Lecture Notes*, Theory of Condensed Matter II

Jörg Schmalian

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Part I
Introduction

This course is concerned with phenomena in quantum condensed matter systems that can be most efficiently analyzed and solved using quantum field theoretical methods. To this end we first physically motivate, introduce, and investigate retarded Green's functions. We will use the equation of motion method to solve several problems such as itinerant ferromagnetism, superconductivity, and dynamical screening of the Coulomb interaction. For a more systematic analysis of many-body systems we will then introduce the Feynman-diagram technique of thermal Green's functions and, once again, investigate superconductivity, but also disordered systems. Finally we will discuss the non-equilibrium version of many-body theory by using the Schwinger-Keldysh approach. As example, we

investigate quantum transport of graphene. Thus, the course is concerned with learning techniques and applying them to solve given many-body problems.

In case of the screening of the Coulomb interaction, we consider for example the Hamiltonian of non-relativistic electrons (no spin-orbit interaction) in a crystalline potential $U(\mathbf{r})$ and with electron-electron interaction $V(\mathbf{r}-\mathbf{r}')$:

$$\begin{aligned} H &= \int d^d r \sum_\alpha \psi_\alpha^\dagger(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} - \mu + U(\mathbf{r}) \right) \psi_\alpha(\mathbf{r}) \\ &= \frac{1}{2} \sum_{\alpha\beta} \int d^d r d^d r' \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta^\dagger(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') \psi_\beta(\mathbf{r}') \psi_\alpha(\mathbf{r}) . \end{aligned} \tag{1}$$

Here $\psi_\alpha(\mathbf{r})$ is the fermionic field operator that annihilates an electron with spin α at position $\mathbf{r}$, obeying standard fermionic anti-commutation relation

$$\left[\psi_\alpha(\mathbf{r}), \psi_\beta^\dagger(\mathbf{r}') \right]_+ = \delta_{\alpha\beta} \delta(\mathbf{r}-\mathbf{r}') . \tag{2}$$

If we include a similar Hamiltonian for the motion of the nuclei, along with the electron-nucleus Coulomb interaction, we pretty much have a complete description of a solid within the non-relativistic limit. Thus, it is possible to fully define the *standard model* of condensed matter physics in the introductory lines of a lecture. One might then be tempted to conclude that this area of physics must be conceptually pretty trivial. All that seems left to do is to solve for the eigenstates and eigenvalues of H, a task that one leaves to a gifted programmer or a clever mathematician. However, except for small systems or systems with a large number of conserved quantities, these many-body systems simply cannot be solved exactly. We need to find ways to analyze such an Hamiltonian, or a simplified version of it, that allow to make as rigorous statements as possible. In fact, the beauty of condensed matter theory is to make predictions about new states of matter and universal behavior that is emergent, i.e. that is not obvious if one looks at the initial degrees of freedom of the Hamiltonian. If nothing else, these considerations reveal that simply writing down a fundamental theory, doesn't yield a whole lot of insight that goes beyond the understanding of what the elementary building blocks of this theory are. Emergent phenomena, such as spontaneous symmetry breaking, composite particles, new topological states of matter etc. etc. require a detailed analysis that is primarily guided by experiment and, of course, by some good physical intuition. The author of these lecture notes is rather convinced that this is the same, regardless whether we talk about the physics of a piece of metal, a neutron star, or the universe as a whole.

Part II
Observables and Green's functions

1 Linear response

We consider a system that is, at least initially, in thermodynamic equilibrium. The expectation value of a physical observable is then given by

$$\langle A \rangle = \mathrm{tr}\left(\rho \mathrm{A}\right), \tag{3}$$

with density operator (often called density matrix)

$$\rho = \frac{1}{Z} e^{-\beta H}. \tag{4}$$

$Z = \mathrm{tr} e^{-\beta H}$ is the partition function and $\beta = \frac{1}{k_B T}$ the inverse temperature. In what follows we will use a system of units where $k_B = 1$, i.e. we measure temperatures in energy units. The generalization to the grand canonical ensemble with chemical potential μ is straightforward. The density operator is then given as $\rho_{\mathrm{eq}} = \frac{1}{Z_g} e^{-\beta(H-\mu N)}$, where N is the particle number operator. As we will mostly use the grand canonical ensemble, we will often call $H - \mu N$ the Hamiltonian and continue to use the letter H. Determining such an expectation value is a formidable task in many body theory and we will do this during this course.

A scenario that occurs very frequently and that offers significant insight into the inner workings of a complex condensed matter systems is based on the measurement of an observable that follows some external perturbation. Such an approach yields dynamical information, in fact it even allows to theoretically study the stability of a state of matter with regards to a spontaneous symmetry breaking. To this end we consider a system coupled to an external field that is characterized by the interaction part of the Hamiltonian $W(t)$, i.e. the Hamiltonian

$$H_{\mathrm{tot}} = H + W(t) \tag{5}$$

consists of the Hamiltonian H that describes our system in isolation and the external time dependent perturbation $W(t)$.

A specific example for $W(t)$ is the coupling

$$W(t) = -\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{B}(t) \tag{6}$$

of an external magnetic field to the electron spins

$$\mathbf{S}_i = \frac{\hbar}{2} \sum_{\alpha\beta} c^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta} \tag{7}$$

of a magnetic system. Another example is interaction

$$W(t) = -\sum_i \mathbf{P}_i \cdot \mathbf{E}(t) \tag{8}$$

between the electrical polarization

$$\mathbf{P}_i = e \sum_\alpha c_{i\alpha}^\dagger \mathbf{R}_i c_{i\alpha} \tag{9}$$

and an external electrical field.

As for the time dependence of $W(t)$, we always have in mind a scenario where the system is not affected by the perturbation in the infinite past, i.e. $W(t \to -\infty) \to 0$. A convenient way to realize this is via

$$\begin{aligned} \mathbf{E}(t) &= \lim_{\delta \to 0^+} \mathbf{E}_0 \exp\left(-i(\omega + i\delta)t\right) \\ \mathbf{B}(t) &= \lim_{\delta \to 0^+} \mathbf{B}_0 \exp\left(-i(\omega + i\delta)t\right), \end{aligned} \tag{10}$$

i.e. we include an infinitesimal positive imaginary part to the frequency of an oscillatory time dependence. In the case of a more general time dependence we would write

$$W(t) = \lim_{\delta \to 0^+} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} W(\omega) e^{-i(\omega + i\delta)t}. \tag{11}$$

Next we consider the time evolution of the observable that follows as a consequence of the applied external perturbation

$$\langle A \rangle_t = \mathrm{tr}\left(\rho(\mathrm{t})\,\mathrm{A}\right), \tag{12}$$

where the density matrix obeys the von Neuman equation

$$i\hbar \frac{\partial}{\partial t} \rho(t) = \left[H + W(t), \rho(t)\right]. \tag{13}$$

Note, in case of $\rho(t)$ and $W(t)$ we are analyzing the time dependence of operators that are in the Schrödinger picture. As a reminder, the von Neuman equation follows for an arbitrary density matrix $\rho(t) = \sum_i |\Psi_{\mathrm{tot},i}(t)\rangle\, p_i\, \langle \Psi_{\mathrm{tot},i}(t)|$ from the Schrödinger equation of the many body wave function $|\Psi_{\mathrm{tot},i}(t)\rangle$ with Hamiltonian H_{tot}. The dynamics of observables is then a consequence of the time dependence of the density matrix. This is indicated by the subscript t of $\langle A \rangle_t$.

As discussed, the perturbation is absent in the infinite past and we assume the system was in equilibrium for $t \to -\infty$:

$$\rho(t \to -\infty) = \rho = \frac{1}{Z} e^{-\beta H}. \tag{14}$$

In most cases the external perturbation is small and we can confine ourselves to changes in $\langle A \rangle_t$ that are linear in $W(t)$. This regime is referred to as linear

response. The subsequent formalism can be (and has been) extended to include higher order non-linearities. Here we will, however, only consider the leading order, linear effects.

To proceed we go to the interaction representation

$$\rho\left(t\right)=e^{-iHt/\hbar}\rho^{(I)}\left(t\right)e^{iHt/\hbar}. \tag{15}$$

Note, $\rho^{(I)}\left(t\right)$ corresponds to the interaction picture of the Hamiltonian H_{tot}. The Hamiltonian of our system of interest is of course H ($W\left(t\right)$ is only used to probe this system). If considered with regards to H, $\rho^{(I)}\left(t\right)$ corresponds to the Heisenberg picture. This is the reason why we will below state that operators are taken in the Heisenberg picture.

Performing the time derivative gives

$$i\hbar\frac{\partial\rho\left(t\right)}{\partial t}=\left[H,\rho\left(t\right)\right]+e^{-iHt/\hbar}i\hbar\frac{\partial\rho^{(I)}\left(t\right)}{\partial t}e^{iHt/\hbar}. \tag{16}$$

Inserting the von Neuman equation yields

$$i\hbar\frac{\partial\rho^{(I)}\left(t\right)}{\partial t}=\left[W^{(I)}\left(t\right),\rho^{(I)}\left(t\right)\right], \tag{17}$$

which is formally solved by (better, its solution is equivalent to the solution of)

$$\rho^{(I)}\left(t\right)=\rho-\frac{i}{\hbar}\int_{-\infty}^{t}dt'\left[W^{(I)}\left(t'\right),\rho^{(I)}\left(t'\right)\right]. \tag{18}$$

If we return to the Schrödinger picture, it follows

$$\rho\left(t\right)=\rho-\frac{i}{\hbar}\int_{-\infty}^{t}dt'e^{-iH\left(t-t'\right)/\hbar}\left[W\left(t'\right),\rho\left(t'\right)\right]e^{iH\left(t-t'\right)/\hbar}. \tag{19}$$

One can now generate a systematic expansion with regards to $W\left(t\right)$ if one solves this integral equation via recursion. At zeroth order holds of course $\rho\left(t\right)=\rho=\frac{e^{-\beta H}}{Z}$. At first order we can insert this zeroth order solution in the right hand side and obtain

$$\rho\left(t\right)=\rho-\frac{i}{\hbar}\int_{-\infty}^{t}dt'e^{-iH\left(t-t'\right)/\hbar}\left[W\left(t\right),\rho\right]e^{iH\left(t-t'\right)/\hbar}. \tag{20}$$

We can now determine the expectation value of A:

$$\left\langle A\right\rangle_{t}=\left\langle A\right\rangle-\frac{i}{\hbar}\int_{-\infty}^{t}dt'\mathrm{tr}\left(\left[\mathrm{W^{(I)}\left(t'\right),\rho}\right]\mathrm{A^{(I)}\left(t\right)}\right). \tag{21}$$

One can cyclically change the order under the trace operation:

$$\mathrm{tr}\left[\left(\mathrm{W}\rho-\rho\mathrm{W}\right)\mathrm{A}\right]=\mathrm{tr}\left[\left(\mathrm{AW}-\mathrm{WA}\right)\rho\right], \tag{22}$$

which gives

$$\langle A\rangle_t = \langle A\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \left\langle \left[A^{(I)}(t), W^{(I)}(t')\right]\right\rangle . \tag{23}$$

It is useful to introduce (the retarded Green's function)

$$\left\langle\left\langle A^{(I)}(t); B^{(I)}(t')\right\rangle\right\rangle = -\frac{i}{\hbar}\theta(t-t')\left\langle\left[A^{(I)}(t), B^{(I)}(t')\right]\right\rangle \tag{24}$$

such that

$$\boxed{\langle A\rangle_t = \langle A\rangle + \int_{-\infty}^{\infty} dt' \left\langle\left\langle A^{(I)}(t); W^{(I)}(t')\right\rangle\right\rangle .} \tag{25}$$

These considerations demonstrate that the linear response of a physical system is characterized by retarded Green's functions. The interesting result is that we can characterize the deviation from equilibrium (e.g. dissipation in case of the electrical conductivity) in terms of fluctuations of the equilibrium (equilibrium correlation functions). Among others, this will lead us to the fluctuation-dissipation theorem. It will also offer a compact and unifying approach to study the response of a system with regards to an arbitrary external perturbation.

Example, conductivity: as discussed, we have an interaction between the electrical field and the electrical polarization:

$$W^{(I)}(t) = -\sum_i \mathbf{P}_i^{(I)} \cdot \mathbf{E}(t) . \tag{26}$$

with (we will frequently not write down explicitly the limit $\delta \to 0^+$)

$$\mathbf{E}(t) = \mathbf{E}_0 \exp\left(-i\left(\omega + i0^+\right)t\right) . \tag{27}$$

If we are interested in the electrical current it follows

$$\langle j_\alpha\rangle_t = -\sum_i \int_{-\infty}^{\infty} dt' \left\langle\left\langle j_\alpha^{(I)}(t); P_{\beta,i}^{(I)}(t')\right\rangle\right\rangle E_{0,\beta} e^{-i(\omega+i\delta)t'} \tag{28}$$

Before we give further examples and discuss the physical implications of our linear response analysis, we will therefore discuss in some detail the mathematical properties of such functions.

2 Properties of retarded and advanced Green's functions

We learned that the linear response of a physical system that is initially in equilibrium can be formulated in terms of retarded Green's functions:

$$\begin{aligned} G_{A,B}^r(t,t') &= \langle\langle A(t); B(t')\rangle\rangle^r \\ &\equiv -i\theta(t-t')\left\langle\left[A(t), B(t')\right]_\eta\right\rangle . \end{aligned} \tag{29}$$

To simplify our notation we will from now on use a convention where $\hbar = 1$, i.e. frequencies and energies are measured in the same units. We further dropped the superscript (I) for the interaction representation. Keep in mind, that it is anyway the Heisenberg picture if we refer this to the Hamiltonian H of the system we are interested in:

$$A(t) = e^{iHt} A e^{-iHt}. \tag{30}$$

Finally, we introduced

$$[A, B]_\eta = AB + \eta BA \tag{31}$$

to simultaneously analyze the commutator for $\eta = -1$ and the anti-commutator for $\eta = +1$. We will see very soon that this generalization to anti-commutators is sometimes a very sensible thing to do if one considers certain properties of fermions.

The prefactor $\theta(t - t')$ emerged as a natural consequence of causality. The response of the quantity $\langle A \rangle_t$ was only influenced by $W(t')$ with $t' < t$. It is however possible, at least formally, to introduce other Green's functions. Important examples are advanced Green's functions:

$$\begin{aligned} G^a_{A,B}(t, t') &= \langle\langle A(t); B(t') \rangle\rangle^r \\ &\equiv i\theta(t' - t) \left\langle [A(t), B(t')]_\eta \right\rangle \end{aligned} \tag{32}$$

or time-ordered (sometimes called causal) Green's functions -

$$\begin{aligned} G^c_{A,B}(t, t') &= \langle\langle A(t); B(t') \rangle\rangle^c \\ &\equiv -i \langle T_\eta A(t) B(t') \rangle \end{aligned} \tag{33}$$

with time ordering operator

$$T_\eta A(t) B(t') = \theta(t - t') A(t) B(t') - \eta\theta(t' - t) B(t') A(t). \tag{34}$$

Because of our insight that retarded Green's functions determine the linear response, we predominantly investigate this function. The advanced and time-ordered functions can be easily analyzed along the same lines. In fact all functions contain essentially the same information.

2.1 Homogeneity of time

An important property of all of those Green's functions is that they are only functions of the difference $t - t'$. It holds

$$\begin{aligned} G^r_{A,B}(t, t') &= -i\theta(t - t') \left\langle [A(t), B(t')]_\eta \right\rangle \\ &= -i\theta(t - t') \left(\langle A(t) B(t') \rangle + \eta \langle B(t') A(t) \rangle \right) \end{aligned} \tag{35}$$

The correlation functions are explicitly given as

$$\begin{aligned}\langle A(t)B(t')\rangle &= \frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}e^{iHt}Ae^{-iHt}e^{iHt'}Be^{-iHt'}\right)\\ &= \frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}e^{iH(t-t')}Ae^{-iH(t-t')}B\right)\\ &= \langle A(t-t')B(0)\rangle \end{aligned} \tag{36}$$

and similar for $\langle B(t')A(t)\rangle = \langle B(0)A(t-t')\rangle$. Thus, it follows

$$\boxed{G^r_{A,B}(t,t') = G^r_{A,B}(t-t').} \tag{37}$$

The reason why we could demonstrate this behavior is that the thermal average, with Boltzmann weight $e^{-\beta H}$ and the unitary time evolution, with e^{-iHt} commute. They are both governed by the same Hamiltonian. Physically it corresponds to the fact that there is no preferred absolute time in a system that is in equilibrium. An implication is that any stationary distribution function, even those that are not in equilibrium but that yield states without preferred time point must have a density matrix $\rho = \rho(H, X_i)$ that only depends on the Hamiltonian and maybe on other conserved quantities X_i of the system with $[H, X_i] = 0$.

2.2 Equation of motion

The fundamental equation of motion of quantum mechanics is the Schrödinger equation. For operators that are not explicitly time dependent in the Schrödinger picture, the Schrödinger equation is equivalent to the Heisenberg equation[1]:

$$i\partial_t A(t) = [A(t), H]_- . \tag{38}$$

This enables us to determine the equation of motion that follows from the Schrödinger equation.

We start from

$$\begin{aligned} i\partial_t G^r_{A,B}(t) &= \partial_t\left\{\theta(t)\left\langle [A(t), B(0)]_\eta\right\rangle\right\}\\ &= \delta(t)\left\langle [A,B]_\eta\right\rangle + \theta(t)\left\langle [\partial_t A(t), B(0)]_\eta\right\rangle\\ &= \delta(t)\left\langle [A,B]_\eta\right\rangle - i\theta(t)\left\langle \left[[A(t),H]_-, B(0)\right]_\eta\right\rangle, \end{aligned} \tag{39}$$

where t now refers to the relative time. The last expression can itself be written as a retarded Green's function

$$G^r_{[A,H]_-,B}(t) = \left\langle\left\langle [A(t),H]_- ; B(t')\right\rangle\right\rangle^r = -i\theta(t)\left\langle\left[[A(t),H]_-, B(0)\right]_\eta\right\rangle$$

and we obtain the equation of motion for retarded Green's functions.

$$\boxed{i\partial_t G^r_{A,B}(t) = \delta(t)\left\langle [A,B]_\eta\right\rangle + G^r_{[A,H]_-,B}(t).} \tag{40}$$

[1] Recall, that we use a system of units with $\hbar = 1$.

Thus, in order to determine one Green's function one needs to know another one. We will see that in case of non-interacting systems the newly generated Green's functions form a closed set, which allows, at least in principle, for a full solution. On the other hand, for a generic interacting many body system a closed solution only exists when one analyzes conserved quantities with $[A, H]_- = 0$ or at least densities of conserved quantities. These aspects will all be discussed in greater detail below.

Because of Eq.(37) follows that we can Fourier transform the Green's function

$$G^r_{AB}(\omega) = \int_{-\infty}^{\infty} dt G^r_{AB}(t)\, e^{i\omega t}. \tag{41}$$

The equation of motion for the Fourier transforms are then easily obtained as

$$\omega G^r_{A,B}(\omega) = \left\langle [A, B]_\eta \right\rangle + G^r_{[A,H]_-,B}(\omega). \tag{42}$$

It is now only an algebraic equation.

If one repeats the same analysis for the advanced and time-ordered Green's functions, one finds identical expressions as in Eqs.(40) and (42). On the other hand, the detailed time dependence of $G^r(t)$, $G^a(t)$, and $G^c(t)$ is obviously very different. From the definition of these quantities follows for example that $G^r(t < 0) = 0$, while $G^a(t > 0) = 0$. Thus, if one wants to determine the correct solution of the equation of motion one must incorporate those boundary conditions appropriately. This also implies that the Fourier transform in Eq.(41) has to be performed with some care. To address these issues we will next analyze the analytic properties of Green's functions in some detail.

2.3 Lehmann representation

In what follows we determine a rigorous representation of $G^r_{AB}(\omega)$ that reveals a lot about the analytic structure of Green's functions. Let $\{|l\rangle\}$ be the exact eigenfunctions of the Hamiltonian with eigenvalues $\{E_l\}$, i.e.

$$H|l\rangle = E_l|l\rangle. \tag{43}$$

Then, we can write a thermal expectation value as

$$\langle A\rangle = \mathrm{tr}(\rho \mathrm{A}) = \frac{1}{Z}\sum_l e^{-\beta E_l} \langle l|A|l\rangle. \tag{44}$$

For a correlation function follows accordingly

$$\begin{aligned}
\langle A(t)\, B(0)\rangle &= \frac{1}{Z}\sum_l e^{-\beta E_l} \langle l|A(t)\, B(0)|l\rangle \\
&= \frac{1}{Z}\sum_l e^{-\beta E_l} \left\langle l\left|e^{iHt}Ae^{-iHt}B\right|l\right\rangle \\
&= \frac{1}{Z}\sum_{l.m} e^{-\beta E_l} e^{it(E_l - E_m)} \langle l|A|m\rangle \langle m|B|l\rangle
\end{aligned} \tag{45}$$

The same analysis can be performed for $\langle B(0) A(t)\rangle$ and yields

$$\begin{aligned}\langle B(0) A(t)\rangle &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_l} e^{-it(E_l-E_m)} \langle l|B|m\rangle \langle m|A|l\rangle \\ &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_m} e^{it(E_l-E_m)} \langle l|A|m\rangle \langle m|B|l\rangle \end{aligned} \quad (46)$$

In order to analyze the frequency dependence of the Fourier transform of the Green's function we first consider the Fourier transform of the correlation functions

$$\langle B(0) A(t)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J(\omega) e^{-i\omega t}. \quad (47)$$

For the inverse transform $J(\omega)$, which we also call the spectral function, follows

$$\begin{aligned} J(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} \langle B(0) A(t)\rangle \\ &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_m} \langle l|A|m\rangle \langle m|B|l\rangle \int_{-\infty}^{\infty} dt e^{it(\omega+E_l-E_m)}. \end{aligned} \quad (48)$$

We use $\int_{-\infty}^{\infty} dt e^{it\omega} = 2\pi\delta(\omega)$ and obtain:

$$\boxed{J(\omega) = \frac{2\pi}{Z}\sum_{l.m} e^{-\beta E_m} \langle l|A|m\rangle \langle m|B|l\rangle \delta(\omega + E_l - E_m).} \quad (49)$$

At $T = 0$ this expression simplifies further. Let us consider a singly degenerate ground state with energy E_0. Then follows $Z_{T\to 0} = e^{-\beta E_0}$. Similarly, in the sum over m only the ground state(s) contribute and we obtain

$$J_{T=0}(\omega) = 2\pi \sum_{l} \langle 0|B|l\rangle \langle l|A|0\rangle \delta(\omega + E_l - E_0). \quad (50)$$

Notice that in case where $B = A^{\dagger}$ follows $\langle l|A|m\rangle \langle m|B|l\rangle = |\langle l|A|m\rangle|^2 \geq 0$. Thus, the spectral function is real with $J(\omega) \geq 0$. With our above results for the two correlation functions follows immediately

$$\langle A(t) B(0)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\beta\omega} J(\omega) e^{-i\omega t}. \quad (51)$$

We use these results to write for our Green's function

$$\begin{aligned} G^r_{AB}(\omega) &= -i\int_{-\infty}^{\infty} dt e^{i\omega t}\theta(t) (\langle A(t) B\rangle + \eta \langle BA(t)\rangle) \\ &= -i\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(e^{\beta\omega'} + \eta\right) J(\omega') \int_{-\infty}^{\infty} dt e^{i(\omega-\omega')t}\theta(t) \end{aligned} \quad (52)$$

To proceed we need to analyze the integral

$$\begin{aligned} f(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}\theta(t) \\ &= \int_{0}^{\infty} dt e^{i\omega t} \\ &= \lim_{\delta\to 0^+}\int_{0}^{\infty} dt e^{i(\omega+i\delta)t} \\ &= \frac{i}{\omega+i0^+}. \end{aligned} \tag{53}$$

To insert the converging factor seems a bit arbitrary. To check that this is indeed the right thing to do, let us perform the inverse transform

$$F(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{ie^{-i\omega t}}{\omega+i0^+}. \tag{54}$$

We want to evaluate this integral using the residue theorem. For $t>0$ we can close the contour in the lower half plane, i.e. the contour encircles the pole at $\omega=-i0^+$. The residue of the pole is 1 (because of the sense of orientation of the contour). For $t<0$ we have to close the contour in the upper half plane. As there is no pole in this half plane, the integral vanishes. Thus, we obtain $F(t)=\theta(t)$ as expected. This analysis also reveals that causality, expressed in terms of the θ-function, implies that we should consider frequencies $\omega+i0^+$ with a small positive imaginary part.

