{ext}(\mathbf{r}, t)$ is also small. The full Hamiltonian in presence of the perturbation is thus

$$\hat{H} = \hat{H}^0 + \int d\boldsymbol{r} \hat{\rho}(\boldsymbol{r}) [\phi^{ext}(\boldsymbol{r}, t) + \phi^{ind}(\boldsymbol{r}, t)]$$
(6.25)

We thus see that the mean field approximation replaces the problem of *interacting* electrons subjected to an *external* perturbation ϕ^{ext} by a problem of *non-interacting* electrons subjected to an *effective* perturbation $\phi^{ext} + \phi^{ind}$. The field ϕ^{ind} is the induced perturbation and comes from the fact that due to the interactions between particles there will be an induced field that will try to modify the deviations in the density that would otherwise be created by the external field.

6.4 Charge response in the random phase approximation

The mean field approximation is very useful: In many situations it will capture the main effects of the feedback due to the interactions. For the Hamiltonian (6.25) we can easily compute the density fluctuation using linear response

$$\rho^{ind}(\mathbf{r},t) = \int d\mathbf{r}_2 dt_2 \chi_0(\mathbf{r} - \mathbf{r}_2, t - t_2) [\phi^{ext}(\mathbf{r}_2, t_2) + \phi^{ind}(\mathbf{r}_2, t_2)]$$
(6.26)

Since $\phi^{ind}(\mathbf{r},t)$ depends on $\rho^{ind}(\mathbf{r},t)$ we have a self consistent integral equation that will allow to determine the average value. The most convenient approach is to analyze the linear response for a given wavevector q and frequency ω

$$\rho^{ind}(\boldsymbol{q},\omega) = \chi_0(\boldsymbol{q},\omega)[\phi^{ext}(\boldsymbol{q},\omega) + \phi^{ind}(\boldsymbol{q},\omega)]$$
(6.27)

Using (6.24) one gets

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$$\phi^{ind}(\boldsymbol{q},\omega) = V(\boldsymbol{q})\rho^{ind}(\boldsymbol{q},\omega) \tag{6.28}$$

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We solve the set Eqs. 6.27 and 6.28 by eliminating $\phi^{ind}(\mathbf{q},\omega)$, and obtain the linear relationship between the induced charge response and the external field

$$\rho^{ind}(\boldsymbol{q},\omega) = \frac{\chi_0(\boldsymbol{q},\omega)\phi^{ext}(\boldsymbol{q},\omega)}{1 - V(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)}$$
(6.29)

Comparing Eq. 6.29 with Eq. 6.14 one obtains the mean field prediction for the charge susceptibility of the interacting electron system

$$\chi_{\rho\rho}^{RPA}(\boldsymbol{q},\omega) = \frac{\chi_0(\boldsymbol{q},\omega)}{1 - V(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)}$$
(6.30)

The index "RPA" for "Random Phase Approximation". Bohm and Pines called it this way because (quoting from Bohm and Pines, Phys. Rev. 82, 625, (1951)) one has to "distinguish between two kinds of response of the electrons to a wave. One of these is in phase with the wave, so that the phase difference between the particle response and the wave producing it is independent of the position of the particle. This is the response which contributes to the organized behavior of the system. The other response has a phase difference with the wave producing it which depends on the position of the particle. Because of the general random location of the particles, this second response tends to average out to zero when we consider a large number of electrons, and we shall neglect the contributions arising from this. This procedure we call the random phase approximation." The Random Phase result is quite remarkable since now the charge susceptibility is expressed in terms of known quantities namely the Fourier transform of the interaction potential $V(\mathbf{q})$ and the *independent* electrons susceptibility $\chi_0(\mathbf{q},\omega)$. This formula will thus allow us to explore in details the consequences of the interactions between particles on the various susceptibilities.

6.5 Dielectric function

Assume that an external charge density $\rho^{ext}(\mathbf{r},t) = \rho^{ext}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$ is added to the system. As a result of the Coulomb interaction $V(\mathbf{q}) = 4\pi q_e^2/|\mathbf{q}|^2$ the external charge generates the potential $\phi^{ext}(\mathbf{q},\omega) = V(\mathbf{q})\rho^{ext}(\mathbf{q},\omega)$. The displacement field is defined as the corresponding electric field: $q_e \mathbf{D} = -\nabla \phi^{ext}$, so that $q_e \mathbf{D} = -i\mathbf{q}\phi^{ext}$. This external potential induces a density response $\rho^{ind}(\mathbf{q},\omega)$ in the system, which in turn also generates a potential $\phi^{ind}(\mathbf{q},\omega) = V(\mathbf{q})\rho^{ind}(\mathbf{q},\omega)$. The total electric field in the solid is given by the gradient of the potential emanating from all (external and induced) charge: $q_e \mathbf{E} = -\nabla \phi^{ext} - \nabla \phi^{ind} = -i\mathbf{q}\phi^{ext} - i\mathbf{q}\phi^{ind}$. The dielectric function for wavevector \mathbf{q} and frequency ω is defined as the material dependent constant of proportionality between displacement field \mathbf{D} and electric field \mathbf{E}

$$\boldsymbol{D}(\boldsymbol{q},\omega) = \epsilon(\boldsymbol{q},\omega)\boldsymbol{E}(\boldsymbol{q},\omega) \tag{6.31}$$

which, with the help of the fields and densities introduced above we write as

$$\epsilon(\boldsymbol{q},\omega) = \frac{1}{1 + \rho^{ind}(\boldsymbol{q},\omega)/\rho^{ext}(\boldsymbol{q},\omega)} = \frac{1}{1 + \phi^{ind}(\boldsymbol{q},\omega)/\phi^{ext}(\boldsymbol{q},\omega)}$$
(6.32)