It follows for the Green's function

$$G^r_{AB}(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\left(e^{\beta\omega'}+\eta\right)J(\omega')}{\omega-\omega'+i0^+}. \tag{55}$$

Inserting the spectral function yields the so called Lehmann representation:

$$G^r_{AB}(\omega) = \frac{1}{Z}\sum_{l.m}\frac{\left(e^{-\beta E_l}+\eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{\omega+E_l-E_m+i0^+} \tag{56}$$

which reveals that a retarded Green's function, once considered with complex frequency argument ω, is analytic everywhere, except infinitesimally below the real axis. In fact one can consider the function

$$\boxed{G_{AB}(z) = \frac{1}{Z}\sum_{l.m}\frac{\left(e^{-\beta E_l}+\eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{z+E_l-E_m},} \tag{57}$$

with complex argument z and the retarded function is given by

$$G^r_{AB}(\omega) = G_{AB}\left(\omega+i0^+\right). \tag{58}$$

Repeating our analysis for the advanced Green's function yields

$$G^a_{AB}(\omega) = G_{AB}\left(\omega - i0^+\right). \tag{59}$$

If one keeps in mind that under the integral holds

$$\frac{1}{\omega + i0^+} = \mathcal{P}\frac{1}{\omega} - i\pi\delta(\omega), \tag{60}$$

where the principle value of $\frac{1}{\omega}$ is meant in the first term, we obtain:

$$\begin{aligned} G^r_{AB}(\omega) - G^a_{AB}(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\left(e^{\beta\omega'} + \eta\right) J(\omega') \\ &\times \left(\frac{1}{\omega - \omega' + i0^+} - \frac{1}{\omega - \omega' - i0^+}\right) \\ &= -i\left(e^{\beta\omega} + \eta\right) J(\omega) \end{aligned} \tag{61}$$

For $B = A^\dagger$, where the product of the two matrix elements is real, the advanced function is the complex conjugate of the retarded function. Considering once again the frequent situation where $B = A^\dagger$ it holds

$$J(\omega) = -2n_\eta(\omega)\,\mathrm{Im}G^r_{AA^\dagger}(\omega), \tag{62}$$

where

$$n_\eta(\omega) = \frac{1}{e^{\beta\omega} + \eta} \tag{63}$$

is, depending on whether we use the commutator or anti-commutator, the Bose or Fermi function, respectively.

In case of $B = A^\dagger$ we also obtain the famous Kramers-Kronig relation

$$\boxed{G^r_{AA^\dagger}(\omega) = -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}G^r_{AA^\dagger}(\omega')}{\omega - \omega' + i0^+},} \tag{64}$$

which reveals that the information about the Green's function is fully contained in its imaginary part, a result that is a consequence of the constraints brought about by causality. This result also allows for the analysis the function $G(z)$ introduced above and yields

$$G_{AA^\dagger}(z) = -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}G^r_{AA^\dagger}(\omega')}{z - \omega'}. \tag{65}$$

Finally, we can use our results to determine expectation values of correlation functions via

$$\begin{aligned} \langle BA(t)\rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J(\omega)\, e^{-i\omega t} \\ &= -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} n_\eta(\omega) \frac{G^r_{AB}(\omega) - G^a_{AB}(\omega)}{2i} e^{-i\omega t}. \end{aligned} \tag{66}$$

In particular, we can use this expression to determine static expectation values (e.g. in case of $B = A^\dagger$)

$$\left\langle A^\dagger A \right\rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} n_\eta(\omega) \operatorname{Im} G^r_{AA^\dagger}(\omega).$$

The previous results finally allow for a proper interpretation of the equation of motion in frequency representation. We obtain a Green's function with proper boundary conditions if we simply analyze

$$\boxed{\left(\omega + i0^+\right) G^r_{A,B}(\omega) = \left\langle [A,B]_\eta \right\rangle + G^r_{[A,H]_-,B}(\omega).} \tag{67}$$

This immediately guarantees that the back-transform $G^r_{AB}(t)$ obeys the correct boundary condition and vanishes for $t < 0$.

As will be discussed in greater detail, one can also show easily that Green's functions obey certain sum rules, the easiest of which is

$$\int_{-\infty}^{\infty} d\omega G^r_{A,B}(\omega) = -i\pi \left\langle [A,B]_\eta \right\rangle. \tag{68}$$

3 Photoemission and single particle Green's function

Photoemission is a widely used experimental approach to study the electronic properties of solids. It is based on the photoelectric effect that was initially discussed by Einstein. The irradiation of a solid with light gives rise to the emission of electrons. In what follows we discuss this effect within a many-body theory.

Let the many-body wave function prior to the irradiation be the initial state $\left|\Psi^N_m\right\rangle = |m\rangle$ where we explicitly denote that we are considering a system with N particles. Let the final state be given as $\left|\Psi^N_f\right\rangle$. The corresponding energies are E^N_m and E^N_f. The transition probability per unit time between the two states is then given by Fermi's golden rule

$$w = 2\pi \left|\left\langle \Psi^N_f \left| V \right| \Psi^N_m \right\rangle\right|^2 \delta\left(\omega - E^N_f + E^N_m\right). \tag{69}$$

The perturbation caused by the irradiation is of the form

$$V = -\mathbf{P} \cdot \mathbf{E}_0. \tag{70}$$

Since the polarization is a single particle operator, i.e. an operator that we can write in the form:

$$V = \sum_{\mathbf{k},\mathbf{k}'\alpha\alpha'} d^{\alpha,\alpha'}_{\mathbf{k},\mathbf{k}'} \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}'\alpha'}, \tag{71}$$

where $\psi^\dagger_{\mathbf{k}\alpha}$ is the creation operator of an electron with momentum $\mathbf{k}$ and spin α and $d^{\alpha,\alpha'}_{\mathbf{k},\mathbf{k}'} = -\left\langle \mathbf{k}\alpha \left| \mathbf{P} \right| \mathbf{k}'\alpha' \right\rangle \cdot \mathbf{E}_0$ refers to the dipole matrix element.

The key assumption of the usual description of photoemission is the so called sudden approximation, where we assume that the excited photoelectron does not couple to the remaining $N-1$ electron system, i.e. it is excited highly above the Fermi energy of the solid and rapidly leaves the system. This is at least consistent with the usual view that photoelectrons originate only from a few top-most layers of the solid near the surface. Thus, we write

$$\left|\Psi_f^N\right\rangle = \psi_{\mathbf{k}_f\beta}^\dagger \left|\Psi_l^{N-1}\right\rangle \tag{72}$$

is the photoelectron added to one of the eigenstates of the $N-1$-particle system. At the same time we assume $\psi_{\mathbf{k}_f\beta}\left|\Psi_m^N\right\rangle = 0$, i.e. the photoelectron state is not mixed into any of the relevant initial states of the system. The emphasis in the last term is on "relevant". At $T=0$, the only relevant initial state is the ground state, and for finite temperatures we are only interested in states with excitation energy $E_m - E_0 \approx k_B T$.

It follows

$$w = 2\pi \left| \left\langle \Psi_l^{N-1} \left| \psi_{\mathbf{k}_f\beta} \sum_{\mathbf{k},\mathbf{k}'\alpha\alpha'} d_{\mathbf{k},\mathbf{k}'}^{\alpha,\alpha'} \psi_{\mathbf{k}\alpha}^\dagger \psi_{\mathbf{k}'\alpha'} \right| \Psi_m^N \right\rangle \right|^2 \delta\left(\omega - E_f^N + E_m^N\right) \tag{73}$$

Since $\psi_{\mathbf{k}_f\beta}\left|\Psi_m^N\right\rangle = 0$, it must hold that $\alpha = \beta$ and $\mathbf{k} = \mathbf{k}_f$, i.e.

It follows

$$w = 2\pi \left| \left\langle \Psi_l^{N-1} \left| \sum_{\mathbf{k},\alpha} d_{\mathbf{k}_f,\mathbf{k}}^{\beta,\alpha} \psi_{\mathbf{k}\alpha} \right| \Psi_m^N \right\rangle \right|^2 \delta\left(\omega - E_f^N + E_m^N\right) \tag{74}$$

We now sum over all initial states $\left|\Psi_m^N\right\rangle = |m\rangle$ with initial probability $p_m = \frac{1}{Z} e^{-\beta E_m}$ and over all final states $\left|\Psi_l^{N-1}\right\rangle = |l\rangle$, and take into account that the final energy $E_f^N = \epsilon_{\mathbf{k}_f} + E_l^{N-1}$ is the sum photoelectron energy $\epsilon_{\mathbf{k}_f}$ and of the energy E_l^{N-1} of the remaining $N-1$ many body state. It follows for the intensity

$$I_{\mathbf{k}_f\beta}(\omega) = \frac{2\pi}{Z} \sum_{lm} e^{-\beta E_m} \left| \left\langle l \left| \sum_{\mathbf{k},\alpha} d_{\mathbf{k}_f,\mathbf{k}}^{\beta,\alpha} \psi_{\mathbf{k}\alpha} \right| m \right\rangle \right|^2 \delta\left(\omega - \epsilon_{\mathbf{k}_f} - E_l + E_m\right) \tag{75}$$

We recognize this result as the spectral function of a retarded Green's function with

$$\begin{aligned} A &= \sum_{\mathbf{k},\alpha} d_{\mathbf{k}_f,\mathbf{k}}^{\beta,\alpha} \psi_{\mathbf{k}\alpha} \\ B &= A^\dagger \end{aligned} \tag{76}$$

If we recall our earlier result that $J(\omega) = -2n_\eta(\omega)\,\mathrm{Im}G_{AA^\dagger}^r(\omega)$ it seems most natural to use for the photoelectron spectrum of occupied states a quantity that

is proportional to the Fermi function $n_+(\omega) = f(\omega) = \left(e^{\beta\omega}+1\right)^{-1}$. Thus we opt for the anticommutator Green's function with $\eta = +1$ and define

$$\boxed{G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = -i\theta(t-t')(t)\left\langle\left[\psi_{\mathbf{k}\alpha}(t),\psi^\dagger_{\mathbf{k}'\alpha'}(0)\right]_+\right\rangle,} \tag{77}$$

such that

$$I_{\mathbf{k}_f\beta}(\omega) = -2f\left(\omega-\epsilon_{\mathbf{k}_f}\right)\sum_{\mathbf{k}\mathbf{k}',\alpha\alpha'} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}}\mathrm{Im}G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}\left(\omega-\epsilon_{\mathbf{k}_f}\right)d^{\alpha',\beta*}_{\mathbf{k}',\mathbf{k}_f}. \tag{78}$$

Thus, except for the dipole matrix elements, the photoemission intensity is determined by the imaginary part of the retarded fermion Green's function.

Let us consider a system of non-interacting fermions with Hamiltonian

$$H = \sum_{\mathbf{k}\alpha}\left(\varepsilon_{\mathbf{k}}-\mu\right)\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}. \tag{79}$$

μ is the chemical potential. In order to determine the equation of motion, for $G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega)$ we need to evaluate the commutator

$$[\psi_{\mathbf{k}\alpha},H]_- = \left(\varepsilon_{\mathbf{k}}-\mu\right)\psi_{\mathbf{k}\alpha} \tag{80}$$

that is particularly easy for non-interacting particles. It follows

$$\left(\omega+i0^+\right)G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \left\langle\left[\psi_{\mathbf{k}\alpha},\psi^\dagger_{\mathbf{k}'\alpha'}\right]_+\right\rangle + \left(\varepsilon_{\mathbf{k}}-\mu\right)G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) \tag{81}$$

Using the usual anti-commutation properties $\left[\psi_{\mathbf{k}\alpha},\psi^\dagger_{\mathbf{k}'\alpha'}\right]_+ = \delta_{\alpha\alpha'}\delta_{\mathbf{k}\mathbf{k}'}$ it follows

$$G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \delta_{\alpha\alpha'}\delta_{\mathbf{k}\mathbf{k}'}G^r_{\mathbf{k}}(\omega), \tag{82}$$

with

$$\boxed{G^r_{\mathbf{k}}(\omega) = \frac{1}{\omega+i0^+-\varepsilon_{\mathbf{k}}+\mu}.} \tag{83}$$

We observe that without the infinitesimal part in the frequency, there would be a pole of the Green's function at the particle energy $\varepsilon_{\mathbf{k}}-\mu$ relative to the chemical potential. We also easily obtain the imaginary part

$$-\frac{1}{\pi}\mathrm{Im}G^r_{\mathbf{k}}(\omega) = \delta\left(\omega-\varepsilon_{\mathbf{k}}+\mu\right). \tag{84}$$

A sharp peak in the imaginary part is a signature that the system is characterized by a particle, a behavior that will be used later on as well, when we analyze interacting electrons. We could for example use this result to obtain the particle number

$$\begin{aligned}\left\langle\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}\right\rangle &= -\int_{-\infty}^{\infty}\frac{d\omega}{\pi}n_+(\omega)\,\mathrm{Im}G^r_{\mathbf{k}}(\omega).\\ &= \int_{-\infty}^{\infty}d\omega f(\omega)\,\delta\left(\omega-\varepsilon_{\mathbf{k}}+\mu\right)\\ &= f\left(\varepsilon_{\mathbf{k}}-\mu\right).\end{aligned} \tag{85}$$

Thus, as expected we finD that the occupation number of free fermions is given by the Fermi function. It turns out that knowledge of the retarded Green's function is sufficient to determine all thermodynamic properties of a many body system of electrons. We will prove this result below for an interacting electron system.

For the photoemission spectrum follows finally:

$$I_{\mathbf{k}_f\beta}(\omega) = \frac{2}{\pi} f\left(\omega - \epsilon_{\mathbf{k}_f}\right) \sum_{\mathbf{k},\alpha} \left| d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \right|^2 \delta\left(\omega - \epsilon_{\mathbf{k}_f} - \varepsilon_{\mathbf{k}\alpha} + \mu\right). \tag{86}$$

The experiments then probes the occupied states of a solid and can be used to determine the energy-momentum relation. Often, one assumes momentum conservation, at least for the components of the momentum parallel to the surface and finds

$$I_{\mathbf{k}_f\beta}(\omega) \propto f\left(\omega - \epsilon_{\mathbf{k}_f}\right) \delta\left(\omega - \epsilon_{\mathbf{k}_f} - \varepsilon_{\mathbf{k}_f} + \mu\right).$$

4 Green's function for free particles

In case of non-interacting fermions and bosons, one can obtain a closed expression for the Green's functions. To this end we consider a Hamiltonian of the form

$$H = \sum_{ij} h_{ij} c_i^\dagger c_j, \tag{87}$$

where $c_i^\dagger$ and c_j are creation and annihilation operators of fermions or bosons in states with single particle quantum numbers i and j, respectively. Those quantum numbers could be momentum, lattice sites in a solid, spin, or a combination of spin and momentum, depending on the problem at hand. The fact that we confine ourselves to bilinear forms (only two operators) reflects that we consider noninteracting particles. We do, however, not assume that h_{ij} is a diagonal matrix, whose diagonal elements are then the single particle eigenstates. In case of bosons (fermions) we use the well known commutator (anticommutator) relations

$$\begin{aligned} \left[c_i, c_j^\dagger\right]_\eta &= \delta_{ij}, \\ \left[c_i, c_j\right]_\eta &= \left[c_i^\dagger, c_j^\dagger\right]_\eta = 0, \end{aligned} \tag{88}$$

with $\eta = -1$ ($\eta = -1$).

We first determine the so called single particle Green's functions[2]

$$G^r_{ij}(t) = -i\theta(t) \left\langle \left[c_i(t), c_j^\dagger\right]_\eta \right\rangle. \tag{89}$$

[2]To simplify our notation we use $G^r_{ij}(t)$ instead of $G^r_{c_i c_j^\dagger}(t)$.

For the analysis of the equation of motion we have to analyze the commutator

$$[c_i, H]_- = \sum_{lm} h_{lm} \left[c_i, c_l^\dagger c_m\right]_- \tag{90}$$

It holds

$$\begin{aligned}\left[c_i, c_l^\dagger c_m\right]_- &= c_i c_l^\dagger c_m - c_l^\dagger c_m c_i \\ &= -\eta c_l^\dagger c_i c_m + \delta_{il} c_m - c_l^\dagger c_m c_i \\ &= \eta^2 c_l^\dagger c_m c_i + \delta_{il} c_m - c_l^\dagger c_m c_i \\ &= \delta_{il} c_m, \end{aligned} \tag{91}$$

which yields

$$[c_i, H]_- = \sum_m h_{im} c_m, \tag{92}$$

regardless of whether we consider bosons or fermions.

For our equation of motion follows then

$$\left(\omega + i0^+\right) G_{ij}^r(\omega) = \delta_{ij} + \sum_m h_{im} G_{mj}^r(\omega). \tag{93}$$

We see that the equation of motion closes in the sense that only Green's functions of the type defined in Eq.(89) are needed. It is also natural to introduce a matrix $\hat{G}(\omega)$ with matrix elements $G_{ij}(\omega)$ and similarly $\hat{h}$ for the matrix representation of the Hamiltonian with elements h_{ij}. Then follows[3]

$$\omega \hat{G}(\omega) = \hat{1} + \hat{h} \cdot \hat{G}(\omega), \tag{94}$$

or

$$\left(\omega - \hat{h}\right) \hat{G}(\omega) = \hat{1}. \tag{95}$$

This leads to

$$\boxed{\hat{G}(\omega) = \left(\omega - \hat{h}\right)^{-1}.} \tag{96}$$

Thus, in order to determine the Green's function of a non-interacting gas of fermions or bosons, it is sufficient to diagonalize a matrix in the space of single-particle quantum numbers. This can be a non-trivial task on its own, e.g. for disordered systems where h_{ij} are realizations subject to a certain disorder distribution function. In systems with translation invariance the single-particle eigenstates of the Hamiltonian are plane-waves with eigenvalues $\varepsilon_{\mathbf{k}}$ that depend on the specific dispersion relation of the problem (e.g. $\varepsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu$ for solutions of the Schrödinger equation). This immediately determines the eigenvalues of the Green's function

$$G_{\mathbf{k}}^r(\omega) = \frac{1}{\omega + i0^+ - \varepsilon_{\mathbf{k}}}, \tag{97}$$

[3]We drop the index r for the retarded function with the understanding that it follows via $\omega \to \omega + i0^+$.

a result that we obtained earlier already for free fermions.

In a solid, with discrete translation invariance, the eigenstates are the bands $\varepsilon_{\mathbf{k},n}$ where the momenta are from the first Brillouin zone and we find accordingly $G^r_{\mathbf{k},n}(\omega) = \frac{1}{\omega + i0^+ - \varepsilon_{\mathbf{k},n}}$.

4.1 Perturbation theory and Dyson equation

An important application of our matrix formalism can be made for systems where we can write

$$h_{ij} = \varepsilon_i^0 \delta_{ij} + V_{ij}, \tag{98}$$

i.e. we are in the eigenbasis of a bare Hamiltonian $\hat{h}^0$ with eigenvalues ε_i^0, while an additional perturbation is off-diagonal.

This suggests to write

$$\begin{aligned} \hat{G}^{-1} &= \omega - \hat{h}^0 - \hat{V} \\ &= \hat{G_0}^{-1} - \hat{V}, \end{aligned} \tag{99}$$

where $\hat{G_0}^{-1} = \omega - \hat{h}^0$ is the Green's function of the bare Hamiltonian, i.e. the bare Green's function. It is a fully diagonal matrix, i.e. we have

$$G_{0,ij}(\omega) = \frac{\delta_{ij}}{\omega - \varepsilon_i^0}. \tag{100}$$

Eq.(99) is called the Dyson equation for single particle systems, i.e. for systems without interactions. We can multiply Eq.(99) from the left with $\hat{G}_0$ and from the right with $\hat{G}$ and obtain

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}. \tag{101}$$

A perturbation theory in $\hat{V}$ can now be generated by iterating this equation repeatedly

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 \hat{V} \hat{G}_0 \cdots . \tag{102}$$

4.2 Higher order correlation functions

The knowledge of $G^r_{ij}(\omega)$ yields immediate information about expectation values of the form $\left\langle c_i^\dagger c_j \right\rangle$. Suppose we want to know something about a more complicated expectation value, such as $\left\langle c_j^\dagger c_k^\dagger c_l c_i \right\rangle$, we can equally find closed expressions for the corresponding Green's functions. To this end we analyze $G_{AB} = G_{i,jkl}$ with $A = c_i$ and $B = c_j^\dagger c_k^\dagger c_l$.

The equation of motion follows immediately, as the commutator with the Hamiltonian is the same

$$\omega G_{i,jkl}(\omega) = \left\langle \left[c_i, c_j^\dagger c_k^\dagger c_l \right]_\eta \right\rangle + \sum_m h_{im} G_{m,jkl}(\omega). \tag{103}$$

The remaining commutator or anticommutator is easily calculated as:

$$\begin{aligned}\left[c_i, c_j^\dagger c_k^\dagger c_l\right]_\eta &= c_i c_j^\dagger c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= -\eta c_j^\dagger c_i c_k^\dagger c_l + \delta_{ij} c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= c_j^\dagger c_k^\dagger c_i c_l - \eta \delta_{ik} c_j^\dagger c_l + \delta_{ij} c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= \delta_{ij} c_k^\dagger c_l - \eta \delta_{ik} c_j^\dagger c_l. \end{aligned} \tag{104}$$

This yields for the equation of motion the result:

$$\omega G_{i,jkl}(\omega) = \delta_{ij} \left\langle c_k^\dagger c_l \right\rangle - \eta \delta_{ik} \left\langle c_j^\dagger c_l \right\rangle + \sum_m h_{im} G_{m,jkl}(\omega). \tag{105}$$

If we use our earlier result for the single particle Green's function we can write this as

$$\sum_m \left(\hat{G}(\omega)^{-1}\right)_{im} G_{m,jkl}(\omega) = \delta_{ij} \left\langle c_k^\dagger c_l \right\rangle - \eta \delta_{ik} \left\langle c_j^\dagger c_l \right\rangle, \tag{106}$$

which can be multiplied by $G_{si}(\omega)$ and summed over i. It follows

$$G_{i,jkl}(\omega) = G_{ij}(\omega) \left\langle c_k^\dagger c_l \right\rangle - \eta G_{ik}(\omega) \left\langle c_j^\dagger c_l \right\rangle \tag{107}$$

These functions can now be used to determine the expectation values $\left\langle c_j^\dagger c_k^\dagger c_l c_i \right\rangle$ and it follows

$$\boxed{\left\langle c_j^\dagger c_k^\dagger c_l c_i \right\rangle = \left\langle c_j^\dagger c_i \right\rangle \left\langle c_k^\dagger c_l \right\rangle - \eta \left\langle c_j^\dagger c_l \right\rangle \left\langle c_k^\dagger c_i \right\rangle.} \tag{108}$$

Thus, we are able to express a more complicated expectation value in terms of simpler ones, a procedure that is correct for arbitrarily complex operators. In fact the last result is the simplest case of a more general statement that goes under the name of Wick theorem.

5 Screening of the Coulomb interaction

In what follows we want to investigate a first non-trivial problem in many-body theory, the screening of the long-range electron-electron Coulomb interaction. Before we go into the details we summarize our conventions for the Fourier transformation between real space and momentum space. We consider always a large but finite volume V together with some sort of boundary conditions that imply discrete momentum values $\mathbf{k}$, where two neighboring points are separated by $\Delta k = \frac{2\pi}{V^{1/d}}$. For an arbitrary function $f(\mathbf{r})$ we then use the convention

$$f_{\mathbf{k}} = \int d^d r f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{109}$$

with back transform

$$f(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} f_{\mathbf{k}}. \tag{110}$$

Here we used that $\int d^d r e^{i\mathbf{k}\cdot\mathbf{r}} = V\delta_{\mathbf{k},\mathbf{0}}$ and $\frac{1}{V}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} = \delta(\mathbf{r})$. Note, that those are not the only conventions used in the literature. Frequently one finds a prefactor $1/\sqrt{V}$ in front of both, the sum and the integral in the above definitions. The justification of our choice is that it allows without problems to take the limit $V \to \infty$, where $\frac{1}{V}\sum_{\mathbf{k}} \cdots \to \int d^d k \cdots$ and $V\delta_{\mathbf{k},\mathbf{0}} \to \delta(\mathbf{k})$. With this convention follows for example for fermionic operators:

$$\psi_{\mathbf{k}\alpha} = \int d^d r \psi_\alpha(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{111}$$

that $[\psi_\alpha(\mathbf{r}), \psi_\beta(\mathbf{r}')]_+ = \delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')$ implies

$$\left[\psi_{\mathbf{k}\alpha}, \psi^\dagger_{\mathbf{k}'\beta}\right]_+ = \delta_{\alpha\beta} V \delta_{\mathbf{k},\mathbf{k}'}. \tag{112}$$

For the Hamiltonian of a free electron system

$$H = \int d^d r \sum_\alpha \psi^\dagger_\alpha(\mathbf{r}) \varepsilon(-i\nabla) \psi_\alpha(\mathbf{r}) \tag{113}$$

follows accordingly

$$H_0 = \frac{1}{V}\sum_{\mathbf{k}\alpha} \varepsilon(\mathbf{k}) \psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}. \tag{114}$$

Another relevant quantity to be Fourier transformed is the density

$$\rho(\mathbf{r}) = \sum_\alpha \psi^\dagger_\alpha(\mathbf{r}) \psi_a(\mathbf{r}). \tag{115}$$

It follows

$$\begin{aligned}
\rho_{\mathbf{q}} &= \sum_\alpha \int d^d r \psi^\dagger_\alpha(\mathbf{r}) \psi_a(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \\
&= \frac{1}{V^2}\sum_{\alpha\mathbf{k}\mathbf{k}'} \int d^d r e^{-i\mathbf{r}\cdot(\mathbf{q}+\mathbf{k}-\mathbf{k}')} \psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}'\alpha} \\
&= \frac{1}{V}\sum_{\alpha\mathbf{k}} \psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha}.
\end{aligned} \tag{116}$$

Another famous example for a Fourier transformation is for the Coulomb interaction

$$\int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{1}{|\mathbf{r}|} = \frac{4\pi}{q^2}. \tag{117}$$

5.1 Density response and dielectric function

Let us consider a system of electrons exposed to the external electric potential as perturbation

$$W(t) = \int d^3 r \rho^{\rm el}(\mathbf{r}) \varphi^{\rm ext}(\mathbf{r}, t), \tag{118}$$

where the external time and space dependent potential $\varphi^{\rm ext}(\mathbf{r}, t)$ couples to the electron charge density

$$\rho^{\rm el}(\mathbf{r}) = -e \sum_{\alpha} \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_a(\mathbf{r}). \tag{119}$$

Here we used that electrons are negatively charged, i.e. we work with $e > 0$. Below it will be more convenient to work with the particle density introduced in Eq.(115), i.e. $\rho^{\rm el}(\mathbf{r}) = -e\rho(\mathbf{r})$.

If we are interested in the induced electron charges we can use our linear response formalism:

$$\begin{aligned} \left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle_t &= \left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle + \int_{-\infty}^{\infty} dt' \left\langle\!\left\langle \rho^{\rm el}(\mathbf{r}, t); W(t') \right\rangle\!\right\rangle. \\ &= \left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle + e^2 \int_{-\infty}^{\infty} dt' d^3 r' \left\langle\!\left\langle \rho(\mathbf{r}, t); \rho(\mathbf{r}', t') \right\rangle\!\right\rangle \varphi^{\rm ext}(\mathbf{r}', t') \end{aligned} \tag{120}$$

Thus, the dynamics of induced charges is determined by the retarded density-density Green's function

$$\begin{aligned} \chi(\mathbf{r}, \mathbf{r}', t) &= -\left\langle\!\left\langle \rho(\mathbf{r}, t); \rho(\mathbf{r}', 0) \right\rangle\!\right\rangle \\ &= i\theta(t) \left\langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', 0)]_- \right\rangle. \end{aligned} \tag{121}$$

If we assume that our system is translation invariant, $\chi(\mathbf{r}, \mathbf{r}', t)$ becomes a function of $\mathbf{r} - \mathbf{r}'$ only. In addition the equilibrium density $\left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle = \rho_0^{\rm el}$ becomes independent on $\mathbf{r}$. It follows

$$\left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle_t = \rho_0^{\rm el} - e^2 \int_{-\infty}^{\infty} dt' d^3 r' \chi(\mathbf{r} - \mathbf{r}', t - t') \varphi^{\rm ext}(\mathbf{r}', t'). \tag{122}$$

A solid is electrically neutral. The electron charges are then compensated by the positive charges of the ions. A popular model to describe the ionic charges is the so-called jellium model. Here one assumes a uniform positive background charge $\rho_{\rm ion}$ of the ions that is, on the time scale of the electrons, fixed. Charge neutrality implies that $\rho^{\rm ion} + \rho_0^{\rm el} = 0$. The total induced charge

$$\rho^{\rm ind}(\mathbf{r}, t) = \left\langle \rho^{\rm el}(\mathbf{r}) \right\rangle_t + \rho^{\rm ion} \tag{123}$$

in our solid is then related to the external potential via

$$\rho^{\rm ind}(\mathbf{r}, t) = -e^2 \int_{-\infty}^{\infty} dt' d^3 r' \chi(\mathbf{r} - \mathbf{r}', t - t') \varphi^{\rm ext}(\mathbf{r}', t'). \tag{124}$$

As required by charge neutrality, the total induced charge vanishes without the external potential.

The above relation between $\rho^{\text{ind}}(\mathbf{r},t)$ and $\varphi^{\text{ext}}(\mathbf{r}',t')$ is a convolution with respect to the temporal and spatial arguments. This can be simplified by going to momentum and frequency space according to:

$$F(\mathbf{q},\omega) = \int d^3r \int dt e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega t)} F(\mathbf{r},t). \tag{125}$$

It follows:

$$\rho^{\text{ind}}(\mathbf{q},\omega) = -e^2 \chi(\mathbf{q},\omega)\,\varphi^{\text{ext}}(\mathbf{q},\omega). \tag{126}$$

The perturbation $W(t)$ can alternatively be written as

$$W(t) = \int d^3r d^3r' \frac{\rho^{\text{el}}(\mathbf{r})\,\rho^{\text{ext}}(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}, \tag{127}$$

where the external charges are simply the sources of the external potential

$$\varphi^{\text{ext}}(\mathbf{r},t) = \int d^3r' \frac{\rho^{\text{ext}}(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}, \tag{128}$$

i.e. it is the solution of the Poisson equation with external charges as sources:

$$\nabla^2 \varphi^{\text{ext}}(\mathbf{r},t) = -4\pi\rho^{\text{ext}}(\mathbf{r},t). \tag{129}$$

This formulation allows to make contact with the usual formulation of the electrodynamics of continua where the sources of the electric field are all charges, external and internal ones

$$\nabla\cdot\mathbf{E} = 4\pi\left(\rho^{\text{ind}} + \rho^{\text{ext}}\right), \tag{130}$$

while the displacement field is introduced as the field that has only the external charges as sources

$$\nabla\cdot\mathbf{D} = 4\pi\rho^{\text{ext}}. \tag{131}$$

The linearized relation between the two fields is

$$\mathbf{D}(\mathbf{r},t) = \int_{-\infty}^{\infty} dt' d^3r' \varepsilon(\mathbf{r}-\mathbf{r}',t-t')\,\mathbf{E}(\mathbf{r}',t'). \tag{132}$$

with dielectric function ε. Once again we assumed translation invariance and the homogeneity of time. We then obtain after Fourier transformation

$$\mathbf{D}(\mathbf{q},\omega) = \varepsilon(\mathbf{q},\omega)\,\mathbf{E}(\mathbf{q},\omega). \tag{133}$$

The above equations for the electric field and the displacement field become in Fourier space

$$\begin{aligned} i\mathbf{q}\cdot\mathbf{E}(\mathbf{q},\omega) &= 4\pi\left(\rho^{\text{ind}}(\mathbf{q},\omega) + \rho^{\text{ext}}(\mathbf{q},\omega)\right) \\ i\mathbf{q}\cdot\mathbf{D}(\mathbf{q},\omega) &= 4\pi\rho^{\text{ext}}(\mathbf{q},\omega). \end{aligned} \tag{134}$$

Expressing $\mathbf{D}(\mathbf{q},\omega)$ in the second equation by $\varepsilon(\mathbf{q},\omega)\,\mathbf{E}(\mathbf{q},\omega)$ allows us to write

$$\rho^{\mathrm{ind}}(\mathbf{q},\omega) = \left(\frac{1}{\varepsilon(\mathbf{q},\omega)} - 1\right)\rho^{\mathrm{ext}}(\mathbf{q},\omega). \tag{135}$$

Thus, the dielectric function relates the external sources to the induced charges. On the other hand, Eq.(126) established a relation between the induced charges and the external potential. As discussed, the external charge density and the external potential are related by the Poisson equation, which becomes in Fourier space

$$q^2\varphi^{\mathrm{ext}}(\mathbf{q},\omega) = 4\pi\rho^{\mathrm{ext}}(\mathbf{q},\omega). \tag{136}$$

With this relation we obtain

$$\rho^{\mathrm{ind}}(\mathbf{q},\omega) = \left(\frac{1}{\varepsilon(\mathbf{q},\omega)} - 1\right)\frac{4\pi}{q^2}\varphi^{\mathrm{ext}}(\mathbf{q},\omega). \tag{137}$$

Comparing this with Eq.(126) yields

$$\boxed{\frac{1}{\varepsilon(\mathbf{q},\omega)} = 1 - \frac{4\pi e^2}{q^2}\chi(\mathbf{q},\omega).} \tag{138}$$

Thus, the retarded density-density Green's function $\chi(\mathbf{q},\omega)$ determines the dielectric function. An interesting implication of this result is that the dielectric function diverges for for $q \to 0$ if $\chi(\mathbf{q},\omega)$ does not vanish at least as q^2. We will see by explicitly analyzing the density-density response function that this is indeed the case and leads to a qualitative change in the space dependence of the effective Coulomb interaction, i.e. the screening of the Coulomb interaction. More specifically, Eq.(138) allows to study the effective potential

$$\varphi(\mathbf{q},\omega) = \frac{1}{\varepsilon(\mathbf{q},\omega)}\varphi^{\mathrm{ext}}(\mathbf{q},\omega) \tag{139}$$

that has as sources the total charge, i.e.

$$\nabla^2\varphi(\mathbf{r},t) = -4\pi\left(\rho^{\mathrm{ind}}(\mathbf{r},t) + \rho^{\mathrm{ext}}(\mathbf{r},t)\right).$$

If we consider for example a single point-charge as source, we have $\rho^{\mathrm{ext}}(\mathbf{r},t) = e\delta(\mathbf{r})$, which yields $\rho^{\mathrm{ext}}(\mathbf{q},\omega) = 2\pi e\delta(\omega)$ and finally $\varphi^{\mathrm{ext}}(\mathbf{q},\omega) = 2\pi e\delta(\omega)\frac{4\pi}{q^2}$. This yields after back Fourier transformation with regards to frequency a time-independent potential:

$$\varphi(\mathbf{q},t) = \frac{4\pi e}{\varepsilon(\mathbf{q},\omega=0)\,q^2}. \tag{140}$$

Another interesting scenario occurs when

$$\varepsilon(\mathbf{q},\omega) \doteq 0. \tag{141}$$

If there are momenta and frequencies where this obeyed, an infinitesimal external charge or potential will induce a large charge response. Below we will see that this gives rise to plasma oscillations of the electron system.

5.2 Density response of non-interacting electrons

A central quantity in our analysis of the Coulomb interaction is the retarded density-density Green's function (times -1):

$$\chi(\mathbf{r},t) = i\theta(t)\left\langle\left[\rho(\mathbf{r},t),\rho(\mathbf{0},0)\right]_-\right\rangle, \tag{142}$$

with electron density $\rho(\mathbf{r},t) = \sum_\alpha \psi_\alpha^\dagger(\mathbf{r},t)\,\psi_a(\mathbf{r},t)$. The Fourier transform of this function with regards to the spatial degrees of freedom is

$$\begin{aligned}\chi_{\mathbf{q}}(t) &= i\theta(t)\frac{1}{V}\sum_{\mathbf{q}'}\left\langle\left[\rho_{\mathbf{q}}(t),\rho_{-\mathbf{q}'}(0)\right]_-\right\rangle \\ &= -\frac{1}{V}\sum_{\mathbf{q}'}\langle\langle\rho_{\mathbf{q}}(t);\rho_{-\mathbf{q}'}\rangle\rangle\end{aligned}$$

In what follows we first determine this function for a system of noninteracting electrons with Hamiltonian

$$H = \frac{1}{V}\sum_{\mathbf{k}\alpha}\varepsilon_{\mathbf{k}}\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}\alpha}. \tag{143}$$

Recall that our result for the single particle Green's function

$$G_{\mathbf{k},\mathbf{k}'}(t) = -i\theta(t)\left\langle\left[\psi_{\mathbf{k}\alpha}(t),\psi_{\mathbf{k}'\alpha}^\dagger\right]_+\right\rangle \tag{144}$$

is

$$G_{\mathbf{k},\mathbf{k}'}(\omega) = \frac{V\delta_{\mathbf{k},\mathbf{k}'}}{\omega-\varepsilon(\mathbf{k})}, \tag{145}$$

as follows from the equation of motion.

To determine the density-density Green's function it is convenient to analyze the general two-particle Green's function

$$\left\langle\left\langle\psi_{\mathbf{k}\alpha}^\dagger(t)\,\psi_{\mathbf{k}+\mathbf{q}\alpha}(t);\psi_{\mathbf{k}'\beta}^\dagger\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle. \tag{146}$$

The equation of motion requires the analysis of the commutator

$$\left[\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}+\mathbf{q}\alpha},\psi_{\mathbf{k}'\beta}^\dagger\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right]_- = V\delta_{\alpha\beta}\left(\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}'-\mathbf{q}'\beta}-\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}'}\psi_{\mathbf{k}'\beta}^\dagger\psi_{\mathbf{k}+\mathbf{q}\alpha}\right).$$

This yields with

$$\left\langle\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}'\alpha}\right\rangle = V\delta_{\mathbf{k}',\mathbf{k}}f(\varepsilon_{\mathbf{k}}) \tag{147}$$

and Fermi function $f(\varepsilon)$ the result:

$$\begin{aligned}\omega\left\langle\left\langle\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}+\mathbf{q}\alpha};\psi_{\mathbf{k}'\beta}^\dagger\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle &= V^2\delta_{\alpha\beta}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta_{\mathbf{q},\mathbf{q}'}\left(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}\right) \\ &+ \left(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}\right)\left\langle\left\langle\psi_{\mathbf{k}\alpha}^\dagger\psi_{\mathbf{k}+\mathbf{q}\alpha};\psi_{\mathbf{k}'\beta}^\dagger\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle.\end{aligned}$$

This can be solved and leads to

$$\left\langle\left\langle \psi^{\dagger}_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha};\psi^{\dagger}_{\mathbf{k}'\beta}\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle = \frac{V^2\delta_{\alpha\beta}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta_{\mathbf{q},\mathbf{q}'}\left(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}\right)}{\omega-\varepsilon_{\mathbf{k}+\mathbf{q}}+\varepsilon_{\mathbf{k}}}.$$

Because of $\delta_{\mathbf{q},\mathbf{q}'}$ follows in particular

$$\chi_{\mathbf{q}}\left(\omega\right) = -\frac{1}{V}\left\langle\left\langle \rho_{\mathbf{q}};\rho_{-\mathbf{q}}\right\rangle\right\rangle. \tag{148}$$

Inserting the result for the two-particle Green's function gives after a few steps

$$\boxed{\chi^{r}_{\mathbf{q}}\left(\omega\right) = \frac{1}{V}\sum_{\alpha\mathbf{k}}\frac{f_{\mathbf{k}+\mathbf{q}}-f_{\mathbf{k}}}{\omega+i0^{+}-\varepsilon_{\mathbf{k}+\mathbf{q}}+\varepsilon_{\mathbf{k}}},} \tag{149}$$

where we returned to the case of the retarded function.

5.3 Evaluation of the Lindhard function

As we will see next, the density-density response function Eq.(149) can be written in the form

$$\chi^{r}_{\mathbf{q}}\left(\omega\right) = \rho_F L\left(\frac{q}{2k_F},\frac{\omega}{4\varepsilon_F}\right) \tag{150}$$

with so called Lindhard function $L\left(Q,\nu\right)$ that is dimensionless and only depends on dimensionless arguments. We observe that the natural length scale is the inverse Fermi wave vector $1/k_F$ and the characteristic energy scale is the Fermi energy. The natural scale for the density response itself is, as we already noticed above, the density of states at the Fermi level.

Let us evaluate $\chi^{r}_{\mathbf{q}}\left(\omega\right)$ of Eq.(149). First, we notice the general property

$$\chi^{r}_{\mathbf{q}=\mathbf{0}}\left(\omega\neq 0\right) = 0. \tag{151}$$

On the other hand we can take the static limit $\omega = 0$. For small $\mathbf{q}$ follows that

$$\begin{aligned}\chi^{r}_{\mathbf{q}\to\mathbf{0}}\left(\omega=0\right) &= -\frac{1}{V}\sum_{\alpha\mathbf{k}}\frac{\partial f_{\mathbf{k}}}{\partial\varepsilon_{\mathbf{k}}} \\ &= -2\int\frac{d^dk}{\left(2\pi\right)^d}\frac{\partial f_{\mathbf{k}}}{\partial\varepsilon_{\mathbf{k}}} = -\int d\varepsilon\rho\left(\varepsilon\right)\frac{\partial f\left(\varepsilon\right)}{\partial\varepsilon}.\end{aligned} \tag{152}$$

At $T=0$ holds $-\frac{\partial f(\varepsilon)}{\partial\varepsilon} = \delta\left(\varepsilon-\varepsilon_F\right)$ with Fermi energy ε_F. Thus, we find

$$\chi^{r}_{\mathbf{q}\to\mathbf{0}}\left(\omega=0\right) = \rho_F \tag{153}$$

with density of states at the Fermi energy ρ_F. We observe that the limits $\mathbf{q}\to\mathbf{0}$ and $\omega\to 0$ do not commute for a system with finite density of states at the Fermi surface.

For the imaginary part holds

$$\mathrm{Im}\chi^r_{\mathbf{q}}(\omega) = -2\pi \int \frac{d^3k}{(2\pi)^3} \left(f_{\mathbf{k+q}} - f_{\mathbf{k}}\right) \delta\left(\omega - \varepsilon_{\mathbf{k+q}} + \varepsilon_{\mathbf{k}}\right). \tag{154}$$

If one analyses $\mathrm{Im}\chi^r_{\mathbf{q}}(-\omega)$, substitutes $\mathbf{k} = -\mathbf{k}' - \mathbf{q}$ and uses $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$, it follows that

$$\mathrm{Im}\chi^r_{\mathbf{q}}(\omega) = -\mathrm{Im}\chi^r_{\mathbf{q}}(-\omega). \tag{155}$$

Thus, it is sufficient to analyze $\omega \geq 0$.

Since $\langle\langle \rho_{\mathbf{q}}; \rho_{-\mathbf{q}} \rangle\rangle$ involves two operators with $\rho_{-\mathbf{q}} = \rho^\dagger_{\mathbf{q}}$, we can use the Kramers-Kronig transformation to determine the real part:

$$\begin{aligned} \mathrm{Re}\chi^r_{\mathbf{q}}(\omega) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\epsilon \frac{\mathrm{Im}\chi^r_{\mathbf{q}}(\epsilon)}{\omega - \epsilon} \\ &= -\frac{2}{\pi}\mathcal{P}\int_{0}^{\infty} d\epsilon \frac{\epsilon \mathrm{Im}\chi^r_{\mathbf{q}}(\epsilon)}{\omega^2 - \epsilon^2}, \end{aligned} \tag{156}$$

where we used in the last step that the imaginary part is an odd function. As the real part only depends on ω^2, it follows immediately that it is an even function of frequency:

$$\mathrm{Re}\chi^r_{\mathbf{q}}(\omega) = \mathrm{Re}\chi^r_{\mathbf{q}}(-\omega). \tag{157}$$

For a parabolic dispersion $\varepsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu$ and at $T = 0$ one can obtain a closed expression for the Lindhard function and this for $\chi^r_{\mathbf{q}}(\omega)$. We first write our expression as

$$\chi^r_{\mathbf{q}}(\omega) = \frac{1}{V}\sum_{\alpha\mathbf{k}} \left(\frac{f_{\mathbf{k}}}{\omega + i0^+ - \varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k-q}}} - \frac{f_{\mathbf{k}}}{\omega + i0^+ + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k+q}}} \right), \tag{158}$$

where we substituted $\mathbf{k} + \mathbf{q} \to \mathbf{k}$ in the first of the two terms of Eq.(149). We next use

$$\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}\pm\mathbf{q}} = -\frac{q^2}{2m} \mp \frac{kq\mu}{m} \tag{159}$$

with $\mu = \cos\theta$ and obtain:

$$\begin{aligned} \mathrm{Re}\chi^r_{\mathbf{q}}(\omega) &= 2\int_0^{k_F} \frac{k^2 dk}{(2\pi)^2} \int_{-1}^{1} d\mu \left(\frac{1}{\omega + \frac{q^2}{2m} - \frac{kq\mu}{m}} - \frac{1}{\omega - \frac{q^2}{2m} - \frac{kq\mu}{m}} \right) \\ &= \frac{2m}{q}\int_0^{k_F} \frac{kdk}{(2\pi)^2} \int_{-1}^{1} d\mu \left(\frac{1}{\frac{m\omega}{kq} + \frac{q}{2k} - \mu} - \frac{1}{\frac{m\omega}{kq} - \frac{q}{2k} - \mu} \right) \end{aligned}$$

We introduce dimensionless variables used in Eq.(150):

$$\begin{aligned} \nu &= \frac{\omega}{4\varepsilon_F}, \\ Q &= \frac{q}{2k_F}, \end{aligned} \tag{160}$$

as well as $p = \frac{k}{k_F}$ and obtain

$$\mathrm{Re}\chi^r_{\mathbf{q}}(\omega) = \frac{mk_F}{Q}\int_0^1 \frac{pdp}{(2\pi)^2}\int_{-1}^1 d\mu \left(\frac{1}{\frac{\nu}{pQ}+\frac{Q}{p}-\mu} - \frac{1}{\frac{\nu}{pQ}-\frac{Q}{p}-\mu}\right) \tag{161}$$

The density of states of a three dimensional parabolic spectrum is $\rho(\varepsilon) = \frac{\sqrt{2}m^{3/2}}{\pi^2}\sqrt{\varepsilon}$, where we included the spin degeneracy already in $\rho(\epsilon)$. With $\rho_F = \rho(\varepsilon_F)$ follows

$$\rho_F = \frac{mk_F}{\pi^2} \tag{162}$$

such that

$$\mathrm{Re}\chi^r_{\mathbf{q}}(\omega) = \frac{\rho_F}{4Q}\int_0^1 pdp\int_{-1}^1 d\mu \left(\frac{1}{\frac{\nu}{pQ}+\frac{Q}{p}-\mu} - \frac{1}{\frac{\nu}{pQ}-\frac{Q}{p}-\mu}\right) \tag{163}$$

We observe that for the real part it is indeed possible to express the density response in terms of the dimensionless Lindhard function of Eq.(150). We perform the integration over μ and obtain

$$\mathrm{Re}\chi^r_{\mathbf{q}}(\omega) = \frac{\rho_F}{4Q}\int_0^1 pdp\log\left|\frac{\left(p+\frac{\nu}{Q}+Q\right)\left(p+\frac{\nu}{Q}-Q\right)}{\left(p-\frac{\nu}{Q}-Q\right)\left(p-\frac{\nu}{Q}+Q\right)}\right|. \tag{164}$$

In the last step we perform the integration over p and it follows

$$\mathrm{Re}\chi^r_{\mathbf{q}}(\omega) = \rho_F L'\left(\frac{q}{2k_F}, \frac{\omega}{4\varepsilon_F}\right), \tag{165}$$

where the real part of the Lindhard function is given as:

$$\begin{aligned} L'(Q,\nu) &= \frac{1}{2} + \frac{1}{8Q}\left(1-\frac{\nu^2}{Q^2}-Q^2\right)\log\left|\frac{\frac{\nu^2}{Q^2}-(Q+1)^2}{\frac{\nu^2}{Q^2}-(Q-1)^2}\right| \\ &- \frac{\nu}{4Q}\log\left|\frac{\left(\frac{\nu}{Q}+1\right)^2-Q^2}{\left(\frac{\nu}{Q}-1\right)^2-Q^2}\right|. \end{aligned} \tag{166}$$

If we consider $\mathbf{q} = \mathbf{0}$, i.e. $Q = 0$, we find with

$$\lim_{Q\to 0}\frac{1}{8Q}\left(1-\frac{\nu^2}{Q^2}-Q^2\right)\log\left|\frac{\frac{\nu^2}{Q^2}-(Q+1)^2}{\frac{\nu^2}{Q^2}-(Q-1)^2}\right| = \frac{1}{2}$$

and

$$\lim_{Q\to 0}\frac{\nu}{4Q}\log\left|\frac{\left(\frac{\nu}{Q}+1\right)^2-Q^2}{\left(\frac{\nu}{Q}-1\right)^2-Q^2}\right| = 1$$

the desired result that

$$L\left(0,\nu\right)=0. \tag{167}$$

For $\omega=0$, i.e. $\nu=0$ we obtain

$$L_0\left(Q\right)\equiv L'\left(Q,0\right)=\frac{1}{2}\left(1+\frac{1-Q^2}{2Q}\log\left|\frac{1-Q}{1+Q}\right|\right). \tag{168}$$

For large momenta holds $L_0\left(Q\gg1\right)\sim\frac{1}{3Q^2}$ while for small momenta holds $L_0\left(Q\ll1\right)\sim1-\frac{1}{3}Q^2$. For $Q\to1$ the derivative of $L_0\left(Q\right)$ diverges logarithmically, while $L_0\left(Q=1\right)=\frac{1}{2}$ is finite.