In Eq. 6.14 we introduced the definition of the charge susceptibility:

$$\chi_{\rho\rho}(\boldsymbol{q},\omega) = \frac{\rho^{ind}(\boldsymbol{q},\omega)}{\phi^{ext}(\boldsymbol{q},\omega)}$$
(6.33)

We multiply left and right of this expression with the Coulomb interaction $V(\mathbf{q})$ and substitute $V(\mathbf{q})\rho^{ind} = \phi^{ind}$

$$V(\boldsymbol{q})\chi_{\rho\rho}(\boldsymbol{q},\omega) = \frac{V(\boldsymbol{q})\rho^{ind}(\boldsymbol{q},\omega)}{\phi^{ext}(\boldsymbol{q},\omega)} = \frac{\phi^{ind}(\boldsymbol{q},\omega)}{\phi^{ext}(\boldsymbol{q},\omega)}$$
(6.34)

If we now compare Eqs. 6.32 with the righthand member of Eq. 6.34, we see that the dielectric function and the charge susceptibility satisfy the general relation

$$\epsilon(\boldsymbol{q},\omega) = \frac{1}{1 + V(\boldsymbol{q})\chi_{\rho\rho}(\boldsymbol{q},\omega)}$$
(6.35)

Substituting the mean-field approximation for the charge susceptibility, Eq. 6.30, in the general expression for the dielectric function, Eq. 6.35, we obtain the dielectric function in the Random Phase Approximation

$$\epsilon^{RPA}(\boldsymbol{q},\omega) = 1 - V(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega) \tag{6.36}$$

6.6 Static Fields: Screening of the Coulomb interaction

Consider now an external charge perturbation consisting of a single electron at the origin. The corresponding density distribution is of the form

$$\rho^{ext}(\mathbf{r}) = \delta(\mathbf{r}) \tag{6.37}$$

The Fourier transform of this density distribution is

$$\rho^{ext}(\boldsymbol{q}) = 1 \tag{6.38}$$

Each q-component acts as an external source, and the corresponding total induced density at wavevector q is, with the help of Eq. 6.32

$$\rho(\boldsymbol{q}) = \rho^{ind}(\boldsymbol{q}) + \rho^{ext}(\boldsymbol{q}) = \frac{1}{\epsilon(\boldsymbol{q})}$$
(6.39)

The screened potential follows from the Poisson equation $\Delta \phi(\mathbf{r}) = -q_e^2 \rho(\mathbf{r})$. The Fourier transform of this expression is $\phi(\mathbf{q}) = 4\pi q_e^2 \rho(\mathbf{q}) |\mathbf{q}|^{-2}$. With the help of this, and inserting Eq. 6.36, we obtain in the Random Phase Approximation

$$\phi^{RPA}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \frac{4\pi q_e^2}{|\mathbf{q}|^2 - |\mathbf{q}|^2 V(\mathbf{q}) \chi_0(\mathbf{q})} e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{q}$$
(6.40)

In vacuum the correction in the denominator disappears, and one obtains the standard Coulomb potential corresponding to a point-charge in the origin

$$\phi(\mathbf{r}) = \frac{q_e^2}{|\mathbf{r}|} \tag{6.41}$$

In a metal we can use Eq. 6.17 in the limit $\omega \to 0$. For the mathematical procedure we refer to the book of G.D. Mahan, "Many-Particle Physics", Plenum, 1980, and later editions, and just state the result here:

$$\chi_0(\mathbf{q},0) \simeq -\frac{mk_F}{\hbar^2 \pi^2} \left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{1 + q/(2k_F)}{1 - q/(2k_F)} \right| \right]$$
(6.42)

In the long wavelength limit $(q/2k_F \ll 1)$ the second term in the square brackets tends to 1/2and the bare susceptibility becomes the constant

$$\lim_{q \to 0} \chi_0(\mathbf{q}, 0) = -\frac{mk_F}{\hbar^2 \pi^2} \tag{6.43}$$

We will start by considering the most frequently used approximation, the so-called Thomas-Fermi model, where one assumes that the long wavelength result applies to all values of q. Substituting this in Eq. 6.40, together with the bare Coulomb interaction $V(\mathbf{q}) = 4\pi q_e^2 |\mathbf{q}|^{-2}$ we get

$$\phi^{TF}(\mathbf{r}) = \frac{q_e^2}{2\pi^2} \int \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{|\mathbf{q}|^2 + k_0^2} d^3\mathbf{q}$$
(6.44)

with the Thomas-Fermi wavector k_0 defined as

$$k_0^2 \equiv \frac{4q_e^2 m k_{\rm F}}{\pi \hbar^2} = \frac{4}{a_0} \left(\frac{3n}{\pi}\right)^{1/3} \tag{6.45}$$