An interesting application of this result is the response of an ideal gas of fermions to a point-like potential, i.e.

$$V^{\text{ext}}\left(\mathbf{r},t\right)=V_0\delta\left(\mathbf{r}\right). \tag{169}$$

If we use our linear response formalism, it follows for the induced charge-density[4]

$$\left\langle\rho\left(\mathbf{r}\right)\right\rangle_t=\int_{-\infty}^{\infty}dt'\int d^3r'\chi\left(\mathbf{r}-\mathbf{r}',t-t'\right)V^{\text{ext}}\left(\mathbf{r}',t'\right). \tag{170}$$

Performing the integration over $\mathbf{r}'$ yields a time-independent density profile

$$\begin{aligned}\left\langle\rho\left(\mathbf{r}\right)\right\rangle &= V_0\chi\left(\mathbf{r},\omega=0\right)\\ &= \rho_F V_0\int\frac{d^3q}{\left(2\pi\right)^3}L_0\left(\frac{q}{2k_F}\right)e^{i\mathbf{q}\cdot\mathbf{r}}.\end{aligned} \tag{171}$$

We can analytically perform this Fourier transformation

$$\begin{aligned}\int\frac{d^3q}{\left(2\pi\right)^3}L_0\left(\frac{q}{2k_F}\right)e^{i\mathbf{q}\cdot\mathbf{r}} &= \int_0^{\infty}\frac{q^2dq}{\left(2\pi\right)^2}\int_{-1}^{1}d\mu L_0\left(\frac{q}{2k_F}\right)e^{iqr\mu}\\ &= \int_0^{\infty}\frac{qdq}{2\pi^2r}L_0\left(\frac{q}{2k_F}\right)\sin\left(qr\right)\\ &= -\frac{\cos\left(2k_Fr\right)-\frac{\sin(2k_Fr)}{2k_Fr}}{4\pi\left(2k_Fr\right)^3}.\end{aligned} \tag{172}$$

Thus, an impurity potential induces a density variation that is static and that oscillates with a period of twice the Fermi momentum

$$\left\langle\rho\left(\mathbf{r}\right)\right\rangle=-\rho_F V_0\frac{\cos\left(2k_Fr\right)-\frac{\sin(2k_Fr)}{2k_Fr}}{4\pi\left(2k_Fr\right)^3}. \tag{173}$$

These oscillations are called Friedel oscillations after the French physicist Jaques Friedel.

Finally we analyze the imaginary part of the density response. The δ-function in Eq.(154) implies that only states with $\varepsilon_{\mathbf{k}+\mathbf{q}}\geq\varepsilon_{\mathbf{k}}$ contribute. On the

[4]With our above formalism this corresponds to $V^{\text{ext}}\left(\mathbf{r},t\right)=-e\varphi^{\text{ext}}\left(\mathbf{r},t\right)$.

other hand, the combination of Fermi functions implies that the occupancy of the states with momentum $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ is different. Taken together, this implies

$$\begin{aligned} |\mathbf{k}| &< k_F \\ |\mathbf{k}+\mathbf{q}| &> k_F. \end{aligned} \tag{174}$$

Thus, the imaginary part is sensitive to particle-hole excitations with energy ω.

To proceed we use the version of Eq.(154) after the shift of momenta in the first term and obtain

$$\begin{aligned} \mathrm{Im}\chi^r_{\mathbf{q}}(\omega) &= -2\pi \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \left(\delta\left(\omega - \varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}-\mathbf{q}}\right)\right. \\ &\quad \left. -\delta\left(\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}\right)\right). \end{aligned} \tag{175}$$

After analogous steps as for the real part we obtain

$$\begin{aligned} \mathrm{Im}\chi^r_{\mathbf{q}}(\omega) &= -\frac{m}{2\pi q}\int_0^{k_F} kdk \int_{-1}^{1} d\mu \left(\delta\left(\frac{m\omega}{kq} + \frac{q}{2k} - \mu\right)\right. \\ &- \left.\delta\left(\frac{m\omega}{kq} - \frac{q}{2k} - \mu\right)\right). \end{aligned} \tag{176}$$

We can perform the integration over $\mu = \cos\theta$, switch to dimensionless units, and consider the function

$$\mathrm{Im}\chi^r_{\mathbf{q}}(\omega) = \rho_F L''\left(\frac{q}{2k_F}, \frac{\omega}{4\varepsilon_F}\right) \tag{177}$$

with

$$\begin{aligned} L''(Q,\nu) &= \frac{\pi}{2Q}\int_0^1 pdp \left[\theta\left(p + \frac{\nu}{Q} - Q\right)\theta\left(p - \frac{\nu}{Q} + Q\right)\right. \\ &- \left.\theta\left(p + \frac{\nu}{Q} + Q\right)\theta\left(p - \frac{\nu}{Q} - Q\right)\right] \end{aligned} \tag{178}$$

The integration over p finally yields

$$\begin{aligned} L''(Q,\nu) &= \frac{\pi}{4Q}\left\{\left[1 - \left(\frac{\nu}{Q} - Q\right)^2\right]\theta\left(1 - \left(\frac{\nu}{Q} - Q\right)^2\right)\right. \\ &- \left.\left|\left[1 - \left(\frac{\nu}{Q} + Q\right)^2\right]\theta\left(1 - \left(\frac{\nu}{Q} + Q\right)^2\right)\right\}. \end{aligned} \tag{179}$$

The imaginary part is finite between the two curves (we only consider $\nu > 0$ at the moment)

$$\begin{aligned} \nu_1 &= Q + Q^2 \\ \nu_2 &= Q - 1 + (Q-1)^2 \end{aligned}$$

Within this regime and for $\nu_3 < Q(1-Q)$ the imaginary part is simply linear in frequency with

$$L''(Q,\nu) = \frac{\pi\nu}{Q}.$$

5.4 Hartree-Fock analysis of the Coulomb interaction

We finally consider an interacting problem of electrons with long ranged Coulomb interaction. In real space, our Hamiltonian is given as

$$\begin{aligned} H &= \sum_{\alpha} \int d^3 r \psi_{\alpha}^{\dagger}(\mathbf{r}) \varepsilon(-i\nabla) \psi_{\alpha}(\mathbf{r}) \\ &+ \frac{e^2}{2} \sum_{\alpha\alpha'} \int d^3 r d^3 r' \frac{\psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\alpha'}^{\dagger}(\mathbf{r}') \psi_{\alpha'}(\mathbf{r}') \psi_{\alpha}(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}. \end{aligned} \tag{180}$$

Fourier transformation to momentum space yields

$$\begin{aligned} H &= \frac{1}{V} \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} \psi_{\mathbf{k}\alpha}^{\dagger} \psi_{\mathbf{k}\alpha} \\ &+ \frac{1}{2V^3} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\alpha\alpha'} v_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \psi_{\mathbf{k}\alpha}^{\dagger} \psi_{\mathbf{k}'\alpha'}^{\dagger} \psi_{\mathbf{k}'+\mathbf{q}\alpha'} \psi_{\mathbf{k}-\mathbf{q}\alpha} \end{aligned} \tag{181}$$

with interaction matrix element

$$v_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) = \frac{4\pi e^2}{q^2}. \tag{182}$$

The indices $\mathbf{k}$ and $\mathbf{k}'$ are of course not necessary. We included them here to allow for an analysis of more general potentials.

We first analyze the single particle Green's function

$$G_{\mathbf{k}}(t) = \left\langle\left\langle \psi_{\mathbf{k}\alpha}(t) ; \psi_{\mathbf{k}\alpha}^{\dagger} \right\rangle\right\rangle \tag{183}$$

Thus, our first step is to determine the commutator

$$[\psi_{\mathbf{k}\alpha}, H] = \varepsilon_{\mathbf{k}} \psi_{\mathbf{k}\alpha} + \frac{1}{V^2} \sum_{\mathbf{k}'\mathbf{q}\alpha'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \psi_{\mathbf{k}'\alpha'}^{\dagger} \psi_{\mathbf{k}'+\mathbf{q}\alpha'} \psi_{\mathbf{k}-\mathbf{q}\alpha} \tag{184}$$

which gives rise to the equation of motion

$$\begin{aligned} (\omega - \varepsilon_{\mathbf{k}}) \left\langle\left\langle \psi_{\mathbf{k}\alpha} ; \psi_{\mathbf{k}\alpha}^{\dagger} \right\rangle\right\rangle_{\omega} &= 1 + \frac{1}{V^2} \sum_{\mathbf{k}'\mathbf{q}\alpha'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \\ &\times \left\langle\left\langle \psi_{\mathbf{k}'\alpha'}^{\dagger} \psi_{\mathbf{k}'+\mathbf{q}\alpha'} \psi_{\mathbf{k}-\mathbf{q}\alpha} ; \psi_{\mathbf{k}\alpha}^{\dagger} \right\rangle\right\rangle_{\omega} \end{aligned}$$

We see that the interaction between particles generated a more complicated Green's function. If one tries to analyze this, more complicated function one obtains an even worse set of operators in the commutator and, accordingly, an even more complicated Green's function. Thus, we are not able to solve this problem exactly any-longer.

Later we will see that it is efficient to define a so called self-energy via

$$\Sigma_{\mathbf{k}}(\omega) = \frac{\frac{1}{V^2}\sum_{\mathbf{k}'\mathbf{q}\alpha'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \left\langle\left\langle \psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha}; \psi^\dagger_{\mathbf{k}\alpha}\right\rangle\right\rangle_\omega}{\left\langle\left\langle \psi_{\mathbf{k}\alpha}; \psi^\dagger_{\mathbf{k}\alpha}\right\rangle\right\rangle_\omega}, \tag{185}$$

which yields

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}. \tag{186}$$

At this point this definition is not overly useful, but we will see that the self energy has a comparatively easy definition in terms of Feynman diagrams. This form of the Green's function reminds us of the Dyson equation

$$G_{\mathbf{k}}(\omega)^{-1} = G_{0\mathbf{k}}(\omega)^{-1} - \Sigma_{\mathbf{k}}(\omega), \tag{187}$$

that we encountered in case of non-interacting fermions or bosons with bare Green's function $G_{0\mathbf{k}}(\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}}}$. The self energy plays a role of a frequency dependent potential for individual particles.

The form of the self energy suggests to search for an approximation, where one replaces the more complicated Green's function by a factor times the ordinary single particle Green's function.

We can make progress if we recall a result for a more complicated Green's function that we obtained for free particles. Consider $G_{AB} = G_{i,jkl}$ with $A = \psi_i$ and $B = \psi^\dagger_j\psi^\dagger_k\psi_l$, we found

$$G_{i,jkl}(\omega) = G_{ij}(\omega)\left\langle c^\dagger_k c_l\right\rangle - \eta G_{ik}(\omega)\left\langle c^\dagger_j c_l\right\rangle. \tag{188}$$

If we use $G_{AB} = G_{B^\dagger A^\dagger}$, it follows for $G_{B^\dagger A^\dagger} = G_{lkj,i}$ with with $A^\dagger = \psi^\dagger_i$ and $B^\dagger = \psi^\dagger_l\psi_k\psi_j$, we obtain

$$G_{lkj,i}(\omega) = G_{ij}(\omega)\left\langle \psi^\dagger_k\psi_l\right\rangle - \eta G_{ik}(\omega)\left\langle \psi^\dagger_j\psi_l\right\rangle. \tag{189}$$

Of course, these expressions are only correct for non-interacting particles. In what follows we will simply assume that we are allowed to use those relations for interacting particles as well. This implies

$$\begin{aligned}\left\langle\left\langle \psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha}; \psi^\dagger_{\mathbf{k}\alpha}\right\rangle\right\rangle_\omega &= \left\langle\left\langle \psi_{\mathbf{k}\alpha}; \psi^\dagger_{\mathbf{k}-\mathbf{q}\alpha}\right\rangle\right\rangle_\omega \left\langle \psi^\dagger_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}'\alpha'}\right\rangle \\ &-\eta \left\langle\left\langle \psi_{\mathbf{k}\alpha}; \psi_{\mathbf{k}'+\mathbf{q}\alpha'}\right\rangle\right\rangle_\omega \left\langle \psi^\dagger_{\mathbf{k}-\mathbf{q}\alpha}\psi_{\mathbf{k}'\alpha'}\right\rangle\end{aligned} \tag{190}$$

We use that the the Green's functions are diagonal in the momentum and spin indices and obtain with $n_{\mathbf{k}\alpha} = \psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}$:

$$\left\langle\left\langle \psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha}; \psi^\dagger_{\mathbf{k}\alpha}\right\rangle\right\rangle_\omega = G_{\mathbf{k}}(\omega) V\left(\delta_{\mathbf{q},0}\left\langle n_{\mathbf{k}'\alpha'}\right\rangle - \eta\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}\delta_{\alpha\alpha'}\left\langle n_{\mathbf{k}'\alpha}\right\rangle\right)$$

If we insert this into the equation of motion or, alternatively, into our definition for the self energy, we find

$$\begin{aligned}\Sigma_{\mathbf{k}}(\omega) &= \frac{1}{V}\sum_{\mathbf{k}'\mathbf{q}\alpha'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{q})\left(\delta_{\mathbf{q},0}\langle n_{\mathbf{k}'\alpha'}\rangle - \eta\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}\delta_{\alpha\alpha'}\langle n_{\mathbf{k}'\alpha'}\rangle\right) \\ &= \frac{1}{V}\sum_{\mathbf{k}'\alpha'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{0})\langle n_{\mathbf{k}'\alpha'}\rangle - \eta\frac{1}{V}\sum_{\mathbf{k}'} v_{\mathbf{k},\mathbf{k}'}(\mathbf{k}-\mathbf{k}')\langle n_{\mathbf{k}'\alpha}\rangle \quad (191)\end{aligned}$$

This is the Hartree-Fock approximation for the self-energy. The first term corresponds to the Hartree term and the second to the Fock term. The philosophy of it's derivation is indeed the same as in the ordinary, first-quantized formulation of quantum mechanics, where one evaluates expectation values with regards to an assumed Slater determinant, i.e. a free-particle wave function. Here we also evaluated interaction effects in the equation of motion, pretending that the higher order Green's function can be analyzed the same way as for free particles.

There is a simple rule that exists for the evaluation of these higher order Green's function. We consider the operator $\psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha}$ and replace a pair made out of a creation and an annihilation operator, once they are next to each other, by its expectation value. If it is necessary to change the order a minis sign might occur for due to the anti-commutation rules. Thus we approximate

$$\begin{aligned}\psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha} &\approx \left\langle\psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\right\rangle\psi_{\mathbf{k}-\mathbf{q}\alpha} \\ &- \left\langle\psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha}\right\rangle\psi_{\mathbf{k}'+\mathbf{q}\alpha'}. \quad (192)\end{aligned}$$

If we further use that the momenta and spins in the expectation value have to be the same, it follows

$$\begin{aligned}\psi^\dagger_{\mathbf{k}'\alpha'}\psi_{\mathbf{k}'+\mathbf{q}\alpha'}\psi_{\mathbf{k}-\mathbf{q}\alpha} &\approx \delta_{\mathbf{q},0}\langle n_{\mathbf{k}'\alpha'}\rangle\psi_{\mathbf{k}-\mathbf{q}\alpha} \\ &- \delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}\delta_{\alpha\alpha'}\langle n_{\mathbf{k}'\alpha'}\rangle\psi_{\mathbf{k}'+\mathbf{q}\alpha'}. \quad (193)\end{aligned}$$

Inserting this expression into the Green's function yields the above result for the self energy.

If we insert this self energy into the Dyson equation we finally obtain a result for the Green's function within Hartree-Fock approximation. This Green's function can then be used to determine expectation values like $\langle n_{\mathbf{k}'\alpha'}\rangle$. Since the self-energy itself depends on those expectation values, one sees that one is confronted with a self-consistency issue. Thus, one has to assume a certain result for $\langle n_{\mathbf{k}'\alpha'}\rangle$, use this ansatz to determine the self energy and Green's function and check whether resulting $\langle n_{\mathbf{k}'\alpha'}\rangle$ agrees with the initial ansatz. If not, one has to use a better ansatz. A good approach to solve this self-consistency problem is to use the occupation one just obtained and an improved ansatz and iterate this problem until convergence is reached. This self consistency procedure demonstrates that one includes in the Hartree-Fock approach effects to arbitrary order in the interaction. This sounds encouraging, however, one certainly didn't include all effects. Only the first order contribution to the self

energy that is completely contained in the approach. We will discuss these issues later-on during the course.

Returning to the Coulomb problem one should get rather nervous if one looks at the Hartree term. Here one has to analyze the matrix element $v_{\mathbf{kk}}(\mathbf{q}=\mathbf{0})$ while the interaction diverges like q^{-2} for small q. Here the self energy amounts to a shift in energy

$$\delta\epsilon = -\lim_{\mathbf{q}\to 0}\frac{4\pi e}{q^2}\rho_0$$

where $\rho_0 = -e\int\frac{d^3k}{(2\pi)^3}\sum_\alpha\langle n_{\mathbf{k}\alpha}\rangle$ is the electron density in equilibrium. Thus, this energy can be written as

$$\delta\epsilon = -e\int d^3r\frac{\rho_0}{|\mathbf{r}|} \tag{194}$$

Physically this is the Coulomb repulsion of a given electron by all other electrons in the system. This yields an infinite shift of the energy of each individual electron and seems to suggest that the system is not stable. In fact we know that for an infinite system the energy density of a homogeneously charged plasma is infinite because of Coulomb's law. In the real solid this is compensated by the attractive potential that each electron feels because of the positively charged ions. The instability we obtained is solely a consequence of the fact that we forgot to include the positively charged ions in our Hamiltonian. Since $\rho_0 = -\rho_{\text{ion}}$ and because we consider a jellium model with homogeneously charged background, we include this Coulomb interaction by shifting all energies by

$$\delta\epsilon_{\text{ion}} = -e\int d^3r\frac{\rho_{\text{ion}}}{|\mathbf{r}|} \tag{195}$$

in the Hamiltonian ($\varepsilon(\mathbf{k}) \to \varepsilon(\mathbf{k}) + \delta\epsilon_{\text{ion}}$). As a frequency independent self energy does nothing else but correcting the energies in our Hamiltonian, we see that the Hartree term exactly cancels $\delta\epsilon_{\text{ion}}$. Thus, for a Coulomb problem we only need to include the Fock term, which for fermions with $\eta = +1$ is given as

$$\Sigma_{\mathbf{k}} = -\int\frac{d^3k'}{(2\pi)^3}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}\langle n_{\mathbf{k}'\alpha}\rangle$$

It amounts to a correction of the single particle energy, i.e.

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega - \varepsilon^*_{\mathbf{k}}}. \tag{196}$$

with renormalized dispersion

$$\varepsilon^*_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + \Sigma_{\mathbf{k}} \tag{197}$$

As long as the Coulomb interaction does not break the rotational symmetry of the system, the renormalized dispersion will continue to depend on the magnitude of the momentum: $k = |\mathbf{k}|$. Thus, the system will be characterized by a

Fermi momentum k_F. Since the Green's function looks like the one of a free Fermi system, it must furthermore hold at $T = 0$ that $\langle n_{\mathbf{k}\alpha}\rangle = 1$ for $k < k_F$ and $\langle n_{\mathbf{k}\alpha}\rangle = 0$ for $k > k_F$, which yields that k_F must be unchanged by the interaction and is fixed by the total density. If follows

$$\begin{aligned}
\Sigma_k &= -\frac{e^2}{\pi}\int_0^{k_F} k'^2 dk' \int_{-1}^{1} d\mu \frac{1}{k^2 + k'^2 - 2kk'\mu} \\
&= -\frac{e^2}{\pi k}\int_0^{k_F} k' dk' \log\left|\frac{k+k'}{k-k'}\right| \\
&= -\frac{e^2 k_F^2}{\pi k}\int_0^{1} p dp \log\left|\frac{k/k_F + p}{k/k_F - p}\right| \\
&= -\frac{e^2 k_F}{\pi}\left(1 + \frac{1}{2}\frac{(k/k_F)^2 - 1}{k/k_F}\log\left|\frac{k/k_F+1}{k/k_F-1}\right|\right)
\end{aligned}$$

We see that at k_F the self energy is $\Sigma_{k_F} = -\frac{e^2 k_F}{\pi}$. This quantity can alternatively be absorbed in the new chemical potential, needed to obtain the correct density. More interesting is the momentum dependence of the self energy. It holds for k near k_F that

$$\frac{\partial \Sigma_k}{\partial k} = \frac{e^2 k_F}{\pi}\log\left|\frac{2k_F}{k - k_F}\right|, \tag{198}$$

i.e. we obtain a logarithmically divergent correction to the velocity

$$v_k^* = \frac{\partial \varepsilon_k^*}{\partial k} = \frac{k}{m} + \frac{\partial \Sigma_k}{\partial k}. \tag{199}$$

This result played a role in the early stages of the theory of interactions in metals[5] However, the inclusion of higher order processes of the perturbation theory strongly suggests that this divergency is spurious. Nevertheless, the Hartree-Fock approximation is a useful tool to get a first idea about an interacting many-body system.

5.5 The random phase approximation for density correlations

In this final chapter on screening of the Coulomb interaction we determine the density-density Green's function of an interacting system within an approximation that is qualitatively similar to the Hartree-Fock approximation.

In full analogy to the case of non-interacting fermions we analyze the Green's function

$$\left\langle\left\langle \psi^\dagger_{\mathbf{k}\alpha}(t)\,\psi_{\mathbf{k}+\mathbf{q}\alpha}(t)\,;\psi^\dagger_{\mathbf{k}'\beta}\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle. \tag{200}$$

[5] J. C. Slater Phys. Rev. **81**, 385 (1951).