The rightmost relation for k_0 is obtained by inserting the expression for the electron density in 3D, $n = k_F^3/(3\pi^2)$ and the definition of the Bohr radius, $a_0 = \hbar^2/mq_e^2$. The Thomas-Fermi screening length $1/k_0$, represents the natural scale in a metal across which static electric fields are screened. The rotational symmetry of the integrand immediately suggests to use the spherical coordinates. One gets

$$\phi^{TF}(\mathbf{r}) = \frac{q_e^2}{\pi} \int_0^\infty dq \ q^2 \int_{-\pi}^{+\pi} d\theta \sin\theta \frac{1}{q^2 + k_0^2} e^{iqr\cos\theta} = \frac{q_e^2}{i\pi r} \int_0^\infty dq \ q \frac{1}{q^2 + k_0^2} \left[e^{iqr} - e^{-iqr} \right] = \frac{q_e^2}{i\pi r} \int_{-\infty}^\infty dq \ q \frac{1}{q^2 + k_0^2} e^{iqr}$$
(6.46)

There are various ways to finish the calculation, using conventional integration techniques. Let us illustrate however on this simple example the use of integration in the complex plane. Since ris positive, we can replace the integral by an integral over the closed contour of Fig. 6.6 without changing the value of the integral. One has thus

$$\phi^{TF}(\mathbf{r}) = \frac{q_e^2}{i\pi r} \oint_C dz \frac{z}{z^2 + k_0^2 r^2} e^{iz}$$
(6.47)

One can rewrite the fraction as

$$\frac{z}{z^2 + k_0^2 r^2} e^{iz} = \frac{1}{2} \left[\frac{e^{iz}}{z + ik_0 r} + \frac{e^{iz}}{z - ik_0 r} \right]$$
(6.48)

which shows directly the two poles $z = \pm i k_0 r$. Only the upper pole is inside the contour. Using the residue theorem one gets

$$\phi^{TF}(\mathbf{r}) = \frac{q_e^2}{i\pi r} \frac{1}{2} \left[2i\pi e^{-k_0 r} + 0 \right]$$

After cleaning up the expression, we obtain the potential

$$\phi^{TF}(\boldsymbol{r}) = \frac{q_e^2}{r} e^{-k_0 r}$$
(6.49)

known as the Yukawa potential. One sees that the Coulomb potential in a solid is not long range anymore, but decays extremely rapidly beyond the length $1/k_0$, called the screening length. This drastic change of behavior comes from the fact that electrons being mobile can come and surround the external charge q_e . As long as this charge produces a visible potential it will attract or repel the electrons, until their cloud of charge exactly compensates the external charge. We thus have the paradoxical result that in a solid the Coulomb interaction is short range, and of range $1/k_0$. This means that two charges that are beyond the length $1/k_0$ will



Figure 6.6: Contour for computing the integral. The circle of infinite radius gives a zero contribution to the integral since the integrand decays fast enough with the radius. The integral over the contour is thus equal to the integral on the real axis. Only the poles inside the contour contribute to the residue theorem.

essentially not see each other. As can be expected $1/k_0^2$ is proportional to the density of states at the Fermi level: one needs to have electrons that can be excited to be able to screen.

Eq. 6.45 expresses that the Thomas-Fermi screening length, k_0^{-1} , is proportional to the squareroot of the average distance between the electrons ($\sim n^{-1/3}$). These two length scales are equal when the density is

$$n_0 = \frac{192}{\pi a_0^3} = 4.3 \cdot 10^{26} cm^{-3} \tag{6.50}$$

For densities higher than n_0 the Thomas-Fermi screening length is longer than the distance between the electrons. In this limit the screening is well described by the Yukawa form, Eq. 6.49.

In the opposite case where $n < n_0$ we need to consider that on length scales shorter than the distance between the electrons, it becomes important to take into account the q dependence of Eq. 6.42. The mathematics is a bit cumbersome and will not be treated here. The bottom line is that the static screening of a Fermi liquid oscillates with a period given by the Fermi wavelength ! This phenomenon, discovered by Jacques Friedel, is known as "Friedel oscillations" of the charge screening. We take aluminum as an example. With 3 conduction electrons per atom this metal has the highest free electron density of common metals; yet the free electron density $n = 2.1 \cdot 10^{23}$ cm⁻³ is well below n_0 . Consequently Friedel oscillations are expected to impact the short range screening of common metals. Nevertheless the Thomas-Fermi model remains a good approximation at long distances, and this model is commonly used to describe metallic screening in Fermi liquids.

6.7 Normal sound

Sound waves are propagating fluctuations of density $n(\mathbf{r}, t)$, and pressure $p(\mathbf{r}, t)$ around their equilibrium values n and p. The pressure gradient at the space coordinate \mathbf{r} constitutes a force

acting on the liquid present at the same coordinate. By virtue of Newtons equation this has the effect to accelerate the local current $j(\mathbf{r}, t)$:

$$-\nabla p(\boldsymbol{r},t) = m\partial_t \boldsymbol{j}(\boldsymbol{r},t) \tag{6.51}$$

The definition of the compressibility κ in a compressible liquid, Eq. 1.22, provides the following relation between density and pressure gradients:

$$\nabla p(\mathbf{r}, t) = \frac{1}{\kappa n} \nabla n(\mathbf{r}, t)$$
(6.52)

Combining Eqs. 6.51 and 6.52 we can eliminate the pressure and obtain a relation between current acceleration and density gradient

$$\partial_t \boldsymbol{j}(\boldsymbol{r},t) = -\frac{1}{\kappa nm} \nabla n(\boldsymbol{r},t)$$
(6.53)

The current and the density distributions are also related through the continuity equation

$$\nabla \cdot \boldsymbol{j}(\boldsymbol{r},t) = -\partial_t n(\boldsymbol{r},t) \tag{6.54}$$