The additional calculation is the determination of the commutator recall that we already used the commutator $\left[\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha}, H_C\right]_-$ where H_C is the Coulomb-interaction in the Hamiltonian H. It holds

$$\begin{aligned}\left[\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha}, H_C\right]_- &= \sum_{\mathbf{k}_1\mathbf{q}_1\alpha_1} v(\mathbf{q})\left(\psi^\dagger_{\mathbf{k}\alpha}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1-\mathbf{q}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha}\right.\\ &- \left.\psi^\dagger_{\mathbf{k}+\mathbf{q}_1\alpha}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1+\mathbf{q}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}\alpha}\right), \qquad (201)\end{aligned}$$

where we used that $v(\mathbf{q}) = v(-\mathbf{q})$. Just like in the case of the Hartree-Fock approximation, we express certain operators in the Green's function by expectation values. For the first term in the above commutator follows

$$\begin{aligned}\psi^\dagger_{\mathbf{k}\alpha}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1-\mathbf{q}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha} &\approx \langle n_{\mathbf{k}_1\alpha_1}\rangle \delta_{\mathbf{q}_1,0}\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha}\\ &+ \langle n_{\mathbf{k}\alpha}\rangle \delta_{\mathbf{q}_1,-\mathbf{q}}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1-\mathbf{q}_1\alpha_1}\\ &- \langle n_{\mathbf{k}\alpha}\rangle \delta_{\mathbf{k},\mathbf{k}_1-\mathbf{q}_1}\delta_{\alpha\alpha_1}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha}\\ &- \langle n_{\mathbf{k}_1\alpha_1}\rangle \delta_{\mathbf{k}_1,\mathbf{k}+\mathbf{q}+\mathbf{q}_1}\delta_{\alpha\alpha_1}\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}_1-\mathbf{q}_1\alpha}, \qquad (202)\end{aligned}$$

where we "contracted" two operators that are next to each other to their expectation value. The minus signs are a result of the fact that we had to bring operators next to each other.

$$\begin{aligned}\psi^\dagger_{\mathbf{k}+\mathbf{q}_1\alpha}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1+\mathbf{q}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}\alpha} &\approx \langle n_{\mathbf{k}_1\alpha_1}\rangle \delta_{\mathbf{q}_1,0}\psi^\dagger_{\mathbf{k}+\mathbf{q}_1\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha}\\ &+ \langle n_{\mathbf{k}\alpha}\rangle \delta_{\mathbf{q}_1,\mathbf{q}}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1+\mathbf{q}_1\alpha_1}\\ &- \langle n_{\mathbf{k}\alpha}\rangle \delta_{\mathbf{k},\mathbf{k}_1}\delta_{\alpha\alpha_1}\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}+\mathbf{q}\alpha}\\ &- \langle n_{\mathbf{k}_1\alpha_1}\rangle \delta_{\mathbf{k}_1,\mathbf{k}+\mathbf{q}}\delta_{\alpha\alpha_1}\psi^\dagger_{\mathbf{k}+\mathbf{q}_1\alpha}\psi_{\mathbf{k}_1+\mathbf{q}_1\alpha}, \qquad (203)\end{aligned}$$

Inserting these approximate expressions into the equation of motion yields

$$\begin{aligned}(\omega - E_{\mathbf{k},\mathbf{q}})\left\langle\left\langle\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}+\mathbf{q}\alpha}; \psi^\dagger_{\mathbf{k}'\beta}\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle &= V^2\delta_{\alpha\beta}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta_{\mathbf{q},\mathbf{q}'}(f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}})\\ &+ (f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}})\sum_{\mathbf{k}_1\alpha_1}(v(\mathbf{q}) - v(\mathbf{k}-\mathbf{k}_1)\delta_{\alpha\alpha_1})\\ &\times \left\langle\left\langle\psi^\dagger_{\mathbf{k}_1\alpha_1}\psi_{\mathbf{k}_1+\mathbf{q}\alpha_1}; \psi^\dagger_{\mathbf{k}'\beta}\psi_{\mathbf{k}'-\mathbf{q}'\beta}\right\rangle\right\rangle\end{aligned}$$

where

$$E_{\mathbf{k},\mathbf{q}} = \varepsilon^*_{\mathbf{k}+\mathbf{q}} - \varepsilon^*_{\mathbf{k}}$$

are the Hartree-Fock corrected single particle energies. In what follows we will ignore these Hartree-Fock corrections. It turns out that the term with $v(\mathbf{k}-\mathbf{k}_1)$ cannot be expressed in terms of the density-density correlation function. It corresponds to other degrees of freedom but the density, which are coupled to density fluctuations via the Coulomb interaction. A frequent assumption is that those degrees of freedom are not coherently coupled to density fluctuations and

will be damped out rapidly. In what follows we will also ignore this term. This is called the random phase approximation.

It follows for the density-density Green's function

$$\chi_{\mathbf{q}}(\omega) = \chi_{\mathbf{q}}^{(0)}(\omega)\left(1 - v(\mathbf{q})\chi_{\mathbf{q}}(\omega)\right) \tag{204}$$

which can be solved and yields

$$\boxed{\chi_{\mathbf{q}}(\omega) = \frac{\chi_{\mathbf{q}}^{(0)}(\omega)}{1 + v(\mathbf{q})\chi_{\mathbf{q}}^{(0)}(\omega)},} \tag{205}$$

where

$$\chi_{\mathbf{q}}^{(0)}(\omega) = \frac{1}{V}\sum_{\alpha\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\omega + i0^+ - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}} \tag{206}$$

is the density-density Green's function of free particles that can be expressed in terms of the Lindhard function.

If we combine our relation Eq.(138) between dielectric function with the density Green's function with Eq.(205), it follows

$$\varepsilon(\mathbf{q},\omega) = 1 + \frac{4\pi e^2}{q^2}\chi_{\mathbf{q}}^{(0)}(\omega) \tag{207}$$

Let us first analyze the response to a static test charge, i.e. the limit $\omega = 0$. In this limit follows

$$\varepsilon(\mathbf{q},0) = \frac{q^2 + 4\pi e^2 \rho_F L_0\left(\frac{q}{2k_F}\right)}{q^2} \tag{208}$$

with

$$L_0(Q) = \frac{1}{2}\left(1 + \frac{1-Q^2}{2Q}\log\left|\frac{1-Q}{1+Q}\right|\right). \tag{209}$$

In the long wave length limit follows $L_0(Q \ll 1) \sim 1 - \frac{1}{3}Q^2$ and we obtain

$$\varepsilon(\mathbf{q},0) = \frac{q^2\left(1 - \frac{2\pi e^2\rho_F}{3k_F^2}\right) + 4\pi e^2\rho_F}{q^2}. \tag{210}$$

If we are in the limit of a good metal, we would expect that the typical kinetic energy is larger than the typical Coulomb interaction, i.e.

$$\frac{k_F^2}{2m} \gg \frac{e^2}{\lambda_F} \tag{211}$$

with Fermi wave number $\lambda_F = \frac{2\pi}{k_F}$. This yields $\frac{2\pi e^2\rho_F}{3k_F^2} \ll 1$ and we obtain

$$\boxed{\varepsilon(\mathbf{q},0) = \frac{q^2 + q_{TF}^2}{q^2},} \tag{212}$$

with Thomas-Fermi wave vector q_{TF} determined by

$$q_{TF}^2 = 4\pi e^2 \rho_F. \tag{213}$$

We can now determine the electric potential of a static point charge

$$\begin{aligned} \varphi(\mathbf{q}, t) &= \frac{4\pi e}{\varepsilon(\mathbf{q}, \omega = 0)\, q^2}. \\ &= \frac{4\pi e}{q^2 + q_{TF}^2}, \end{aligned} \tag{214}$$

which yields a long distance dependence in coordinate space

$$\varphi(\mathbf{r}, t) = \frac{e^2}{|\mathbf{r}|} e^{-q_{TF}|\mathbf{r}|}. \tag{215}$$

Thus, the interaction of charges is screened beyond the Thomas-Fermi length q_{TF}^{-1}.

Finally we can analyze whether we can fulfill the condition $\varepsilon(\mathbf{q}, \omega) = 0$, which amounts to a resonant response to an infinitesimal external charge perturbation.

$$1 + \frac{4\pi e^2}{q^2} \rho_F L\left(\frac{q}{2k_F}, \frac{\omega}{4\varepsilon_F}\right) = 0 \tag{216}$$

In the long wavelength limit we can expand the Lindhard function for small momenta but arbitrary energies. It holds

$$L(Q \ll 1, \nu) = -\frac{Q^2}{3\nu^2} - \frac{Q^4}{5\nu^4} \cdots. \tag{217}$$

This yields

$$\omega^2 = \frac{16\pi}{3} e^2 \rho_F \frac{\epsilon_F^2}{k_F^2} \left(1 + \frac{12\epsilon_F^2 q^2}{5k_F^4 \omega^2}\right). \tag{218}$$

The coefficient

$$\frac{16\pi}{3} e^2 \rho_F \frac{\epsilon_F^2}{k_F^2} = \frac{4}{3\pi} e^2 \frac{k_F^3}{m}$$

can be expressed in terms of the particle density $n = \int_{k<k_F} \frac{d^3k}{(2\pi)^3} = \frac{k_F^3}{3\pi^2}$ and it follows

$$\omega^2 = \omega_{pl}^2 + \frac{3}{5m^2} q^2 \tag{219}$$

with plasma frequency

$$\omega_{pl}^2 = \frac{4\pi n e^2}{m}. \tag{220}$$

Since the imaginary part of the Lindhard function vanishes at small q and finite ω, these collective modes are undamped. The correspond to the emergent response of a charged fluid to an external charge perturbation. The plasma frequency of usual metals is in the regime of several electron volts, i.e. it is a very high frequency collective mode.

Part III
Diagrammatic perturbation theory at finite T

In the previous chapters we learned that retarded Green's function can be determined from an analysis of the equation of motion. The approach is very straightforward and powerful for non-interaction systems. However, as soon as one wants to incorporate effects of interactions, the method is not very transparent and efficient. An elegant alternative is the analysis of Green's functions using Feynman diagrams. A diagrammatic perturbation theory can be developed for time ordered Green's functions. Historically the formulation was done first for the so called causal Green's function

$$\begin{aligned} G^c_{A,B}(t,t') &= \langle\langle A(t);B(t')\rangle\rangle^c \\ &\equiv -i\langle TA(t)B(t')\rangle, \end{aligned} \tag{221}$$

with time ordering operator

$$TA(t)B(t') = \theta(t-t')A(t)B(t') - \eta\theta(t'-t)B(t')A(t). \tag{222}$$

While these functions can be efficiently determined in terms of Feynman diagrams, it holds that they are analytic functions in the complex plane only in the limit $T=0$. For this reason we will not discuss causal Green's function further. Instead, an elegant and very efficient approach valid also at finite temperatures can be developed in terms of Matsubara. Before we discuss Matsubara functions we briefly summarize the concept of the S-matrix, as it will play an important role in our subsequent analysis.

Let us consider a Hamiltonian

$$H = H_0 + V \tag{223}$$

that consists of a free part H_0 and an interaction part V. The time evolution is governed by

$$e^{-iH(t-t')} = e^{-iH_0t}S(t,t')e^{iH_0t'} \tag{224}$$

which defines the S-matrix. With this definition follows for the time dependence of an arbitrary operator in Heisenberg representation

$$\begin{aligned} A(t) &= e^{iHt}Ae^{-iHt} \\ &= S^\dagger(t,0)e^{-iH_0t}Ae^{-iH_0t}S(t,0) \\ &= S^\dagger(t,0)\tilde{A}(t)S(t,0) \end{aligned} \tag{225}$$

where

$$\tilde{A}(t) = e^{-iH_0t}Ae^{-iH_0t}. \tag{226}$$

In order to determine the S-matrix we consider the time derivative of

$$S(t,t') = e^{iH_0 t} e^{-iH(t-t')} e^{-iH_0 t'}. \tag{227}$$

It holds

$$\begin{aligned}
\partial_t S(t,t') &= iH_0 e^{iH_0 t} e^{-iH(t-t')} e^{-iH_0 t'} \\
&- e^{iH_0 t} (iH) e^{-iH(t-t')} e^{-iH_0 t'} \\
&= e^{iH_0 t} (iH_0 - iH) e^{-iH(t-t')} e^{-iH_0 t'} \\
&= -e^{iH_0 t} (iV) e^{-iH_0 t} e^{iH_0 t} e^{-iH(t-t')} e^{-iH_0 t'} \\
&= -i\tilde{V}(t) S(t,t')
\end{aligned} \tag{228}$$

To determine the S-matrix we have to include the boundary condition

$$S(t,t) = 1. \tag{229}$$

The solution of the above differential equation is

$$S(t,t') = Te^{-i\int_{t'}^{t} dt'' \tilde{V}(t'')}. \tag{230}$$

Let us demonstrate that this is indeed the correct solution. The boundary condition is clearly obeyed. Next, we expand the exponential function:

$$S(t,t') = \sum_{n=0}^{\infty} S_n(t,t') \tag{231}$$

with

$$S_n = \frac{(-i)^n}{n!} T \int_{t'}^{t} dt_n \cdots \int_{t'}^{t} dt_2 \int_{t'}^{t} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{232}$$

There are $n!$ possibilities to order of the time variables t_i. We could for example relabel the t_i such that the earliest is called t_1, followed by t_2 etc. Then holds

$$S_n = (-i)^n T \int_{t'}^{t} dt_n \cdots \int_{t'}^{t_3} dt_2 \int_{t'}^{t_2} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{233}$$

Of course with this specific relabeling we may also skip the time ordering operation, i.e.

$$S_n = (-i)^n \int_{t'}^{t} dt_n \cdots \int_{t'}^{t_3} dt_2 \int_{t'}^{t_2} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{234}$$

It follows

$$\partial_t S_n(t,t') = -i\tilde{V}(t) S_{n-1}(t,t'), \tag{235}$$

where obviously holds that $S_{-1}(t,t')=0$. This yields

$$\begin{aligned}\partial_t S(t,t') &= -i\tilde{V}(t)\sum_{n=0}^{\infty} S_{n-1}(t,t') \\ &= -i\tilde{V}(t)\sum_{n=-1}^{\infty} S_n(t,t') \\ &= -i\tilde{V}(t)S(t,t').\end{aligned}$$

Thus, we found the correct solution.

6 The Matsubara function

The Matsubara function is motivated by the close analogy between time evolution and thermal averaging. One introduces

$$A(\tau) = e^{\tau H} A e^{-\tau H} \tag{236}$$

and defines

$$\mathcal{G}_{AB}(\tau,\tau') = -\langle TA(\tau)B(\tau')\rangle. \tag{237}$$

with

$$TA(\tau)B(\tau') = \theta(\tau-\tau')A(\tau)B(\tau') - \eta\theta(\tau'-\tau)B(\tau')A(\tau). \tag{238}$$

It is immediately evident why one often refers to the Matsubara approach as the imaginary time approach with

$$t \to -i\tau. \tag{239}$$

It is easy to show that the Green's function is homogeneous with regards to time, i.e. that

$$\mathcal{G}_{AB}(\tau,\tau') = \mathcal{G}_{AB}(\tau-\tau'). \tag{240}$$

This follows again from the fact that the "time-evolution" and the thermal averaging is governed by the Hamiltonian H.

6.1 Periodicity of the Matsubara function and Matsubara frequencies

Next we analyze the detailed time dependence of $\mathcal{G}_{AB}(\tau)$ and show that it is an periodic (anti-periodic) function for bosonic (fermionic) Green's functions. We consider an arbitrary integer m and consider values of τ that obey:

$$m\beta < \tau < (m+1)\beta. \tag{241}$$

It then follows that

$$\mathcal{G}_{AB}(\tau - m\beta) = -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H} TA(\tau-m\beta)B\right)$$

Since $\tau - m\beta > 0$ we can drop the time ordering symbol:

$$\begin{aligned}
\mathcal{G}_{AB}(\tau - m\beta) &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}e^{(\tau-m\beta)H}Ae^{-(\tau-m\beta)H}B\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{(\tau-(m+1)\beta)H}Ae^{-(\tau-m\beta)H}B\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}Be^{(\tau-(m+1)\beta)H}Ae^{-(\tau-(m+1)\beta)H}\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}BA(\tau-(m+1)\beta)\right) \qquad (242)
\end{aligned}$$

If $\tau < 0$ holds

$$BA(\tau) = -\eta TA(\tau)B.$$

Since $\tau - (m+1)\beta < 0$ it follows

$$\begin{aligned}
\mathcal{G}_{AB}(\tau - m\beta) &= \frac{\eta}{Z}\mathrm{tr}\left(e^{-\beta H}TA(\tau-(m+1)\beta)B\right) \\
&= -\eta\mathcal{G}_{AB}(\tau-(m+1)\beta) \qquad (243)
\end{aligned}$$

In particular follows for $m = -1$ that:

$$\mathcal{G}_{AB}(\tau) = -\eta\mathcal{G}_{AB}(\tau+\beta). \qquad (244)$$

Matsubara functions are periodic (anti-periodic) for bosonic (fermionic) choice of the time ordering. Since both functions are periodic with period 2β we can always expand in the Fourier series

$$\mathcal{G}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\mathcal{G}(\omega_n) \qquad (245)$$

where $e^{-2i\beta\omega_n} = 1$, i.e. $\omega_n = n\pi/\beta$. The Fourier coefficients are:

$$\mathcal{G}(\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau}. \qquad (246)$$

This incorporates the information with regards to the period 2β. We do however have even more information. It holds

$$e^{-i\beta\omega_n} = -\eta. \qquad (247)$$

In case of $\eta = -1$, i.e. for bosons, we know that the period is in fact β. Thus, only the Matsubara frequencies with $\omega_n = 2n\pi/\beta$ contribute. For fermionic functions we have $\mathcal{G}(\tau+\beta) = -\mathcal{G}(\tau)$, i.e. $e^{-i\beta\omega_n} = -1$, such that now only odd multiples of π/β contribute and we have $\omega_n = (2n+1)\pi/\beta$. For the Fourier coefficients follows then

$$\begin{aligned}
\mathcal{G}(\omega_n) &= \frac{1}{2}\int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau} - \frac{\eta}{2}\int_{-\beta}^{0} d\tau\mathcal{G}(\tau+\beta)e^{i\omega_n\tau} \\
&= \frac{1-\eta e^{-i\omega_n\beta}}{2}\int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau} \\
&= \int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau}. \qquad (248)
\end{aligned}$$

In summary, we have discrete Matsubara frequencies that are distinct for bosonic and fermionic propagators:

$$\boxed{\omega_n = \begin{cases} 2n\pi/\beta & \text{for bosons} \\ (2n+1)\,\pi/\beta & \text{for fermions} \end{cases}}. \tag{249}$$

6.2 Relation to the retarded function

All this looks rather artificial as no obvious relation to reality seems to exist between the Matsubara functions and physical observables. However, if we repeat the same steps that led to the spectral representation of the retarded Green's function it follows:

$$\begin{aligned} \mathcal{G}_{AB}(\omega_n) &= -\frac{1}{Z}\int_0^\beta d\tau e^{i\omega_n\tau}\mathrm{tr}\left(e^{(\tau-\beta)H}Ae^{-\tau H}B\right) \\ &= -\frac{1}{Z}\sum_{lm}\int_0^\beta d\tau e^{i\omega_n\tau}e^{(\tau-\beta)E_l}e^{-\tau E_m}\langle l|A|m\rangle\langle m|B|l\rangle \\ &= \frac{1}{z}\sum_{lm}\frac{e^{-\beta E_l}-e^{-\beta E_m}e^{i\beta\omega_n}}{i\omega_n+E_l-E_m}\langle l|A|m\rangle\langle m|B|l\rangle \end{aligned} \tag{250}$$

Since $e^{i\beta\omega_n} = -\eta$, it follows

$$\boxed{\mathcal{G}_{AB}(\omega_n) = \frac{1}{Z}\sum_{l.m}\frac{\left(e^{-\beta E_l}+\eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{i\omega_n+E_l-E_m}} \tag{251}$$

If we compare this with the general Lehmann representation that was derived earlier, it follows

$$\mathcal{G}_{AB}(\omega_n) = G_{AB}(z = i\omega_n). \tag{252}$$

We already discussed that we can define Green's function in the entire complex plane and that the only source for non-analyticity is the real axis. Now we see that the Matsubara function yields the complex Green's function at the purely imaginary Matsubara frequencies. Thus, if we determine the Matsubara function, we can determine the retarded function via analytic continuation

$$i\omega_n \to \omega + i0^+. \tag{253}$$

Thus, knowledge of the Matsubara function allows for the determination of the retarded function.

This immediately yields information about the single-particle Matsubara Green's function. Consider the Hamiltonian

$$H_0 = \sum_\alpha \int \frac{d^dk}{(2\pi)^d}\varepsilon_{\mathbf{k}}\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}. \tag{254}$$

We obtain for the Fourier transform of

$$\mathcal{G}_{0\mathbf{k}}(\tau) = -\left\langle T\psi_{\mathbf{k}\alpha}(\tau)\,\psi^{\dagger}_{\mathbf{k}\alpha}\right\rangle_0 \tag{255}$$

that

$$\mathcal{G}_{0,\mathbf{k}}(\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}}. \tag{256}$$

Here we indicate with $\langle\cdots\rangle_0$ that the average is with regards to the Hamiltonian H_0.

6.3 Evolution with imaginary time

We already introduced the time dependence introduces

$$A(\tau) = e^{\tau H} A e^{-\tau H} \tag{257}$$

which can be used to determine the equation of motion

$$\begin{aligned} \partial_\tau A(\tau) &= HA(\tau) - A(\tau)H \\ &= -[A(\tau), H] \end{aligned} \tag{258}$$

For our subsequent analysis we will use

$$e^{\tau H} e^{-\tau H} = 1, \tag{259}$$

i.e.

$$\left(e^{\tau H}\right)^{-1} = e^{-\tau H}. \tag{260}$$

In full analogy of the S-matrix we can introduce

$$\mathcal{S}(\tau,\tau') = e^{H_0\tau} e^{-H(\tau-\tau')} e^{-H_0\tau'}. \tag{261}$$

The time evolution of the full Hamiltonian is written as

$$e^{-H(\tau-\tau')} = e^{-H_0\tau}\mathcal{S}(\tau,\tau')\,e^{H_0\tau;}. \tag{262}$$

In distinction to the real-time S-matrix, $\mathcal{S}(\tau,\tau')$ is not unitary. It does however hold

$$\mathcal{S}(\tau,\tau) = 1 \tag{263}$$

as well as

$$\begin{aligned} \mathcal{S}(\tau_1,\tau_2)\,\mathcal{S}(\tau_2,\tau_3) &= e^{H_0\tau_1} e^{-H(\tau_1-\tau_2)} e^{-H_0\tau_2} e^{H_0\tau_2} e^{-H(\tau_2-\tau_3)} e^{-H_0\tau_3} \\ &= \mathcal{S}(\tau_1,\tau_3). \end{aligned} \tag{264}$$

Using $\tau_3 = \tau_1$, this implies in particular that

$$\mathcal{S}(\tau_1,\tau_2) = \mathcal{S}(\tau_2,\tau_1)^{-1}. \tag{265}$$

The time evolution of the full Hamiltonian is written as

$$\begin{aligned} A(\tau) &= e^{\tau H} e^{-\tau H_0} \tilde{A}(\tau) e^{\tau H_0} e^{-\tau H} \\ &= \mathcal{S}(0,\tau)\, \tilde{A}(\tau)\, \mathcal{S}(\tau,0)\,, \end{aligned} \tag{266}$$

where

$$\tilde{A}(\tau) = e^{\tau H_0} A e^{-\tau H_0}. \tag{267}$$

The equation of motion for the imaginary-time version of the S-matrix follows in full analogy to the case with real times

$$\begin{aligned} -\partial_\tau \mathcal{S}(\tau,\tau') &= -e^{H_0\tau}(H_0 - H) e^{-H(\tau-\tau')} e^{-H_0\tau'} \\ &= \tilde{V}(\tau)\, \mathcal{S}(\tau,\tau')\,. \end{aligned} \tag{268}$$

The solution of this operator differential equation is obtained along the lines discussed above and yields

$$\mathcal{S}(\tau,\tau') = T e^{-\int_{\tau'}^{\tau} d\tau'' \tilde{V}(\tau'')}.$$

This result can for example we used to express the partition function or Green's functions in a manner that is well suited for a perturbation theory. In case of the partition function holds:

$$\begin{aligned} Z &= \mathrm{tr} e^{-\beta H} \\ &= \mathrm{tr}\left(e^{-\beta H_0} \mathcal{S}(\beta,0)\right) \\ &= Z_0 \langle \mathcal{S} \rangle_0 \end{aligned} \tag{269}$$

with our earlier definition for the average w.r.t. H_0 and with

$$\mathcal{S} \equiv \mathcal{S}(\beta,0) = e^{-\int_0^{\beta} d\tau'' \tilde{V}(\tau'')}. \tag{270}$$

Thus, we can express the fully interacting partition sum in terms of expectation values of the noninteracting problem. The same reasoning can be performed for the single particle Green's function as

$$\begin{aligned} \mathcal{G}_{\mathbf{k}}(\tau) &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H} T \psi_{\mathbf{k}\alpha}(\tau)\, \psi^\dagger_{\mathbf{k}\alpha}(0)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0} \mathcal{S}(\beta,0)\, \mathcal{S}(0,\tau)\, \tilde{\psi}_{\mathbf{k}\alpha}(\tau)\, \mathcal{S}(\tau,0)\, \tilde{\psi}^\dagger_{\mathbf{k}\alpha}(\tau')\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0} T \mathcal{S}(\beta,\tau)\, \tilde{\psi}_{\mathbf{k}\alpha}(\tau)\, \mathcal{S}(\tau,0)\, \tilde{\psi}^\dagger_{\mathbf{k}\alpha}(0)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0} T \mathcal{S}(\beta,\tau)\, \mathcal{S}(\tau,0)\, \tilde{\psi}_{\mathbf{k}\alpha}(\tau)\, \tilde{\psi}^\dagger_{\mathbf{k}\alpha}(0)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0} T \tilde{\psi}_{\mathbf{k}\alpha}(\tau)\, \tilde{\psi}^\dagger_{\mathbf{k}\alpha}(0)\, \mathcal{S}(\beta,0)\right) \end{aligned} \tag{271}$$

If we combine this with our representation for the partition function we obtain

$$\begin{aligned}\mathcal{G}_{\mathbf{k}}(\tau) &= -\frac{\left\langle T\tilde{\psi}_{\mathbf{k}\alpha}(\tau)\,\tilde{\psi}^{\dagger}_{\mathbf{k}\alpha}(0)\,\mathcal{S}(\beta,0)\right\rangle_0}{\langle\mathcal{S}(\beta,0)\rangle_0} \\ &= -\frac{\left\langle T\tilde{\psi}_{\mathbf{k}\alpha}(\tau)\,\tilde{\psi}^{\dagger}_{\mathbf{k}\alpha}(0)\,\mathcal{S}\right\rangle_0}{\langle\mathcal{S}\rangle_0} \end{aligned} \tag{272}$$

The appeal of this formulation is that we can develop a perturbation theory in the potential V by expanding the exponentials in the numerator and denominator, respectively.