Eqs. 6.53 and 6.54 form a set that can be solved. To achieve this we take the divergence of both sides of Eq. 6.53

$$\partial_t \nabla \cdot \boldsymbol{j}(\boldsymbol{r}, t) = -\frac{1}{\kappa n m} \Delta n(\boldsymbol{r}, t)$$
(6.55)

and the time derivative of both sides of Eq. 6.54:

$$\partial_t \nabla \cdot \boldsymbol{j}(\boldsymbol{r}, t) = -\partial_t^2 n(\boldsymbol{r}, t) \tag{6.56}$$

We now combine Eqs. 6.55 and 6.56, eliminate $\partial_t \nabla \cdot \boldsymbol{j}(\boldsymbol{r},t)$, and thus obtain the equation for the propagation of normal sound

$$\left[\partial_t^2 - c_{ns}^2 \Delta\right] n(\boldsymbol{r}, t) = 0 \tag{6.57}$$

where the normal sound velocity is given by

$$c_{ns} = \frac{1}{\sqrt{\kappa nm}} \tag{6.58}$$

It is easy to solve the normal sound differential equation (Eq. 6.57) using separation of variables, with the result

$$n(\mathbf{r},t) = n_0 e^{i(\omega t - \mathbf{q} \cdot \mathbf{r})}$$

$$\omega = c_{ns} |\mathbf{q}|$$
(6.59)

Let us now consider the limit of weakly interacting fermions. In this case we can use the expressions for density, density of states and compressibility of a Fermi gas (Eqs. 1.10, 1.14 and 1.25). Substitution in Eq. 6.58 gives for the velocity of the "normal sound"

$$c_{ns} = \frac{v_{\rm F}}{\sqrt{3}} \tag{6.60}$$

6.8 General considerations of collective modes of interacting fermions

Let us examine the case when the susceptibility is divergent for some finite frequency ω . For simplicity we consider in this section the case that T = 0. The physics of such a situation is easy to understand. The susceptibility (say of charge) relates the response of the system $\rho(\mathbf{r}, t)$ to an excitation $\phi(\mathbf{r}, t)$. If the excitation is at a given momentum and frequency

$$\phi(\mathbf{r},t) = \phi_0 e^{i(\mathbf{q}\mathbf{r}-\omega t)} \tag{6.61}$$

it means that the response is of the same form

$$\rho(\mathbf{r},t) = \rho_0 e^{i(\mathbf{q}\mathbf{r}-\omega t)} \tag{6.62}$$

but with an amplitude that is given by

$$\rho_0 = \chi(\boldsymbol{q}, \omega)\phi_0 \tag{6.63}$$

Thus if the susceptibility $\chi(\mathbf{q}, \omega)$ is very large it means that even if the amplitude of an external perturbation was extremely small there would be a sizeable fluctuation of the density that would exist in the system. If the susceptibility diverges it means that even if the external perturbation vanishes there would be a mode of oscillations of density that would exist in the solid: i.e. even if $\phi_0 = 0$, ρ_0 would be finite.

The divergence of a susceptibility thus signals the existence of a *collective* mode. The density susceptibility and spin susceptibility give rise to the two collective modes of oscillating particle density and spin density respectively. For a system of electrons, the particle density is equivalent to the charge density. A priori other susceptibilities can diverge leading to other collective modes but the two previous ones are the ones that will in principle occur systematically in an interacting fermionic system. We can thus identify the collective modes by examining the expression (6.30) and finding the values (q, ω) for which it diverges. This condition will give us the dispersion relation of the collective mode. Note that such collective modes represent oscillations in density of the Fermi gas. They are thus quite different from the single particle excitations. In a Fermi liquid we will have quite generally three types of excitations:

- 1. The single particles excitations: they are the Landau quasiparticles, and are characterized by their effective mass m^* and quasiparticle weight Z_k . In the case of electrons they carry a charge q_e and a spin 1/2, and essentially resemble individual electron excitations.
- 2. A collective density oscillation. The total number of particle is constant but the density redistributes in the system. This is a wave of density with a wavevector \boldsymbol{q} and a frequency ω that are related by a dispersion relation $\omega(\boldsymbol{q})$ characteristic of the corresponding mode and given by the divergence of the charge susceptibility. There is no disturbance in the spin density
- 3. A collective mode of spin. This is a spin density wave. The particle density (which in the case of electrons is equivalent to the charge density) is uniform and undisturbed. The dispersion relation of this density wave $\omega(q)$ is given by the divergence of the spin susceptibility

6.9 Zero sound

In the case of 3 He and other fermi-type atomic liquids and gases, the particles are neutral. There is no long-range Coulomb interaction in this case, but instead there is a short-range



Figure 6.7: Graphical solutions for the equation (6.65). For repulsive interactions two solutions are a priori possible but only one of the modes will be undamped and thus corresponds to the zero sound. When the interaction becomes very small the zero sound velocity tends to v_F . The zero sound velocity increases as the repulsion increases and the system becomes stiffer and stiffer.

contact interaction. In coordinate space we approximate this with a δ -function potential of the type $V(\mathbf{r}_1 - \mathbf{r}_2) = U\delta(\mathbf{r}_1 - \mathbf{r}_2)$. In momentum space the interaction is $V(\mathbf{q}) = U$, is independent of the momentum \mathbf{q} transferred in a collision between two particles. The susceptibility in the mean-field approximation is therefore

$$\chi(\boldsymbol{q},\omega) = \frac{\chi_0(\boldsymbol{q},\omega)}{1 - U\chi_0(\boldsymbol{q},\omega)}$$
(6.64)