7 Wick theorem

The formulation of the Matsubara function in the previous section demonstrated that we need to evaluate expectation values of higher order operators with regards to a non-interacting Hamiltonian. In our earlier analysis of retarded Green's functions of free particles we already noticed that higher order Green's functions can be evaluated for free particles. In what follows we develop an efficient formalism to do this for the Matsubara function. We consider a Hamiltonian

$$H_0 = \sum_i \varepsilon_i c_i^{\dagger} c_i, \tag{273}$$

where i stands for an arbitrary set of single particle quantum numbers, for example spin and momentum. We will also use the shorthand notation

$$\alpha_i = c_i \;\text{ or }\; c_i^{\dagger}. \tag{274}$$

7.1 Time evolution of creation and annihilation operators

First we analyze the specific time evolution of the creation and annihilation operator. It holds

$$c_i(\tau) = e^{\tau H_0} c_i e^{-\tau H_0}. \tag{275}$$

We can solve the associated equation of motion

$$\begin{aligned}\partial_\tau c_i(\tau) &= -\left[c_i(\tau), H_0\right] \\ &= -\varepsilon_i c_i(\tau), \end{aligned} \tag{276}$$

which yields

$$c_i(\tau) = e^{-\tau\varepsilon_i} c_i(0) = e^{-\tau\varepsilon_i} c_i. \tag{277}$$

Thus, it follows

$$c_i e^{-\tau H_0} = e^{-\tau H_0} c_i e^{-\tau\varepsilon_i}. \tag{278}$$

An analogous expression follows for

$$c_i^{\dagger}(\tau) = e^{\tau H_0} c_i^{\dagger} e^{-\tau H_0} \tag{279}$$

and yields

$$c_i^\dagger(\tau) = e^{\tau\varepsilon_i} c_i^\dagger \tag{280}$$

as well as

$$c_i^\dagger e^{-\tau H_0} = e^{-\tau H_0} c_i^\dagger e^{\tau\varepsilon_i}. \tag{281}$$

Let us stress our notation. While $c_i^\dagger$ is obviously the hermitian conjugate of c_i, this does not hold that $c_i^\dagger(\tau)$ and $c_i(\tau)$ once $\tau \neq 0$. $c_i^\dagger(\tau)$ merely refers to the time evolution of $c_i^\dagger$, while $(c_i(\tau))^\dagger = c_i^\dagger(-\tau)$.

We can summarize our findings as follows

$$\alpha_i e^{-\tau H_0} = e^{-\tau H_0} \alpha_i e^{s_i \tau \varepsilon_i}, \tag{282}$$

where

$$s_i = \begin{cases} +1 & \text{if} \quad \alpha_i = c_i^\dagger \\ -1 & \text{if} \quad \alpha_i = c_i \end{cases}. \tag{283}$$

7.2 Wick theorem of time-independent operators

Next we proof the Wick-theorem of time-independent operators. We analyze the following expectation value of n creation and n annihilation operators:

$$\langle \alpha_1 \alpha_2 \cdots \alpha_{2n} \rangle_0 = \frac{1}{Z_0} \mathrm{tr}\left(e^{-\beta H_0} \alpha_1 \alpha_2 \cdots \alpha_{2n} \right). \tag{284}$$

Our goal is to proof that

$$\begin{aligned} \langle \alpha_1 \alpha_2 \cdots \alpha_{2n} \rangle_0 &= \Big\{ \overbrace{\alpha_1 \alpha_2} \overbrace{\alpha_3 \alpha_4} \cdots \overbrace{\alpha_{2n-1} \alpha_{2n}} \\ &+ \overbrace{\alpha_1 \alpha_2 \alpha_3 \alpha_4} \cdots \overbrace{\alpha_{2n-1} \alpha_{2n}} \\ &+ \cdots \Big\}, \end{aligned} \tag{285}$$

where the sum goes over all possible pairwise contractions. A contraction is defined as

$$\overbrace{\alpha_i \alpha_j} = \langle \alpha_i \alpha_j \rangle_0 \tag{286}$$

and interchanging contracted operators produces a sign η,

$$\overbrace{\alpha_i \alpha_j \alpha_k \alpha_l} = -\eta \overbrace{\alpha_i \alpha_k} \overbrace{\alpha_j \alpha_l}, \tag{287}$$

where $\eta = +1$ for fermions and $\eta = -1$ for bosons. It also holds

$$\begin{aligned} [\alpha_i, \alpha_j]_\eta &= \alpha_i \alpha_j + \eta \alpha_j \alpha_i \\ &= \begin{cases} \delta_{ij} & \text{for} \quad \left[c_i, c_j^\dagger\right]_\eta \\ \eta \delta_{ij} & \text{for} \quad \left[c_i^\dagger, c_j\right]_\eta \\ 0 & \text{for} \quad [c_i, c_j]_\eta \text{ or } \left[c_i^\dagger, c_j^\dagger\right]_\eta \end{cases}. \end{aligned} \tag{288}$$

To proof this statement we use

$$\alpha_i\alpha_j = -\eta\alpha_j\alpha_i + \left[\alpha_i,\alpha_j\right]_\eta . \tag{289}$$

and write

$$\begin{aligned}\alpha_1\alpha_2\alpha_3\cdots\alpha_{2n} &= \left[\alpha_1,\alpha_2\right]_\eta \alpha_3\cdots\alpha_{2n} \\ &- \eta\alpha_2\alpha_1\alpha_3\cdots\alpha_{2n}.\end{aligned} \tag{290}$$

If we look at the second term, we find similarly

$$\begin{aligned}\alpha_2\alpha_1\alpha_3\cdots\alpha_{2n} &= \alpha_2\left[\alpha_1,\alpha_3\right]_\eta \cdots\alpha_{2n} \\ &- \eta\alpha_2\alpha_3\alpha_1\cdots\alpha_{2n}.\end{aligned} \tag{291}$$

If we repeat this $2n-1$ times, it follows

$$\begin{aligned}\alpha_1\alpha_2\cdots\alpha_{2n} &= \sum_{j=2}^{2n}(-\eta)^{j-2}\,\alpha_2\cdots\alpha_{j-1}\left[\alpha_1,\alpha_j\right]_\eta\alpha_{j+1}\cdots\alpha_{2n} \\ &+ (-\eta)^{2n-1}\,\alpha_2\alpha_3\cdots\alpha_{2n}\alpha_1.\end{aligned} \tag{292}$$

It holds of course that $(-\eta)^{2n-1} = -\eta$.

Next we perform the thermodynamic average

$$\begin{aligned}\left\langle\alpha_2\alpha_3\cdots\alpha_{2n}\alpha_1\right\rangle_0 &= \frac{1}{Z_0}\mathrm{tr}\left(e^{-\beta H_0}\alpha_2\alpha_3\cdots\alpha_{2n}\alpha_1\right) \\ &= \frac{e^{s_1\beta\varepsilon_1}}{Z_0}\mathrm{tr}\left(e^{-\beta H_0}\alpha_1\alpha_2\alpha_3\cdots\alpha_{2n}\right) \\ &= \left\langle\alpha_1\alpha_2\alpha_3\cdots\alpha_{2n}\right\rangle_0 .\end{aligned} \tag{293}$$

Here we used our previous result Eq.(282). From Eq.292 follows then

$$\left\langle\alpha_1\alpha_2\alpha_3\cdots\alpha_{2n}\right\rangle_0 = \sum_{j=2}^{2n}(-\eta)^{j-2}\left\langle\alpha_2\cdots\alpha_{j-1}\,\frac{\left[\alpha_1,\alpha_j\right]_\eta}{1+\eta e^{s_1\beta\varepsilon_1}}\,\alpha_{j+1}\cdots\alpha_{2n}\right\rangle_0 . \tag{294}$$

Since we are dealing with free particles, it holds of course that

$$\begin{aligned}\left\langle c_i^\dagger c_j\right\rangle_0 &= \frac{\delta_{ij}}{e^{\beta\varepsilon_i}+\eta} = \frac{\eta\delta_{ij}}{1+\eta e^{\beta\varepsilon_i}}, \\ &= \frac{\left[c_i^\dagger,c_j\right]_\eta}{1+\eta e^{\beta\varepsilon_i}} = \frac{\left[c_i^\dagger,c_j\right]_\eta}{1+\eta e^{s_i\beta\varepsilon_i}}\end{aligned} \tag{295}$$

as well as

$$\begin{aligned}\left\langle c_i c_j^\dagger\right\rangle_0 &= \delta_{ij} - \eta\left\langle c_j^\dagger c_i\right\rangle_0 = \frac{\delta_{ij}}{1+\eta e^{-\beta\varepsilon_l}}. \\ &= \frac{\left[c_i,c_j^\dagger\right]_\eta}{1+\eta e^{s_i\beta\varepsilon_i}},\end{aligned} \tag{296}$$

while $\left\langle c_i^\dagger c_j^\dagger \right\rangle_0 = \langle c_i c_j \rangle_0 = 0$. With our definition of a contraction, it follows then

$$\frac{[\alpha_i, \alpha_j]_\eta}{1+\eta e^{s_i \beta \varepsilon_i}} = \overbrace{\alpha_i \alpha_j}. \tag{297}$$

which leads to:

$$\langle \alpha_1 \alpha_2 \alpha_3 \cdots \alpha_{2n} \rangle_0 = \sum_{j=2}^{2n} (-\eta)^{j-2} \langle \alpha_2 \cdots \alpha_{j-1} \; \overbrace{\alpha_1 \alpha_j} \; \alpha_{j+1} \cdots \alpha_{2n} \rangle_0 . \tag{298}$$

The contraction itself is, as we just saw, only a number.

We further define, as intermediate steps of the analysis, contractions between operators that are not neighbors, i.e.

$$\begin{aligned} \alpha_i \overbrace{\alpha_j \alpha_k} \alpha_l &= -\eta \overbrace{\alpha_j \alpha_i \alpha_k} \alpha_l \\ &= -\eta \alpha_i \overbrace{\alpha_j \alpha_l} \alpha_k \\ &= \overbrace{\alpha_j \alpha_i \alpha_l \alpha_k} \end{aligned} \tag{299}$$

i.e. we modify the sign of the expression by $-\eta$, depending on whether we performed an even or odd number of exchanges. Then follows

$$\begin{aligned} \langle \alpha_1 \alpha_2 \alpha_3 \cdots \alpha_{2n} \rangle_0 &= \sum_{j=2}^{2n} \overbrace{\alpha_1 \alpha_j} \, (-\eta)^{j-2} \langle \alpha_2 \cdots \alpha_{j-1} \; \alpha_{j+1} \cdots \alpha_{2n} \rangle_0 . \\ &= \sum_{j=2}^{2n} \left\langle \overbrace{\alpha_1 \alpha_2 \cdots \alpha_{j-1} \alpha_j} \alpha_{j+1} \cdots \alpha_{2n} \right\rangle_0 \end{aligned} \tag{300}$$

We can now repeat the procedure for the remaining operators and obtain the sum over all possible pairwise contractions, which proves Wick's theorem.

Two examples are:

$$\begin{aligned} \left\langle c_1^\dagger c_2 c_3^\dagger c_4 \right\rangle_0 &= \overbrace{c_1^\dagger c_2} \overbrace{c_3^\dagger c_4} + \overbrace{c_1^\dagger \overbrace{c_2 c_3^\dagger} c_4} \\ &= \left\langle c_1^\dagger c_2 \right\rangle_0 \left\langle c_3^\dagger c_4 \right\rangle_0 + \left\langle c_1^\dagger c_4 \right\rangle_0 \left\langle c_2 c_3^\dagger \right\rangle_0 \end{aligned} \tag{301}$$

and

$$\begin{aligned} \left\langle c_1^\dagger c_2^\dagger c_3 c_4 \right\rangle_0 &= \overbrace{c_1^\dagger \overbrace{c_2^\dagger c_3} c_4} + \overbrace{\overbrace{c_1^\dagger c_2^\dagger} c_3 c_4} \\ &= \left\langle c_1^\dagger c_4 \right\rangle_0 \left\langle c_2^\dagger c_3 \right\rangle_0 - \eta \left\langle c_1^\dagger c_3 \right\rangle_0 \left\langle c_2 c_4^\dagger \right\rangle_0 . \end{aligned}$$

7.3 Wick theorem for time dependent operators

Our next step is to consider time dependent expectation values of the sort

For the evaluation of $\mathcal{G}_{\mathbf{k}}(\tau)$ and even for the partition function $Z = Z_0 \langle \mathcal{S} \rangle_0$, we consider time dependent expectation values

$$\left\langle T c_{i_1}(\tau_1) \cdots c_{i_n}(\tau_n) c^\dagger_{j_n}(\tau'_n) \cdots c_{j_1}(\tau'_1) \right\rangle_0 . \tag{302}$$

In analogy to our previous notation we use the shorthand

$$\alpha_i(\tau) = c_i(\tau) \quad \text{or} \quad c^\dagger_i(\tau) . \tag{303}$$

Our results for the time dependence of the operators yields

$$\alpha_i(\tau) = e^{s_i \tau \varepsilon_i} \alpha_i , \tag{304}$$

where we remind that

$$s_i = \begin{cases} +1 & \text{if} \quad \alpha_i = c^\dagger_i \\ -1 & \text{if} \quad \alpha_i = c_i \end{cases} . \tag{305}$$

Thus, we want to analyze

$$\langle T \alpha_1(\tau_1) \alpha_2(\tau_2) \cdots \alpha_{2n}(\tau_{2n}) \rangle_0 = e^{\sum_{j=1}^{2n} s_j \tau_j \varepsilon_j} \langle T \alpha_1 \alpha_2 \cdots \alpha_{2n} \rangle_0 \tag{306}$$

Here the time ordering operator arranges the time independent α_i corresponding to the associated time τ_i. Let us for the time beeing assume that the operators are already time ordered, i.e. that

$$\tau_1 > \tau_2 > \cdots \tau_{2n} . \tag{307}$$

Then we only have to analyze

$$\langle \alpha_1 \alpha_2 \cdots \alpha_{2n} \rangle_0 \tag{308}$$

for which we can use the above Wick theorem.

To proceed we define the contraction of time dependent operators

$$\alpha_i \overbrace{(\tau_i) \alpha_j(\tau_j)} \equiv \langle T \alpha_i(\tau_i) \alpha_j(\tau_j) \rangle_0 \tag{309}$$

which we can for $\tau_i > \tau_j$ always write as

$$\alpha_i \overbrace{(\tau_i) \alpha_j(\tau_j)} = e^{\tau_i s_i \varepsilon_i + \tau_j s_j \varepsilon_j} \overbrace{\alpha_i \alpha_j} \tag{310}$$

This implies

$$\begin{aligned} \langle T \alpha_1(\tau_1) \alpha_2(\tau_2) \cdots \alpha_{2n}(\tau_{2n}) \rangle_0 \quad = \quad & \Big\{ \alpha_1 \overbrace{(\tau_1) \alpha_2(\tau_2)} \alpha_3 \overbrace{(\tau_3) \alpha_4(\tau_4)} \cdots \alpha_{2n-1} \overbrace{(\tau_{2n-1}) \alpha_{2n}(\tau_{2n})} \\ + \quad & \alpha_1 \overbrace{(\tau_1) \alpha_2 \overbrace{(\tau_2) \alpha_3 \overbrace{(\tau_3) \alpha_4(\tau_4)}} \cdots \alpha_{2n-1} \overbrace{(\tau_{2n-1}) \alpha_{2n}(\tau_{2n})} \\ + \quad & \cdots \Big\} , \end{aligned} \tag{311}$$

where the sum goes again over all possible pairwise contractions and each crossing of contraction brackets amount to a factor $-\eta$.

In our analysis we made the asssumption that the operators are already time ordered. Suppose this is not the case. Then we need to perform p changes in the order of the operators, amounting to a factor $(-\eta)^p$. This resulting expression can then be analyzed using Wick's theorem. We can then reorder the operators to return to the original, not-time ordered order. However, given our sign-rules for contractions, this also just amounts to another factor $(-\eta)^p$. The total factor is then $(-\eta)^{2p} = 1$. Thus, the above expansion is equally valid even if the operators are not yet time ordered. These insigts can alternatively be written as that the higher order Green;s function

$$\mathcal{G}_0^{(n)}\left(i_1, \cdots i_n; j_1 \cdots j_n\right) = (-1)^n \left\langle T c_{i_1} \cdots c_{i_n} c_{j_n}^\dagger \cdots c_{j_1} \right\rangle_0, \tag{312}$$

can be expressed as

$$\mathcal{G}_0^{(n)}\left(i_1, \cdots i_n; j_1 \cdots j_n\right) = \sum_P (-\eta)^P \mathcal{G}_0\left(i_1; j_{P(1)}\right) \cdots \mathcal{G}_0\left(i_n; j_{P(n)}\right). \tag{313}$$

The sum $\sum_P$ runs over all possible permutations of the indices and P itself is the order of the permutation (i.e. it is even or odd, depending on whether an even or odd number of pairwise exchanges had to be done to achieve the permutation). example, it holds

$$\mathcal{G}_0^{(2)}\left(i_1, i_2; j_1 j_2\right) = \mathcal{G}_0\left(i_1; j_1\right) \mathcal{G}_0\left(i_2; j_2\right) - \eta \mathcal{G}_0\left(i_1; j_2\right) \mathcal{G}_0\left(i_2; j_1\right). \tag{314}$$

8 Diagrammatic expansion of the partition function

We established already that the partition function can be written as

$$Z = Z_0 \left\langle \mathcal{S} \right\rangle_0$$

with

$$\mathcal{S} \equiv \mathcal{S}\left(\beta, 0\right) = T e^{-\int_0^\beta d\tau'' \tilde{V}\left(\tau''\right)}. \tag{315}$$

Thus, we obtain

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int d\tau_1 \cdots d\tau_n \left\langle T V\left(\tau_1\right) \cdots V\left(\tau_n\right) \right\rangle_0. \tag{316}$$

Let us specify the interaction as

$$V\left(\tau\right) = \frac{1}{2} \sum_{klmn} v\left(k, l; n, m\right) c_k^\dagger\left(\tau\right) c_l^\dagger\left(\tau\right) c_m\left(\tau\right) c_n\left(\tau\right) \tag{317}$$

The n-th term in the perturbation expansion is then

$$\begin{aligned}\delta_n &= \frac{(-1)^n}{n!2^n}\int d\tau_1\cdots d\tau_n \sum_{k_1 l_1 m_1 n_1}\cdots\sum_{k_n l_n m_n n_n} v\left(k_1,l_1;m_1,n_1\right)\ldots v\left(k_n,l_n;m_n,n_n\right)\\ &\times \left\langle T c^\dagger_{k_1}\left(\tau_1\right) c^\dagger_{l_1}\left(\tau_1\right) c_{m_1}\left(\tau_1\right) c_{n_1}\left(\tau_1\right)\cdots c^\dagger_{k_n}\left(\tau_n\right) c^\dagger_{l_n}\left(\tau_n\right) c_{m_n}\left(\tau_n\right) c_{n_n}\left(\tau_n\right)\right\rangle_0 \quad (318)\end{aligned}$$

The time ordered expectation value can now be evaluated using Wick's theorem and be expressed in terms of the known non-interacting Green's function.

8.1 Ring diagrams

The partition function inthe ring approximation is:

$$\frac{Z}{Z_0} \approx 1 - \frac{1}{2}\frac{V}{(2\pi)^3}\int d^3q \sum_n \log\left(1 - v(\mathbf{q})\Pi(\mathbf{q},\Omega_n)\right).$$

Let us now take a closer look at the object $\Pi(\mathbf{q},\Omega_n)$ inside the logarithm. We will first focus on the Matsubara summation, therefore we suppress all momentum dependences. It will be straightforward to restore these later. Then $\Pi(\Omega_m)$ is given by the expression

$$\Pi(\Omega_m) = T\sum_n \mathcal{G}_1(\omega_n)\mathcal{G}_2(\omega_n+\Omega_m),$$

where the indices $1,2$ refer to the suppressed variables. As was derived before, the Matsubara Green's functions $\mathcal{G}(\omega_n)$ are equal to the complex Green's functions $G(z)$ evaluated at $z = i\omega_n$. We use this and rewrite the sum as a contour integral. This provides us with the formula

$$\begin{aligned}\Pi(\Omega_m) &= T\sum_n G_1(i\omega_n)G_2(i\omega_n+i\Omega_m)\\ &= -\oint\frac{dz}{2\pi i}f(z)G_1(z)G_2(z+i\Omega_m), \quad (319)\end{aligned}$$

where $f(z) = \frac{1}{e^{\beta z}+1}$ is the Fermi function. The contour integral is taken as shown in the figure. We now want to deform this contour and transform it into a real integration. In doing this we have to be careful, since the complex Green's function has poles on the real-axis. This in turn means that we have to avoid the real axis, since our integrand contains $G_1(z)$. On the other hand, the integrand also contains $G_2(z+i\Omega_m)$, thus we must avoid the horizontal line that goes through $z = -i\Omega_m$ also. We therefore choose a contour as shown in the figure. Clearly this contour gives the same result as the previous one, since we enclose the same poles as before.
As usual, the semicircular arcs do not contribute to the integrals. Therefore only the four horizontal lines have to be taken into account. Let us first consider the two horizontal paths at the bottom. These two paths run in opposite directions

and are infinitesimally displaced relative to each other. We parametrize the two paths by $z = \epsilon + i0^+$ and $z = \epsilon - i0^+$ respectively. Since $f(z)$ and $G_2(z)$ do not have poles near these paths we can ignore the infinitesimal shifts in these functions. Then the sum of the two integrals yields for the contour C_l, along the two lower paths the value

$$-\oint_{\mathcal{C}_l} \frac{dz}{2\pi i} f(z)G_1(z)G_2(z+i\Omega_m) = -\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} f(\epsilon)G_2(\epsilon+i\Omega_m)\left[G_1(\epsilon+i0^+) - G_1(\epsilon-i0^+)\right].$$

Similarly, the two paths on the top are parametrized by $z = -i\Omega_m + i0^+ + \epsilon$ and $z = -i\Omega_m - i0^+ + \epsilon$. Here $f(z)$ and $G_1(z)$ are analytic near these two paths, thus we can ignore the infinitesimal shifts for these functions. Thus we have

$$-\oint_{\mathcal{C}_u} \frac{dz}{2\pi i} f(z)G_1(z)G_2(z+i\Omega_m) = -\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} f(\epsilon-i\Omega_m)G_1(\epsilon-i\Omega_m)\left[G_2(\epsilon+i0^+) - G_2(\epsilon-i0^+)\right].$$

Thus the total contribution to $\Pi(\Omega_M)$ is given by

$$\begin{aligned}\Pi(\Omega_m) &= -\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} f(\epsilon)G_2(\epsilon+i\Omega_m)\left[G_1(\epsilon+i0^+) - G_1(\epsilon-i0^+)\right] \\ &\quad -\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} f(\epsilon)G_1(\epsilon-i\Omega_m)\left[G_2(\epsilon+i0^+) - G_2(\epsilon-i0^+)\right],\end{aligned}$$

where in the second integrand we used the fact that $f(\epsilon - i\Omega_m) = \frac{1}{e^{\beta(\epsilon-i\Omega_m)}+1} = \frac{1}{e^{\beta\epsilon}+1} = f(\epsilon)$. Now we recall that $G_1(\epsilon+i0^+) - G_1(\epsilon-i0^+) = 2i\mathrm{Im}[G_1(\epsilon+i0^+)] = 2iG''_{r1}(\epsilon)$, i.e. the imaginary part of the retarded Green's function and this holds analogously for G_2. Then we are left with

$$\Pi(\Omega_m) = -\int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} f(\epsilon)G_2(\epsilon+i\Omega_m)G''_{r1}(\epsilon) - \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} f(\epsilon)G_1(\epsilon-i\Omega_m)G''_{r2}(\epsilon).$$

Finally we go over to the retarded $\Pi_r(\Omega)$ by making the substitution

$$i\Omega_m = \Omega + i0^+.$$

This gives us

$$\Pi_r(\Omega) = -\int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} f(\epsilon)G_{r2}(\epsilon+\Omega)G''_{r1}(\epsilon) - \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} f(\epsilon)G^*_{r1}(\epsilon-\Omega)G''_{r2}(\epsilon).$$

Let us now look first at the imaginary part of this expression for $\Pi_r(\Omega)$. This gives us

$$\begin{aligned}
\mathrm{Im}[\Pi_r(\Omega)] &= -\left[\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)G''_{r2}(\epsilon+\Omega)G''_{r1}(\epsilon) - \int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)G^{''}_{r1}(\epsilon-\Omega)G''_{r2}(\epsilon)\right] \\
&= -\left[\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)G''_{r2}(\epsilon+\Omega)G''_{r1}(\epsilon) - \int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon+\Omega)G^{''}_{r1}(\epsilon)G''_{r2}(\epsilon+\Omega)\right] \\
&= -\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}\left(f(\epsilon)-f(\epsilon+\Omega)\right)G''_{r2}(\epsilon+\Omega)G''_{r1}(\epsilon).
\end{aligned}$$

We notice the following remarkable fact. If we are at low temperatures, the Fermi function is nearly a step function and $f(\epsilon)-f(\epsilon+\Omega)$ will only be finite, if ϵ and $\epsilon+\Omega$ have different signs, in other words, when one excitation corresponds to a particle and the other to a hole. Intuitively, such particle-hole excitations correspond to the diagram shown.