The condition for a collective mode is similar as for the plasmon, namely $\chi(\boldsymbol{q},\omega) = \infty$. In order to satisfy this equation we need to find lines of constant $\operatorname{Re} \chi_0(\boldsymbol{q},\omega)$ in the (\boldsymbol{q},ω) plane, satisfying

$$\operatorname{Re}\chi_0(\boldsymbol{q},\omega) = \frac{1}{U} \tag{6.65}$$

In 3 dimensions one can calculate from Eq. 6.17 4

$$\operatorname{Re} \chi_{0}(\boldsymbol{q}, \omega) \simeq \frac{mk_{\mathrm{F}}}{\hbar^{2}\pi^{2}} \left[-1 + \frac{\omega}{2qv_{\mathrm{F}}} \ln \left| \frac{1 + \omega/qv_{\mathrm{F}}}{1 - \omega/qv_{\mathrm{F}}} \right| \right]$$

$$\operatorname{Im} \chi_{0}(\boldsymbol{q}, \omega) \simeq \begin{cases} 0 &, \quad \omega > qv_{\mathrm{F}} \\ \frac{-mk_{\mathrm{F}}\omega}{2\pi\hbar^{2}qv_{\mathrm{F}}} &, \quad \omega < qv_{\mathrm{F}} \end{cases}$$
(6.66)

Equation (6.65) can easily be solved graphically using the expression for the bare susceptibility, Eq. 6.66, as indicated on Fig. 6.7. Since in the limit of weak interaction $1/U \rightarrow \infty$, the condition Eq. 6.65 is met for $\omega/qv_{\rm F} \rightarrow 1$. We see that two solutions could in principle exist

 $^{^{4}}$ This is a somewhat tedious calculation, for which we refer to G.D. Mahan, "Many-Particle Physics", Plenum, 1980, and later editions.

Sect. 6.10



Figure 6.8: (top) The zero sound corresponds to an anisotropic deformation of the Fermi surface that will retain its shape and propagate. (bot) In the normal sound all anisotropies are washed out by the scattering of the quasiparticles, and thus only expansions and contractions of the Fermi surface are possible.

for repulsive interactions U > 0. However, only one of the modes has a velocity larger than $v_{\rm F}$. According to the second condition (6.66) the mode for which $c < v_{\rm F}$ leads to an imaginary part, and it thus damped. We thus see that the collective mode has a dispersion relation for which the frequency ω is proportional to the wavevector q. This is identical to what one expects for a sound wave propagating in the system. Accordingly this collective mode is called zero sound. We will later compare it to the propagation of a normal sound in the system. If we denote c_{zs} the sound velocity of this mode we see that

$$c_{zs} = v_{\rm F} \tag{6.67}$$

is simply the Fermi velocity. We thus see that due to the interactions a modulation of the density $\hat{\rho}(r,t) = \hat{\rho}_0 \cos(\mathbf{qr} - \omega t)$ can propagate in the system.

6.10 The differences between zero sound and normal sound

In the previous sections we have obtained two different results for the propagation of sound in a neutral Fermi liquid: zero sound and normal sound, each having a different velocity. They correspond to two different internal ways of having a wave of density propagating in the system. Zero sound is characteristic of a quantum fluid and does not exist in a classical gas. To understand the difference between the two types of sound requires not only a determination of the velocity, and the knowledge that both modes correspond to a propagating wave of density, but also how exactly the excitations are distributed in the system to create this type of density wave. The precise calculation would carry us too far, so we will only describe the results qualitatively.



Figure 6.9: Observation of the zero sound in 3 He. At high temperature the velocity is the one of the normal sound, and as the temperature is lowered and the scattering decreases, the velocity increases to the one of the zero sound. After Abel, Phys Rev Lett 17, 74 (1966).

The main difference between a Fermi liquid and a normal gas, is the separation that exists between interaction acting on the quasiparticles and the scattering among the quasiparticles. In a normal system, both effects are directly related. In a perfect gas there are no interactions and no scattering, but as the interactions are introduced in a real gas, both the interaction effects and the scattering of the particles grow essentially in the same way. This is not the case, as we already saw, in a Fermi liquid. Since the excitations interact with the soup of the ground state, one can have strong interaction effects on the quasiparticles while being in an essentially collisionless regime for the quasiparticles. It means that contrary to the case of a normal gas one can have excitations around the Fermi surface that will be of a particular shape and that will be able to retain their shape without being "redistributed" by collision. This difference is at the essence of the difference between the normal sound and the zero sound.

The normal sound corresponds to a situation where the scattering is high. Thus in each portion of the system, excitations very rapidly reach the only possible equilibrium distribution which is an isotropic one around the Fermi surface.

On the other hand the zero sound corresponds to the limit of low scattering, and other modes are possible. It is possible to show, either from a phenomenological description as was initially done by Landau, or more microscopically, that the distribution of excitation corresponding to the collective mode is of the form

$$\delta n_0(\mathbf{k}) = C\delta(\xi_k) \frac{\cos\theta}{\cos\theta - \omega/qv_{\rm F}} \tag{6.68}$$

where θ is the azimuthal angle with respect to the vector \boldsymbol{q} giving the direction of the wave propagation. This indicates that the excitations are localized close to the Fermi level but correspond to a redistribution of particles around the Fermi surface that is anisotropic and very seriously so if s is close to one. The propagation of this wave is the zero sound. A summary is shown in Fig. 6.8

Of course if the temperature is high enough, the scattering is too high (as we saw it essentially



Figure 6.10: Comparison of the optical data (left , C. N. Presura, Ph.D. thesis, Rijksuniversiteit Groningen, (2003).) and EELS spectra (right, S. Nakai, N. Nuecker, H. Romberg, M. Alexander and J. Fink, Physica Scripta **41**, 596 (1990), reproduced from the original figure with permission of the authors.) of Bi₂Sr₂CaCu₂O₈, both providing $-\text{Im}\epsilon^{-1}(q,\omega)$, where $\epsilon^{-1}(q,\omega) = 1 + V_q \chi_{\rho\rho}(q,\omega)$. The peak positions in both spectra correspond to the plasmaresonance frequency.

grows as T^2), and will finish by killing the anisotropic shape. At high temperatures the zero sound will therefore turn into normal sound.

The existence of zero sound is thus a remarkable prediction and a strong characteristic of the Fermi liquid. Although the difference of velocity between the two modes is small it can be observed in ³He for which the parameters are controlled enough. This is shown in Fig. 6.9.

Let us finish this section by noting that having a "sound" mode with the energy ω going to zero as \boldsymbol{q} goes to zero is in fact a quite general property. This will occur each time the Hamiltonian has a continuous symmetry (here the translation symmetry) and that we consider excitations that corresponds to a spontaneously breaking of this symmetry. In this case one can show that there must be low energy modes (so called Goldstone modes) that have to exist.

6.11 Coulomb interaction: Plasmons

If the case of a gas of charged fermions, the propagating density modes do not follow a linear sound-like dispersion, but instead a gap opens in the collective mode spectrum. This leads to the concept of plasmons that we will now describe in some detail.

The momentum space representation of the Coulomb interaction is given by $V_q = 4\pi q_e^2/q^2$. As discussed in one of the earlier sections, the collective modes exist for frequencies and wavevectors for which $\chi_{\rho\rho}(\boldsymbol{q},\omega) = \infty$, which with the help of Eq. 6.30 implies $1 = V(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)$. We first explore the ω, q space, where $\omega \gg v_F q$, so that we can ignore the imaginary part in the expression of the bare susceptibility, Eq. 6.66. The solutions of $1 = V(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)$ are then

$$1 = \frac{4\pi q_e^2}{q^2} \frac{mk_{\rm F}}{\pi^2 \hbar^2} \left[-1 + \frac{\omega}{2qv_{\rm F}} \ln \left| \frac{1 + \omega/qv_{\rm F}}{1 - \omega/qv_{\rm F}} \right| \right]$$
(6.69)

Since $qv_{\rm F}/\omega \ll 1$, we proceed by making a power series expansion of the righthand side of the

expression. We start by re-arranging the terms as

$$1 + \frac{\pi \hbar^2 q^2}{4mq_e^2 k_{\rm F}} = \frac{\omega}{2qv_{\rm F}} \left(\ln(1 + qv_{\rm F}/\omega) - \ln(1 - qv_{\rm F}/\omega) \right)$$
(6.70)

and expand $\ln(1+x) = x - x^2/2 + x^3/3 - x^4/4 + x^5/5...$ so that

$$1 + \frac{\pi\hbar^2 q^2}{4mq_e^2 k_{\rm F}} = \frac{\omega}{qv_{\rm F}} \left\{ \frac{qv_{\rm F}}{\omega} + \frac{1}{3} \left(\frac{qv_{\rm F}}{\omega}\right)^3 + \frac{1}{5} \left(\frac{qv_{\rm F}}{\omega}\right)^5 \dots \right\}$$
(6.71)

Se now see that the first terms on the left- and right hand side of the expression are both equal to 1. Collecting the remaining terms gives

$$\frac{\pi q^2}{4mq_e^2 k_{\rm F}} = \frac{q^2 v_{\rm F}^2}{3\omega^2} + \frac{q^4 v_{\rm F}^4}{5\omega^4} \dots$$
(6.72)

so that, using the Fermi liquid relations $v_{\rm F}=\hbar k_F/m,$ and $k_F^3/(3\pi^2)=n$, we obtain the following expansion of q

$$\omega^2 = \frac{4\pi nq_e^2}{m} + \frac{3}{5}v_F^2 q^2 + O\left(q^4\right)$$
(6.73)

which means that even when $q \to 0$ there is an oscillation of the charge of the system at the frequency $\omega_p \equiv \sqrt{4\pi n q_e^2/m}$. When q becomes finite this mode disperses in a way that is schematically represented in Note that at small momentum q this mode is undamped since the condition $\omega(q)/q > v_F$ is indeed satisfied. Experimentally plasmons can be measured from optical spectra, or by studying the inelastic scattering of high energy (200 keV) electrons. An example of such measurements is shown in Fig. 6.10

Let us finish by noting that the existence of the plasmon is a quite general and important phenomena. It corresponds to a situation of a system that has a continuum symmetry but is in addition coupled to a gauge field (here the electromagnetic field, since there is the Coulomb interaction). This situation occurs in many physical situations, such as for superconductivity (U(1) symmetry of changing the phase of the wave function)) or particle physics for the standard model. In that case, it is possible to show that the Goldstone modes that one would expect in the absence of gauge field do not appear, but that they are absorbed by the gauge field that becomes massive. This mechanism was identified by P. W. Anderson as being responsible for the existence of the Meissner effect in a superconductor (massive electromagnetic field). It has been extended by Higgs to general symmetry group and is at the heart of the properties of the standard model. It is widely known as the Higgs (or Anderson-Higgs) mechanism, and we will encounter it in several other situations.