Let us now insert the forms of the Green's functions and reintroduce the momentum summations. The complex bare Green's functions are given by

$$\begin{aligned}
G_{r1}(\omega) &= \frac{1}{\omega+i0^+-\epsilon_k} \\
G_{r2}(\omega) &= \frac{1}{\omega+i0^+-\epsilon_{\boldsymbol{k}+\boldsymbol{q}}}.
\end{aligned}$$

We need the imaginary parts of these:

$$\begin{aligned}
G''_{r1}(\omega) &= -\pi\delta(\omega-\epsilon_k) \\
G''_{r2}(\omega) &= -\pi\delta(\omega-\epsilon_{\boldsymbol{k}+\boldsymbol{q}})
\end{aligned}$$

Inserting this into the formula for $\Pi_r(\boldsymbol{q},\Omega)$ we obtain

$$\begin{aligned}
\Pi_r(\boldsymbol{q},\Omega) &= -\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)G_{r2}(\epsilon+\Omega)G''_{r1}(\epsilon) - \int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)G^{*}_{r1}(\epsilon-\Omega)G''_{r2}(\epsilon) \\
&= -\sum_{\boldsymbol{k}}\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)\frac{1}{\epsilon+\Omega+i0^+-\epsilon_{\boldsymbol{k}+\boldsymbol{q}}}\left[-\pi\delta(\epsilon-\epsilon_k)\right] \\
&\quad -\sum_{\boldsymbol{k}}\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)\frac{1}{\epsilon-\Omega-i0^+-\epsilon_k}\left[-\pi\delta(\epsilon-\epsilon_{\boldsymbol{k}+\boldsymbol{q}})\right] \\
&= \sum_{\boldsymbol{k}}\frac{f(\epsilon_k)}{\epsilon_k+\Omega+i0^+-\epsilon_{\boldsymbol{k}+\boldsymbol{q}}} + \sum_{\boldsymbol{k}}\frac{f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}})}{\epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\Omega-i0^+-\epsilon_k} \\
&= \sum_{\boldsymbol{k}}\frac{f(\epsilon_k)-f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}})}{\epsilon_k-\epsilon_{\boldsymbol{k}+\boldsymbol{q}}+\Omega+i0^+}.
\end{aligned}$$

This is the Lindhard function that we already found via the equation-of-motion technique.

Let us now return to the evaluation of partition function. There the correction due to the interaction term had the form

$$T\sum_n \log\left[1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\Omega_n)\right].$$

Recall that Ω_n is now a bosonic Matsubara frequency, i.e. $\Omega_n = \frac{\pi}{\beta}2n$. In converting this sum to a contour integral we must be careful about the pole at Ω_0 of the Bose function. Let us therefore carry out the contour integral as shown in the figure. The contour does not include Ω_0 and instead we add it by hand:

$$T\sum_n \log\left[1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\Omega_n)\right] = \oint_{\mathcal{C}} \frac{dz}{2\pi i} n_B(z)\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},z)\right) + T\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},0)\right),$$

where $n_B(z) = \frac{1}{e^{\beta z}-1}$. Converting the contour integral again to real integrals, we have to be careful this time about the Bose function, since it has a pole at $z = 0$:

$$\begin{aligned}\oint_{\mathcal{C}} \frac{dz}{2\pi i} n_B(z)\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},z)\right) &= \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi i} n_B(\epsilon + i0^+)\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\epsilon + i0^+)\right) \\ &\quad - \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi i} n_B(\epsilon - i0^+)\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\epsilon - i0^+)\right).\end{aligned}$$

Let us now evaluate the Bose function near $z = 0$, i.e. $\epsilon \approx 0$:

$$n_B(\epsilon \pm i0^+) = \frac{1}{\exp(\beta(\epsilon \pm i0^+)) - 1} \approx \frac{T}{\epsilon \pm i0^+}$$

Since $\Pi(\boldsymbol{q}, \epsilon \pm i0^+)$ has no poles near $\epsilon = 0$, the only difficulty in the integrals comes from the difference of the Bose functions, i.e. the difference of the of $n_B(\epsilon \pm i0^+)$:

$$n_B(\epsilon + i0^+) - n_B(\epsilon - i0^+) = -2\pi T i\delta(\epsilon)$$

Away from $\epsilon = 0$ the Bose function is regular and we can replace $n_B(\epsilon \pm i0^+)$ by $n_B(\epsilon)$. This gives

$$\begin{aligned}\oint_{\mathcal{C}} \frac{dz}{2\pi i} n_B(z)\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},z)\right) &= \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi i} n_B(\epsilon)\left[\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\epsilon + i0^+)\right) - \log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\epsilon - i0^+)\right)\right] \\ &\quad - T\log\left(1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},0)\right)\end{aligned}$$

but the last term exactly cancels the zeroth Matsubara term that we added by hand. Thus we are left with the simple result:

$$T\sum_n \log\left[1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\Omega_n)\right] = \int_{-\infty}^{+\infty} \frac{d\epsilon}{\pi} n_B(\epsilon)\mathrm{Im}\log\left[1 - v(\boldsymbol{q})\Pi(\boldsymbol{q},\epsilon + i0^+)\right]$$

9 Diagram rules for the single particle Green's function

Next we perform the diagramatic analysis of the single particle Green's function

$$\mathcal{G}_{\mathbf{k}}(\tau) = -\frac{\left\langle T\tilde{\psi}_{\mathbf{k}\alpha}(\tau)\,\tilde{\psi}^{\dagger}_{\mathbf{k}\alpha}(0)\,\mathcal{S}\right\rangle_0}{\langle\mathcal{S}\rangle_0}. \tag{320}$$

We proceed in full analogy to the analysis of the partition function. When we perform contractions, we also have an external time point τ and external momenta $\mathbf{k}$ and spin variable α where no integration is needed.

10 Fermi liquid theory

The key concept underlying Fermi liquid theory is adiabacity, i.e. the assumption that the low energy excitations of an interacting Fermi system are in one-to-one correspondence to the excitations of a non-interacting Fermi gas. The theory was originally developed for ^{3}He, which at low temperatures is a structureless fermion due to the net spin 1/2 in the nucleus. The proton charge is compensated by the two electrons that form a singlet state and therefore don't contribute to the total spin of the system. One simplifying aspect of ^{3}He, if compared to electrons in solids, is the absence of an underlying crystalline lattice. The bare dispersion is then given in form of the free particle dispersion

$$\varepsilon^{\text{free}}_{\mathbf{k}} = \frac{\hbar k^2}{2m}. \tag{321}$$

The quantum numbers of the excited many-body states of a free Fermi gas are the occupations $n_{\mathbf{k}\sigma}$ of single-particle states; the corresponding single-particle states are characterized by momentum and spin: $|\mathbf{k}\sigma\rangle$.

10.1 quasi-particle excitations

In the ground state we continue to assume that the system is characterized by a filled Fermi sea with

$$n^{(0)}_{\mathbf{k}\sigma} = \theta(k_F - k) \tag{322}$$

where k_F is the same as for an ideal Fermi gas with same density:

$$\begin{aligned}\frac{N}{V} &= 2\int \frac{d^3k}{(2\pi)^3} n^{(0)}_{\mathbf{k}\sigma} \\ &= \frac{1}{\pi^2}\int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2}\end{aligned} \tag{323}$$

which yields $k_F = \left(3\pi^2 N/V\right)^{1/3}$. Excitations are now characterized by changes $\delta n_{\mathbf{k}\sigma}$ of the occupations, i.e.

$$n_{\mathbf{k}\sigma} = n^{(0)}_{\mathbf{k}\sigma} + \delta n_{\mathbf{k}\sigma}. \tag{324}$$

The corresponding change in energy is then given by

$$\delta E = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma}. \tag{325}$$

Since the labeling of quantum numbers is the same compared to the free fermi system, purely statistical aspects, like the entropy, should also only be determined by the corresponding ideal Fermi gas expressions:

$$S = -k_B \sum_{\mathbf{k},\sigma} \left(n_{\mathbf{k}\sigma} \log n_{\mathbf{k}\sigma} + (1 - n_{\mathbf{k}\sigma}) \log (1 - n_{\mathbf{k}\sigma}) \right). \tag{326}$$

Maximizing this expression with the condition that $E = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$ and $N = \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma}$, yields

$$n_{\mathbf{k}\sigma} = \frac{1}{e^{\beta \varepsilon_{\mathbf{k}\sigma}} + 1}, \tag{327}$$

where the excitation energy $\varepsilon_{\mathbf{k}\sigma}$ is measured relative to the Fermi energy.

In general, the energy $\varepsilon_{\mathbf{k}\sigma}\left[n_{\mathbf{k}'\sigma'}\right]$ is a functional of the occupations of all states in the system. If we first add only one particle to the ground state, we can safely say that

$$\varepsilon^0_{\mathbf{k}\sigma} \equiv \varepsilon_{\mathbf{k}\sigma}\left[n^0_{\mathbf{k}'\sigma'}\right] \tag{328}$$

is the dispersion of the single particle, where $n^0_{\mathbf{k}\sigma} = \theta\left(k_F - k\right)$. Near E_F we make the assumption

$$\varepsilon^0_{\mathbf{k}\sigma} = v\left(k - k_F\right), \tag{329}$$

where the parameter $v = k_F/m^*$ is often expressed in terms of the effective mass m^*. This immediately leads to the density of states

$$\rho_F = \frac{m^* k_F}{\pi^2 \hbar^2}, \tag{330}$$

that is modified by the factor m^*/m compared to the free fermion expression. An immediate consequence of this modified density of states emerges for the heat capacity

$$\begin{aligned} C &= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}\sigma} \frac{d}{dT} n_{\mathbf{k}\sigma} = \rho_F \int_{-\infty}^{\infty} d\varepsilon \varepsilon \frac{d}{dT} \frac{1}{e^{\varepsilon/(k_B T)} + 1} \\ &= \gamma T, \end{aligned} \tag{331}$$

where

$$\gamma = \frac{\pi^2 k_B^2}{3} \rho_F = \frac{m^*}{m} \gamma_{\text{free}}. \tag{332}$$

Here, γ_{free} is the heat capacity of non-interacting fermions.

A key additional aspect of the Landau theory is that in case of excitations with more than one particle, the changes in the occupations $\delta n_{\mathbf{k}\sigma}$ will lead to changes $\delta\varepsilon_{\mathbf{k}\sigma}$ of the quasi-particle energies. Thus one writes generally

$$\varepsilon_{\mathbf{k}\sigma} = \varepsilon^0_{\mathbf{k}\sigma} + \delta\varepsilon_{\mathbf{k}\sigma} \tag{333}$$

where

$$\delta\varepsilon_{\mathbf{k}\sigma} = \frac{1}{N}\sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'}. \tag{334}$$

$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$ is a phenomenological interaction parameter that determines the extend to which the energy of state $|\mathbf{k},\sigma\rangle$ is affected by a change in population $\delta n_{\mathbf{k}'\sigma'}$ of $|\mathbf{k}',\sigma'\rangle$. If we do not want to have a preference of one spin direction over the other (in the absence of an external magnetic field) we write

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f^s_{\mathbf{k},\mathbf{k}'} + \sigma\sigma' f^a_{\mathbf{k},\mathbf{k}'}. \tag{335}$$

In addition we assume that all relevant momenta are on the Fermi surface, i.e. $\mathbf{k} = k_F\mathbf{e}_{\mathbf{k}}$ and $\mathbf{k}' = k_F\mathbf{e}_{\mathbf{k}'}$ where $\mathbf{e}^2_{\mathbf{k}} = \mathbf{e}^2_{\mathbf{k}'} = 1$ are unit vectors. In an isotropic system like ^{3}He, with no preferred direction, one expects that $f^{s,a}_{\mathbf{k},\mathbf{k}'}$ only depend on the angle θ between $\mathbf{k}$ and $\mathbf{k}'$, i.e. on $\cos\theta_{\mathbf{k},\mathbf{k}'} = \mathbf{e}_{\mathbf{k}}\cdot\mathbf{e}_{\mathbf{k}'}$:

$$f^{s,a}_{\mathbf{k},\mathbf{k}'} = f^{s,a}\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right). \tag{336}$$

Since $f^{s,a}$ are of dimension energy, dimensionless quantities follow via

$$F^{s,a} = \rho_F f^{s,a}. \tag{337}$$

We expand $F^{s,a}\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right)$ in Legendre polynomials

$$F^{s,a}\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right) = \sum_{l=0}^{\infty} F^{s,a}_l P_l\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right) \tag{338}$$

and use the usual representation in terms of spherical harmonics

$$F^{s,a}\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right) = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{F^{s,a}_l}{2l+1}Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right)Y^*_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right). \tag{339}$$

The orthogonality of the Legendre polynomials

$$\frac{1}{2}\int_{-1}^{1} d\cos\theta P_l\left(\cos\theta\right)P_{l'}\left(\cos\theta\right) = \frac{\delta_{l,l'}}{2l+1} \tag{340}$$

allows for the representation

$$\begin{aligned} F_l^{s,a} &= \frac{2l+1}{2}\int_{-1}^{1} d\cos\theta F^{s,a}\left(\cos\theta\right) P_{l'}\left(\cos\theta\right) \\ &= \frac{2l+1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta F^{s,a}\left(\cos\theta\right) P_{l'}\left(\cos\theta\right) \\ &= \frac{2l+1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \int d\varepsilon F^{s,a}\left(\cos\theta\right) P_{l'}\left(\cos\theta\right)\delta\left(\varepsilon\right) \\ &= \frac{2\left(2l+1\right)}{\rho_F}\frac{1}{N}\sum_{\mathbf{k}'} F^{s,a}_{\mathbf{k},\mathbf{k}'} P_l\left(\cos\theta_{\mathbf{k},\mathbf{k}'}\right)\delta\left(\varepsilon_{\mathbf{k}}\right). \end{aligned} \tag{341}$$

10.2 Susceptibilities

Suppose we are at $T = 0$ we add an external perturbation of the type

$$\delta\varepsilon^0_{\mathbf{k}\sigma} = \left(v_l^s + \sigma v_l^a\right) Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right), \tag{342}$$

where the spherical harmonic determines the directional dependence on the momentum and $v_l^{s,a}$ are the amplitudes of the perturbation. In case of an external magnetic field holds $\delta\varepsilon^0_{\mathbf{k}\sigma} = -\sigma\mu_B B$, i.e. we have $m = l = 0$ and, due to $Y_{00} = 4\pi$, $v_0^a = -\sigma\mu_B B/4\pi$ and $v_0^s = 0$. A change in the chemical potential $\delta\mu$ amounts to $\delta\varepsilon^0_{\mathbf{k}\sigma} = -\delta\mu$, i.e. $m = l = 0$ and $v_0^s = -\delta\mu/4\pi$ and $v_0^a = 0$. In general we can introduce the susceptibility

$$\chi_l^{s,a} = -\frac{\partial^2 E}{\partial\left(v_l^{s,a}\right)^2}. \tag{343}$$

In particular, this allows us to determine physical observables like the magnetic susceptibility

$$\chi_s = \frac{1}{V}\left.\frac{\partial M}{\partial B}\right|_{B=0} \tag{344}$$

with magnetization $M = \mu_B\sum_{\mathbf{k},\sigma}\sigma n_{\mathbf{k}\sigma}$. Another option is the charge susceptibility

$$\chi_c = \frac{1}{V}\left.\frac{\partial N}{\partial\left(\delta\mu\right)}\right|_{\delta\mu=0} \tag{345}$$

with particle number $N = \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma}$. χ_c is closely related to the compressibility

$$\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} = n^{-2}\frac{\partial n}{\partial\mu}.$$

which holds for a system where the free energy can be written as $F\left(V,N\right) = Nf\left(n\right)$, where $n = N/V$ is the particle density.

In case of a free Fermi gas follows

$$\begin{aligned} \chi_s^0 &= \mu_B^2\rho_F^0 \\ \chi_c &= \rho_F^0. \end{aligned} \tag{346}$$

where the mass in the density of states ρ_F^0 is m, not m^*.

Since fermions of a Fermi liquid are interacting there is no reason that an external field or chemical potential change will change the quasiparticle energies $\varepsilon_{\mathbf{k}\sigma}$ in the exact same fashion as $\delta\varepsilon_{\mathbf{k}\sigma}^0$. Thus, we assume

$$\begin{aligned}\delta\varepsilon_{\mathbf{k}\sigma} &= \delta\varepsilon_{\mathbf{k}\sigma}^0 + \frac{1}{N}\sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'} \\ &= \left(t_l^s + \sigma t_l^a\right) Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right), \end{aligned} \tag{347}$$

where in general $t_l^{s,a} \neq v_l^{s,a}$. Suppose there is such an energy shift, then we can determine the associated particle density shift from Eq.327

$$\begin{aligned} n_{\mathbf{k}\sigma} &= \frac{1}{e^{\beta\left(\varepsilon_{\mathbf{k}\sigma}^0 + \delta\varepsilon_{\mathbf{k}\sigma}\right)} + 1} \\ &= \theta\left(k_F - k\right) - \delta\left(\varepsilon_{\mathbf{k}\sigma}^0\right)\delta\varepsilon_{\mathbf{k}\sigma}, \end{aligned} \tag{348}$$

which yields

$$\delta n_{\mathbf{k}\sigma} = -\delta\left(\varepsilon_{\mathbf{k}\sigma}^0\right)\delta\varepsilon_{\mathbf{k}\sigma}. \tag{349}$$

This result can now be inserted into Eq.347 which yields

$$\delta\varepsilon_{\mathbf{k}\sigma} = \delta\varepsilon_{\mathbf{k}\sigma}^0 - \frac{1}{N}\sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta\left(\varepsilon_{\mathbf{k}'\sigma'}^0\right)\delta\varepsilon_{\mathbf{k}'\sigma'} \tag{350}$$

or equivalently

$$t_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) = v_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) - \frac{1}{N}\sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta\left(\varepsilon_{\mathbf{k}'\sigma'}^0\right) t_l^{\sigma'} Y_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right) \tag{351}$$

Now we can use the above expansion of $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$ in spherical harmonics

$$\begin{aligned} t_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) &= v_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) - \frac{\rho_F}{2}\int d\Omega_{\mathbf{k}'}\sum_{\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} t_l^{\sigma'} Y_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right) \\ &= v_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) - \frac{\rho_F}{2}\int \frac{d\Omega_{\mathbf{k}'}}{4\pi}\sum_{\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} t_l^{\sigma'} Y_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right) \\ &= v_l^\sigma Y_{lm}\left(\mathbf{e}_{\mathbf{k}}\right) - \frac{1}{2}\int d\Omega_{\mathbf{k}'}\sum_{\sigma'}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \frac{F_{l'}^s + \sigma\sigma' F_{l'}^a}{2l+1} \\ &\quad \times Y_{l'm'}\left(\mathbf{e}_{\mathbf{k}}\right) Y_{l'm'}^*\left(\mathbf{e}_{\mathbf{k}'}\right) t_l^{\sigma'} Y_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right) \end{aligned} \tag{352}$$

We use the orthogonality of the spherical harmonics

$$\int d\Omega_{\mathbf{k}'} Y_{l'm'}^*\left(\mathbf{e}_{\mathbf{k}'}\right) Y_{lm}\left(\mathbf{e}_{\mathbf{k}'}\right) = \delta_{ll'}\delta_{mm'} \tag{353}$$

and obtain

$$t_l^\sigma = v_l^\sigma - \frac{1}{2}\sum_{\sigma'} t_l^{\sigma'}\frac{F_l^s + \sigma\sigma' F_l^a}{2l+1}. \tag{354}$$

If we consider for example a change in the chemical potential with, $v_0^\sigma = -\delta\mu/4\pi$, it follows for $t_0^\sigma = t_0$ spin independent, that

$$t_0 = v_0 - t_0 F_0^s \tag{355}$$

which leads to

$$t_0 = \frac{v_0}{1+F_0^s}. \tag{356}$$

It is now straightforward to determine the charge susceptibility via

$$\begin{aligned} \chi_c &= \frac{1}{V}\frac{\partial N}{\partial(\delta\mu)} = -\frac{1}{4\pi}\frac{1}{V}\frac{\partial N}{\partial v_0} \\ &= -\frac{1}{4\pi}\frac{1}{V}\frac{\partial N}{\partial t_0}\frac{\partial t_0}{\partial v_0} \\ &= -\frac{1}{1+F_0^s}\frac{1}{4\pi}\frac{1}{V}\frac{\partial N}{\partial t_0}. \end{aligned} \tag{357}$$

To determine $\frac{-1}{4\pi}\frac{1}{V}\frac{\partial N}{\partial t_0}$ we use

$$n_{\mathbf{k}\sigma} = \frac{1}{e^{\beta\left(\frac{k_F}{m^*}(k-k_F)+4\pi t_0\right)}+1}$$

The derivative of $N = \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma}$ with respect to t_0 can be performed, e.g. by resorting to our above result for the charge susceptibility of a free electron gas (with the difference that we need to consider the effective mass, not the bare mass). It follows $\frac{-1}{4\pi}\frac{1}{V}\frac{\partial N}{\partial t_0} = \rho_F$ and we obtain

$$\chi_c = \frac{\rho_F}{1+F_0^s}$$

Thus, the charge susceptibility is different from the free fermi gas value in two ways. First, in the density of states the mass m is replaced by the effective mass m^*. In addition the interactions lead to an overall coefficient $(1+F_0^s)^{-1}$. The theory is therefore stable as long as $F_0^s < -1$. If $F_0^s \to -1$ the system will undergo a transition to a regime where different densities phase segregate.

As will be discussed in a homework assignment, if the system in Gallilei invariant, one can further derive a relationship between the effective mass m^* and the Landay parameter F_1^s:

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s. \tag{358}$$

11 Conservation laws and Ward-Identities

Next we will address the implication of conservation laws within the many body description of condensed matter systems. Within quantum mechanics, conservation laws are generally associated with an operator O that commutes with the Hamiltonian

$$[O, H] = 0. \tag{359}$$

Whenever we have to deal with a conserved quantity, it is often natural to introduce an associated density $\rho(\mathbf{r},t)$, such that

$$O=\int_V d^d r\rho(\mathbf{r},t). \tag{360}$$

The density then obeys a continuity equation

$$\partial_t\rho+\nabla\cdot\mathbf{j}=0, \tag{361}$$

which determines the associated current density in the long wave-length limit. Integrating this equation over a volume V yields the Gauss'-theorem

$$\partial_t O=-\int_{\partial V}\mathbf{j}\cdot d\mathbf{S}, \tag{362}$$

where ∂V is the surface of V and $d\mathbf{S}$ refers to the surface element directed along the outward normal of the surface. If the volume V is chosen to correspond to the entire system, the current of a conserved quantity obviously has to vanish.