6.12 Landau Damping

Let us go back to the condition giving the damping of the collective modes

$$\operatorname{Im}\chi_0(\boldsymbol{q},\omega) \neq 0 \tag{6.74}$$

Although one can compute it explicitly for some specific dispersion relation ξ as we did in the previous section, let us examine it in general. Writing explicitly the imaginary part one gets

$$\operatorname{Im} \chi_0(\boldsymbol{q}, \omega) = \frac{\pi}{\Omega} \sum_{\boldsymbol{k}} [\xi_k f_{k+q} - \xi_k f_k] \delta(\omega + \xi_k - \xi_{k+q})$$
(6.75)

If one is at T = 0 one thus sees that the imaginary part consists in creating particle hole excitations where one take a particle with momentum k below the Fermi surface, and brings it



Figure 6.11: Plasmon mode (blue) for systems with long range Coulomb interaction. The dispersion relation of the mode tends to a finite frequency ω_p when the density distortion becomes uniform, indicating an oscillation of the density of charge with time. Not that at small q this mode is indeed undamped.

at a higher energy $\xi_{k+q} = \xi_k + \omega$ above the Fermi surface. All other excitations are blocked by the Pauli principle. Since the sum over \mathbf{k} is made of positive terms, to identify the region in the plane (q, ω) where the imaginary part is non zero one must thus find for which values of ω and q one can make such particle-hole excitations. It is easy to see, as shown in Fig. 6.12. that the worse one can make in terms of energy is to use all the available wavevector to "climb" in energy. The maximum difference in energy is in that case

$$\xi_{k+q} - \xi_k \simeq \hbar v_{\rm F} (k+q-k) = \hbar v_{\rm F} q \tag{6.76}$$

This provides an upper limit above which particle-hole excitations of small momentum cannot be created. Note that this condition coincides with the one we found for the free electrons dispersions relation (6.66). This result is in fact quite general. Then it is clear that, as shown in Fig. 6.12 one can make for $0 < q < 2k_{\rm F}$ excitations of arbitrarily low energy simply by bringing the particle from one point of the Fermi surface to the other. When $q > 2k_{\rm F}$ one is in a similar situation than the one for $q \sim 0$ since in that case $q - 2k_{\rm F}$ can only be used to "climb" away from the Fermi surface. This time this gives a minimum value for the energy below which a particle-hole excitation cannot exist. These criteria define the particle-hole continuum showed in Fig. 6.13. In this region the imaginary part of χ_0 is non zero and a collective mode entering this region will thus be damped.

6.13 Spin susceptibility and magnons

The interaction in Eq. 6.18 was defined for the charge sector. However, in solids the effective interaction between parallel and anti-parallel spins is in general different. This has to do with the fact that the effective interactions between dressed quasi-particles on a low energy scale are no longer described the bare Coulomb interaction, but rather by screened interactions and more complicated processes which can depend on the spin. Let us define $V_{\parallel}(\mathbf{r})$ and $V_{\perp}(\mathbf{r})$ as the interaction between parallel and anti-parallel spins respectively. The total interaction between



Collective modes

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Figure 6.12: (a) An excitation close to $q \sim 0$ costing the maximum energy. One uses all the q to raise in energy away from the Fermi surface. (b) Excitations of essentially zero energy take an electron just below the Fermi surface and recreate it just above the Fermi surface with a different q this is possible for $q < 2k_{\rm F}$. (c) For $q > 2k_{\rm F}$ the remaining of the wavevector must be used to increase the energy of the particle giving a minimum value before particle-hole excitations can be created.



Figure 6.13: Particle-hole continuum. In this region single particle excitations can be excited. If a collective mode enters this zone, it will thus be damped by Landau damping by exciting particle hole pairs.

the electrons is then

$$H^{(i)} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V_{\parallel}(r_1 - r_2) \left[\hat{\rho}_{\uparrow}(r_1) \hat{\rho}_{\uparrow}(r_2) + \hat{\rho}_{\downarrow}(r_1) \hat{\rho}_{\downarrow}(r_2) \right] + \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 V_{\perp}(r_1 - r_2) \left[\hat{\rho}_{\uparrow}(r_1) \hat{\rho}_{\downarrow}(r_2) + \hat{\rho}_{\downarrow}(r_1) \hat{\rho}_{\uparrow}(r_2) \right]$$
(6.77)

This can be rearranged as follows

$$\begin{split} H^{(i)} &= \frac{1}{2} \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \frac{V_{\parallel}(r_1 - r_2) + V_{\perp}(r_1 - r_2)}{2} \left[\hat{\rho}_{\uparrow}(r_1) + \hat{\rho}_{\downarrow}(r_1) \right] \left[\hat{\rho}_{\uparrow}(r_2) + \hat{\rho}_{\downarrow}(r_2) \right] \\ &+ \frac{1}{2} \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \frac{V_{\parallel}(r_1 - r_2) - V_{\perp}(r_1 - r_2)}{2} \left[\hat{\rho}_{\uparrow}(r_1) - \hat{\rho}_{\downarrow}(r_1) \right] \left[\hat{\rho}_{\uparrow}(r_2) - \hat{\rho}_{\downarrow}(r_2) \right] \end{split}$$

Taking this into account, the charge-charge interaction $V(\mathbf{r})$ in Eq. 6.18 is then given by

$$V(\boldsymbol{r}) = \left[V_{\parallel}(\boldsymbol{r}) + V_{\perp}(\boldsymbol{r}) \right] / 2 \tag{6.78}$$

The spin polarisation is described by the operator

$$\hat{m}(\boldsymbol{r}) = \hat{\rho}_{\uparrow}(\boldsymbol{r}) - \hat{\rho}_{\downarrow}(\boldsymbol{r}) \tag{6.79}$$

which is proportional to the magnetization along the z-axis. The interaction between two spin-densities is given by

$$J(\boldsymbol{r}) = \left[V_{\parallel}(\boldsymbol{r}) - V_{\perp}(\boldsymbol{r}) \right] / 2 \tag{6.80}$$

The corresponding interaction hamiltonian is with this notation

$$\hat{H}^{\text{int}} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 J(\mathbf{r}_1 - \mathbf{r}_2) \hat{m}(\mathbf{r}_1) \hat{m}(\mathbf{r}_2)$$
(6.81)

If the interaction is a pure Coulomb interaction, $V_{\parallel}(\mathbf{r}) = V_{\perp}(\mathbf{r})$, as is the case for a free electron system such as aluminum, we have

$$V(\boldsymbol{q}) = \frac{4\pi q_e^2}{q^2}$$

$$J(\boldsymbol{q}) = 0$$
(6.82)

in other words, the long range part of the interaction drops out of the spin susceptibility. This is quite natural since a disturbance in spin density does not induce an imbalance of the charge, and thus cannot feel the Coulomb interaction. The spin susceptibility is always controlled by short range exchange interactions, usually between neighboring atoms with overlapping charge clouds. The physics of exchange interactions is a vast subject, which in the interest of time we will not dwell upon any further in the present section.

The coupling of an external magnetic field to the spin polarization is described by the Hamiltonian

$$\hat{H}^{\rm p} = \sum_{q} h(q, t) \hat{m}(q) \tag{6.83}$$

Here $h(\mathbf{q}, t)$ is, apart from uninteresting factors, just the magnetic field. Similar as for the charge response, we treat the interaction Eq. 6.18 by using the mean field approximation, from which we get

$$\hat{H}^{\rm MF} = \sum_{q} h^{ind}(\boldsymbol{q}, t) \hat{m}(\boldsymbol{q})$$
(6.84)

where

$$h^{ind}(\boldsymbol{q},t) = J(\boldsymbol{q})m(\boldsymbol{q},t) \tag{6.85}$$

The spin-density can thus be written as a response to the total field $h + h^{ind}$ for the free electron gas. Since for the free electrons gas there is no response of the down spins when there is a perturbation applied to the up spins and vice versa, one has

$$m(\boldsymbol{q},\omega) = \chi_0(\boldsymbol{q},\omega) \left(h(\boldsymbol{q},\omega) + h^{ind}(\boldsymbol{q},\omega) \right)$$
(6.86)

where $\chi_0(\boldsymbol{q},\omega)$ is the "bare" susceptibility, Eq. 6.17, which is the same one for the spin- and charge response. Eq. 6.86 is easily solved, leading to the full susceptibility in the mean-field approximation

$$\chi_{\sigma\sigma}(\boldsymbol{q},\omega) = \frac{m(\boldsymbol{q},\omega)}{h(\boldsymbol{q},\omega)} = \frac{\chi_0(\boldsymbol{q},\omega)}{1 - J(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)}$$
(6.87)

We can easily write the condition for the divergence of the susceptibility. For the spin density waves

$$1 - J(\boldsymbol{q}) \operatorname{Re} \chi_0(\boldsymbol{q}, \omega) = 0$$

Im $\chi_0(\boldsymbol{q}, \omega) = 0$ (6.88)

We see that the condition $\operatorname{Im} \chi_0(\boldsymbol{q}, \omega) = 0$ is in any case mandatory for the susceptibility to diverge. The physical meaning of this condition is clear. Imposing $\operatorname{Im} \chi_0(\boldsymbol{q}, \omega)$ is equivalent to imposing that $\operatorname{Im} \chi(\boldsymbol{q}, \omega) = 0$ as can be directly seen by writing the imaginary part of χ . It is thus equivalent to imposing that there is no dissipation taking place in the system. This is indeed mandatory for a mode to proceed without damping. Indeed in the absence of an external excitation, if there is dissipation taking place it means that the energy must be taken from the density oscillation and that the collective mode will cease to propagate undamped. We thus see that the condition

$$\operatorname{Im}\chi_0(\boldsymbol{q},\omega) = 0 \tag{6.89}$$

corresponds to the absence of damping for the collective mode. This condition is discussed in detail in section Section 6.12. In non magnetically ordered metals, the magnons *are* always Landau damped. It is still possible to have peaks in the $\text{Im}\chi(q,\omega)$, but these are rather broad, and are therefore called "paramagnons". In certain superconducting materials, which are close to a magnetic instability, the paramagnon branch can soften far enough, so that it becomes situated below the superconducting gap. In this case these modes are no longer Landau damped, and show up as sharp lines in the magnetic susceptibility, which can be measured using inelastic neutron scattering.

Another well-known situation where there are sharp collective modes of magnetic polarization, is when the electrons are already spin-polarized in the ground state, in other words, when the system is ferro-magnetic, or anti-ferromagnetic. In this case the collective modes are called "magnons".