Let us consider a system with Hamiltonian

$$H=H_0+V, \tag{363}$$

where

$$H_0=\sum_{\mathbf{k}\alpha}\varepsilon_{\mathbf{k}}\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}. \tag{364}$$

A natural conservation law is associated with charge or particle conservation, i.e. $O=N$. In non-relativistic systems, the conservation of the total spin, i.e. $O=\mathbf{S}$ is another example. One must however keep in mind that the weak relativistic spin-orbit interaction will violate spin-conservation. Let us consider the charge conservation. The associated density is obviously

$$\rho(\mathbf{r},t)=\sum_\alpha\psi^\dagger_\alpha(\mathbf{r},t)\,\psi_\alpha(\mathbf{r},t). \tag{365}$$

In momentum space this coresponds to

$$\rho_{\mathbf{q}}=\frac{1}{N}\sum_{\mathbf{k}\alpha}\psi^\dagger_{\mathbf{k}+\mathbf{q}\alpha}\psi_{\mathbf{k}\alpha}. \tag{366}$$

In order to keep our argumentation sufficiently general, we will consider densities of the form

$$\rho_{\mathbf{q}}=\sum_{\mathbf{k}\alpha\beta}\psi^\dagger_{\mathbf{k}+\frac{\mathbf{q}}{2},\alpha}\phi_{\alpha\beta}(\mathbf{k})\,\psi_{\mathbf{k}-\frac{\mathbf{q}}{2},\beta}, \tag{367}$$

with form factor $\phi_{\alpha\beta}(\mathbf{k})$. The charge density corresponds to $\phi_{\alpha\beta}(\mathbf{k})=\delta_{\alpha\beta}$, and a spin density amounts to the $\phi_{\alpha\beta}(\mathbf{k})=\sigma^j_{\alpha\beta}$ for the three Pauli matrices.

In what follows we consider systems where $[\rho_{\mathbf{q}},V]=0$. This is the case for the charge density with electron-electron Coulomb interaction. In case of the

spin-density it is true for all systems without spin-orbit interaction. In order to obtain the associated current, we evaluate the commutator of $\rho_{\mathbf{q}}$ with the Hamiltonian, where we only need to focus on the commutator with the kinetic energy:

$$[H_0, \rho_{\mathbf{q}}] = \sum_{\mathbf{k}\alpha\beta} \left(\varepsilon_{\mathbf{k}+\frac{\mathbf{q}}{2}} - \varepsilon_{\mathbf{k}-\frac{\mathbf{q}}{2}} \right) \psi^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}\alpha} \phi_{\alpha\beta}(\mathbf{k}) \psi_{\mathbf{k}-\frac{\mathbf{q}}{2}\alpha}. \tag{368}$$

This expression can be expanded for small momenta $\mathbf{q}$ and yields

$$\partial_t \rho_{\mathbf{q}} = i[H_0, \rho_{\mathbf{q}}] = i\mathbf{q} \cdot \sum_{\mathbf{k}\alpha\beta} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \psi^{\dagger}_{\mathbf{k}\alpha} \phi_{\alpha\beta}(\mathbf{k}) \psi_{\mathbf{k}\beta}. \tag{369}$$

Fourier transformation of the continuity-equation yields $\partial_t \rho_{\mathbf{q}} = i\mathbf{q} \cdot \mathbf{j}$ such that

$$\mathbf{j} = \sum_{\mathbf{k}\alpha b} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \psi^{\dagger}_{\mathbf{k}\alpha} \phi_{\alpha\beta}(\mathbf{k}) \psi_{\mathbf{k}\beta}. \tag{370}$$

Next we want to explore the implications of conservation laws for associated Green's functions. To this end we recall that a density-density susceptibility is expressed as

$$\chi_c(\mathbf{q}, \tau) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'\alpha\beta} \left\langle T \psi^{\dagger}_{\mathbf{k}\alpha}(\tau) \psi_{\mathbf{k}+\mathbf{q}\alpha}(\tau) \psi^{\dagger}_{\mathbf{k}'\beta} \psi_{\mathbf{k}'-\mathbf{q}\beta} \right\rangle.$$

Since we consider generalized densities with form factor $\phi_{\alpha\beta}(\mathbf{k})$, it is useful to analyze:

$$Q^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega) = \int d\tau e^{i\Omega\tau} \left\langle T \psi^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}\alpha}(\tau) \psi_{\mathbf{k}-\frac{\mathbf{q}}{2}\beta}(\tau) \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(0) \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(0) \right\rangle. \tag{371}$$

Just like for the retarded function we can exploit the equation of motion

$$\begin{aligned}
\partial_\tau \left\langle T \rho_{\mathbf{q}}(\tau) \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(\tau') \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau'') \right\rangle &= \left\langle T [H(\tau), \rho_{\mathbf{q}}(\tau)] \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(\tau') \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau'') \right\rangle \\
&+ \delta(\tau - \tau') \left\langle T \left[\rho_{\mathbf{q}}(\tau), \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(\tau') \right] \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau'') \right\rangle \\
&+ \delta(\tau - \tau'') \left\langle T \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(\tau') \left[\rho_{\mathbf{q}}(\tau), \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau'') \right] \right\rangle.
\end{aligned}$$

For the commutators follows

$$\begin{aligned}
\left[\rho_{\mathbf{q}}, \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma} \right] &= \sum_{\alpha} \psi^{\dagger}_{\mathbf{k}'+\frac{\mathbf{q}}{2},\alpha} \phi_{\alpha\gamma}(\mathbf{k}'), \\
\left[\rho_{\mathbf{q}}, \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta} \right] &= -\sum_{\beta} \phi_{\delta\beta}(\mathbf{k}') \psi_{\mathbf{k}'-\frac{\mathbf{q}}{2},\beta}.
\end{aligned} \tag{372}$$

We can now insert the density and current and Fourier transform the resulting correlator

$$\begin{aligned}
G^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega, \omega) &= \int d\tau d\tau' e^{i\Omega\tau + \omega\tau''} \\
&\times \left\langle T \psi^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}\alpha}(\tau) \psi_{\mathbf{k}-\frac{\mathbf{q}}{2}\beta}(\tau) \psi^{\dagger}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(0) \psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau'') \right\rangle
\end{aligned}$$

which yields in particular for $Q^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega)$, needed in the determination of susceptibilities, that

$$Q^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega) = T\sum_{\omega} G^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega,\omega)\,. \tag{373}$$

The above equation of motion now leads to the Ward-identity:

$$\sum_{\mathbf{k}\alpha\beta}\left(i\Omega - \left(\varepsilon_{\mathbf{k}+\frac{\mathbf{q}}{2}} - \varepsilon_{\mathbf{k}-\frac{\mathbf{q}}{2}}\right)\right)\phi_{\alpha\beta}(\mathbf{k})\, G^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega,\omega) \quad = \quad \phi_{\delta\gamma}(\mathbf{k}')\left(\mathcal{G}_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\omega) - \mathcal{G}_{\mathbf{k}'-\frac{\mathbf{q}}{2}\gamma}(\omega+\Omega)\right),$$

with usual single particle Green's function

$$\mathcal{G}_{\mathbf{k}\alpha}(\omega) = -\int d\tau e^{i\omega\tau}\left\langle T\psi_{\mathbf{k}'+\frac{\mathbf{q}}{2}\delta}(\tau)\,\psi^{\dagger}_{\mathbf{k}'+\frac{\mathbf{q}}{2},\alpha}(0)\right\rangle.$$

The above Ward identity allows to draw conclusions for the two susceptibilities:

$$\begin{aligned}
\chi_{\rho}(\mathbf{q},\Omega) &= T\sum_{\mathbf{k},\mathbf{k}',\omega}\sum_{\alpha\beta\gamma\delta}\phi^{\alpha\beta}(\mathbf{k})\,\phi^{\gamma\delta}(\mathbf{k}')\,G^{(4)\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega,\omega)\\
\chi^{ij}_{J}(\mathbf{q},\Omega) &= T\sum_{\mathbf{k},\mathbf{k}',\omega}\sum_{\alpha\beta\gamma\delta}\phi^{\alpha\beta}(\mathbf{k})\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k_i}\phi^{\gamma\delta}(\mathbf{k}')\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k_j}G^{(4)\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\Omega,\omega)\,.
\end{aligned}$$

In case of the susceptibility χ_ρ of the associated conserved density, it follows from the Ward identity that

$$\begin{aligned}
\chi_{\rho}(\mathbf{q}=\mathbf{0},\Omega\neq 0) &= T\sum_{\mathbf{k}',\omega\gamma\delta}\phi^{\gamma\delta}(\mathbf{k}')\,\frac{\mathcal{G}_{\mathbf{k}'}(\omega)-\mathcal{G}_{\mathbf{k}'}(\omega+\Omega)}{i\Omega}\\
&= 0.
\end{aligned} \tag{374}$$

This identity can be used to check whether a given approximation used to analyze a many body problem respects the corresponding conservation law. Notice, that this is precisely the behavior we found earlier for the Lindhard function. Here it is a behavior caused by charge conservation.

In addition we can draw conclusions about the susceptibility of the associated current-current susceptibility.

$$\chi^{ij}_{J}(\mathbf{q},0)\Big|_{\mathbf{q}=q\mathbf{e}_i\to 0} = -T\sum_{\mathbf{k}',\omega\gamma\delta}\left(\phi^{\gamma\delta}(\mathbf{k}')\right)^2\frac{\partial\mathcal{G}_{\mathbf{k}'}(\omega)}{\partial k'_i}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k'_j}.$$

12 Physics of Graphene

13 Superconductivity

The microscopic theory of superconductivity was formulated by John Bardeen, Leon N. Cooper, and J. Robert Schrieffer. It is among the most beautiful and successful theories in physics. The BCS-theory starts from an effective Hamiltonian of fermionic quasiparticle excitations that interact via a weak attractive

interaction. It yields a ground-state many-body wave function and thermal excitations to describe superconductivity. Historically, the first underlying microscopic mechanism that lead to such an attraction was the exchange of lattice vibrations. In the meantime ample evidence exists, in particular in case of the copper-oxide high-temperature superconductors, for superconductivity that is caused at least predominantly by electronic interactions. Other materials that are candidates for electronically induced pairing are the heavy electron systems, organic charge transfer salts and the iron based superconductors.

13.1 off-diagonal long range order

The initial observation of superconductivity was made by measuring the resistivity $\rho(T)$ of mercury as function of temperature. Below the superconducting transition temperature, T_c, $\rho(T) = 0$ with very high precision. Understanding this drop in the resistivity is a major challenge in a theory of superconductivity. We will return to this problem later. Arguably even more fundamental than the vanishing voltage drop are two central experiments: the Meissner effect and the quantization of the magnetic flux in multiply connected superconductors. The Meissner effect implies that a weak magnetic field is expelled from the bulk of a superconductor. The effect occurs regardless of whether the external field is switched on for temperatures below T_c or before the system is cooled down to enter the superconducting state. This strongly supports the view that a superconductor is in thermal equilibrium. Multiply connected superconducting geometries such as a ring, can however lead to a subtle memory effects. Switching off an external magnetic field for $T < T_c$ leads to magnetic flux trapped in non-superconducting holes. This flux takes values that are integer multiples of the flux quantum

$$\Phi_0 = \frac{h}{2e} \approx 2.067833758(46) \times 10^{-15}\ \mathrm{Tm}^2, \tag{375}$$

where h is Planck's constant and e the magnitude of the electron charge e. By discussing in some detail the concept of off-diagonal long range order we give precise microscopic criteria that lead to the Meissner effect and to flux quantization. A theory of superconductivity consistent with these criteria is therefore guaranteed to correctly describe these fundamental experimental observations. As we will see later, the BCS theory is such a theory.

Off-diagonal long-range order (ODLRO) is a natural generalization of the Bose-Einstein condensation of free bosons to the regime of interacting systems. It was introduced to capture the nontrivial physics of superfluid ^{4}He[**?**, **?**] and later generalized to describe superconductivity and superfluidity of fermions[**?**]. The formal definition is based on the single-particle and two-particle density matrix $\rho^{(1)}$ and $\rho^{(2)}$, respectively:

$$\begin{aligned} \rho^{(1)}_{\alpha\alpha'}(\mathbf{r},\mathbf{r}') &= \left\langle \psi^\dagger_\alpha(\mathbf{r})\,\psi_{\alpha'}(\mathbf{r}')\right\rangle, \\ \rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2) &= \left\langle \psi^\dagger_\alpha(\mathbf{r}_1)\,\psi^\dagger_\beta(\mathbf{r}_2)\,\psi_{\beta'}(\mathbf{r}'_2)\,\psi_{\alpha'}(\mathbf{r}'_1)\right\rangle. \end{aligned} \tag{376}$$

$\psi_\alpha^\dagger(\mathbf{r})$ and $\psi_\alpha(\mathbf{r})$ are the creation and annihilation operators of a boson or fermion at position $\mathbf{r}$ and with spin α, respectively. The operators are in the Schrödinger picture such that the $\rho^{(n)}$ are independent on time in thermal equilibrium. Generalizations to an n-particle density matrix $\rho^{(n)}$ with $n > 2$ or averages with respect to a non-equilibrium scenario are straightforward. Before we define ODLRO, we summarize a few properties of these density matrices. We obtain immediately the expected normalization

$$\mathrm{tr}\rho^{(1)} = \int d^d r \sum_\alpha \rho^{(1)}_{\alpha\alpha'}(\mathbf{r},\mathbf{r}) = N \tag{377}$$

as well as

$$\mathrm{tr}\rho^{(2)} = \int d^d r_1 d^d r_2 \sum_{\alpha\beta} \rho^{(2)}_{\alpha\beta\alpha\beta}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_2) = N(N-1). \tag{378}$$

We first concentrate on spin-less bosons in a translation invariant system and analyze $\rho^{(1)}$. It is a hermitian matrix with respect to the matrix indices $\mathbf{r}$ and $\mathbf{r}'$. If n_p is the p-th real eigenvalue of $\rho^{(1)}$ with eigenvector $\phi_p(\mathbf{r})$, we can expand[6]

$$\rho^{(1)}(\mathbf{r},\mathbf{r}') = \sum_p n_p \phi_p^*(\mathbf{r}')\phi_p(\mathbf{r}). \tag{379}$$

A macroscopic occupation of a single-particle state occurs if there exists one eigenvalue, say n_0, that is of order of the particle number N of the system. This is a natural generalization of Bose-Einstein condensation to interacting systems. Off-diagonal long range order occurs if for large distances $|\mathbf{r}-\mathbf{r}'|$ the expansion, Eq.379, is dominated by a single term (the one with the macroscopic eigenvalue n_0 and eigenfunction $\phi_0(\mathbf{r})$). The condition for ODLRO is therefore

$$\rho^{(1)}(\mathbf{r},\mathbf{r}')\Big|_{|\mathbf{r}-\mathbf{r}'|\to\infty} \to n_0\phi_0^*(\mathbf{r}')\phi_0(\mathbf{r}). \tag{380}$$

For a translation invariant system further holds that $\rho^{(1)}(\mathbf{r},\mathbf{r}') = \rho^{(1)}(\mathbf{r}-\mathbf{r}')$, i.e. the quantum number p corresponds to the momentum vector $\mathbf{p}$. In the

[6]Consider a hermitian matrix A with eigenvectors $\mathbf{x}_{(n)}$ and eigenvalues $\lambda_{(n)}$, i.e.

$$\sum_j A_{ij} x_{(n)j} = \lambda_{(n)} x_{(n)i}.$$

We can consider the matrix A_{ij} for given j as vector with components labelled by i and expand with respect to the complete set of eigenvectors. The same can be done for the other index. This implies

$$A_{ij} = \sum_{pq} \alpha_{(p,q)} x_{(p)i} x^*_{(q)j}.$$

Inserting this expansion into the eigenvalue equation and using the orthogonality and normalization of the eigenvectors ($\sum_j x^*_{(p)j} x_{(q)j} = \delta_{pq}$) it follows

$$\sum_j A_{ij} x_{(n)j} = \sum_p \alpha_{(p,n)} x_{(n)i}.$$

Since the $\mathbf{x}_{(n)}$ are eigenvectors it follows $\alpha_{(p,n)} = \lambda_{(n)}\delta_{p,n}$.

thermodynamic limit holds that $\lim_{\mathbf{r}\to\infty}\rho^{(1)}(\mathbf{r}) = \alpha N/V$ with α a generally complex coefficient where $|\alpha|$ is of order unity. Here V is the volume of the system and we used $\phi_0 \approx \frac{1}{\sqrt{V}}$.

We first consider the case of free bosons where $\phi_p(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{p}\cdot\mathbf{r}}$ and the eigenvalues are given by the Bose-Einstein distribution function:

$$n_{\mathbf{p}} = \frac{1}{e^{\beta(\epsilon(\mathbf{p})-\mu)}-1}. \tag{381}$$

We consider the regime above the Bose-Einstein condensation temperature with

$$k_B T_{\mathrm{BEC}} = 2\pi\varsigma\left(\frac{3}{2}\right)^{-2/3}\frac{\hbar^2}{m}\left(N/V\right)^{2/3}, \tag{382}$$

where $\mu < 0$ and the occupation of all single-particle states behaves in the thermodynamic limit as $\lim_{N\to\infty} n_{\mathbf{p}}/N = 0$. $n_{\mathbf{p}}$ decays for increasing momenta exponentially on the scale $2\pi/\lambda_T$ with thermal de Broglie wave length

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{k_B T m}}. \tag{383}$$

It follows

$$\rho^{(1)}(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{p}} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} = \int \frac{d^3p}{(2\pi)^3} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \tag{384}$$

decays exponentially like e^{-r/λ_T}, implying no ODLRO. On the other hand, in case of a macroscopic occupation $n_{\mathbf{0}} = \alpha N$ of the lowest energy state, i.e. for $\mathbf{p} = \mathbf{0}$, below T_{BEC} follows

$$\rho^{(1)}(\mathbf{r}) = \alpha\frac{N}{V} + \frac{1}{V}\sum_{\mathbf{p}>0} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \tag{385}$$

The second term decays exponentially, with the same reasoning as for $T > T_{BEC}$ while the first term gives rise to ODLRO. Our reasoning is in fact more general. In case of a macroscopic occupation of a momentum state, i.e. $n_{\mathbf{p}_0} = \alpha_0 N$ holds

$$\lim_{\mathbf{r}\to\infty}\rho^{(1)}(\mathbf{r}) = \alpha_0\frac{N}{V}e^{i\mathbf{p}_0\cdot\mathbf{r}} \tag{386}$$

as long as the occupation of all other momentum states decays sufficiently fast for large momenta, they will not contribute in the limit of large $\mathbf{r}$. Thus, we have established that the macroscopic occupation of states is rather generally related to large distant correlations of the one particle density matrix.

Next we discuss some physical implications of this observation and demonstrate that charged bosons with ODLRO are subject to the Meissner effect and flux quantization. The discussion is adapted from Refs.[**?**, **?**] where fermionic

systems were discussed. We start from the Hamiltonian of a system of bosons in a uniform magnetic field $\mathbf{B}$:

$$H = \sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i - \mathbf{r}_j\right). \tag{387}$$

The vector potential can be written as

$$\mathbf{A}\left(\mathbf{r}\right) = \mathbf{A_0}\left(\mathbf{r}\right) + \nabla\varphi\left(\mathbf{r}\right), \tag{388}$$

where $\mathbf{A}_0\left(\mathbf{r}\right) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ and φ is an arbitrary function. The many-body wave function of the problem is $\Psi_\nu\left(\mathbf{r}_1,\cdots,\mathbf{r}_N\right) = \Psi_\nu\left(\mathbf{r}_j\right)$.

Let us perform a spatial displacement $\mathbf{r}_j \to \mathbf{r}_j - \mathbf{a}$ with some length scale $\mathbf{a}$. The boson-boson interaction is invariant with respect to this transformation, while the vector potential transforms as

$$\begin{aligned}
\mathbf{A}\left(\mathbf{r}\right) &\to \mathbf{A}\left(\mathbf{r}-\mathbf{a}\right) \\
&= \mathbf{A}\left(\mathbf{r}\right) - \frac{1}{2}\mathbf{B}\times\mathbf{a} + \nabla\left(\varphi\left(\mathbf{r}-\mathbf{a}\right) - \varphi\left(\mathbf{r}\right)\right) \\
&= \mathbf{A}\left(\mathbf{r}\right) + \nabla\chi_{\mathbf{a}}\left(\mathbf{r}\right),
\end{aligned} \tag{389}$$

with

$$\chi_{\mathbf{a}}\left(\mathbf{r}\right) = \mathbf{a}\cdot\mathbf{A}_0\left(\mathbf{r}\right) + \varphi\left(\mathbf{r}-\mathbf{a}\right) - \varphi\left(\mathbf{r}\right).$$

The displacement can be understood as a gauge transformation. Thus, we can write the Schrödinger equation as it emerges after the transformation:

$$\left(\sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j - \mathbf{a}\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i - \mathbf{r}_j\right)\right)\Psi_\nu\left(\mathbf{r}_j - \mathbf{a}\right) = E_\nu\Psi_\nu\left(\mathbf{r}_j - \mathbf{a}\right)$$

alternatively as

$$\begin{aligned}
\left(\sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i - \mathbf{r}_j\right)\right) & e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j - \mathbf{a}\right) \\
&= E_\nu e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j - \mathbf{a}\right),
\end{aligned}$$

with $\chi_{\mathbf{a}}\left(\mathbf{r}\right)$ given above. In addition to the many-body wave functions $\Psi_\nu\left(\mathbf{r}_j\right)$ we have the alternative choice

$$\Psi'_\nu\left(\mathbf{r}_j\right) = e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j - \mathbf{a}\right). \tag{390}$$

The density matrix can therefore we evaluated using the original or the primed wave functions. For the density matrix expressed in terms of the primed wave functions follows

$$\begin{aligned}
\rho^{(1)}\left(\mathbf{r},\mathbf{r}'\right) &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}\left(\mathbf{r}\right) - \chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)} N\int d^d r_2\cdots d^d r_N \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \\
&\times \Psi^*_\nu\left(\mathbf{r}-\mathbf{a},\mathbf{r}_2-\mathbf{a},\cdots,\mathbf{r}_N-\mathbf{a}\right) \\
&\times \Psi_\nu\left(\mathbf{r}'-\mathbf{a},\mathbf{r}_2-\mathbf{a},\cdots,\mathbf{r}_N-\mathbf{a}\right).
\end{aligned} \tag{391}$$

All other phase factors $\propto \chi_{\mathbf{a}}(\mathbf{r}_j)$ for $j = 2 \cdots N$ cancel. Using periodic boundary conditions we can shift the integration variables $\mathbf{r}_j \to \mathbf{r}_j - \mathbf{a}$ and obtain

$$\rho^{(1)}(\mathbf{r}, \mathbf{r}') = e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}) - \chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)} \rho^{(1)}(\mathbf{r} - \mathbf{a}, \mathbf{r}' - \mathbf{a}). \tag{392}$$

Let us now assume ODLRO, i.e. for large distance between $\mathbf{r}$ and $\mathbf{r}'$ holds Eq.380. This implies

$$\phi_0^*(\mathbf{r}')\,\phi_0(\mathbf{r}) = e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}) - \chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)} \phi_0^*(\mathbf{r}' - \mathbf{a})\,\phi_0(\mathbf{r} - \mathbf{a}) \tag{393}$$

which implies for the eigenfunction of the density operator

$$\phi_0(\mathbf{r}) = f_{\mathbf{a}} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r})} \phi_0(\mathbf{r} - \mathbf{a}), \tag{394}$$

where $f_{\mathbf{a}}$ is a phase factor that is $\mathbf{r}$-independent but displacement dependent. We now perform two successive transformations

$$\begin{aligned} \phi_0(\mathbf{r}) &= f_{\mathbf{b}} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r})} \phi_0(\mathbf{r} - \mathbf{b}) \\ &= f_{\mathbf{a}} f_{\mathbf{b}} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r})} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b})} \phi_0(\mathbf{r} - \mathbf{a} - \mathbf{b}) \end{aligned} \tag{395}$$

Of course, we can also change the order of the displacements:

$$\phi_0(\mathbf{r}) = f_{\mathbf{a}} f_{\mathbf{b}} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r})} e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a})} \phi_0(\mathbf{r} - \mathbf{a} - \mathbf{b}). \tag{396}$$

Since the wave function is single valued, the two phase factors that relate the two wave functions must be the same and we find the condition:

$$e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{b}}(\mathbf{r}) + \chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b}))} = e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{a}}(\mathbf{r}) + \chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}))}, \tag{397}$$

It follows from the above definition of $\chi_{\mathbf{a}}(\mathbf{r})$ that

$$\chi_{\mathbf{b}}(\mathbf{r}) + \chi_{\mathbf{a}}(\mathbf{r} - \mathbf{b}) = \chi_{\mathbf{a}+\mathbf{b}}(\mathbf{r}) + \frac{1}{2}\mathbf{B} \cdot (\mathbf{a} \times \mathbf{b}). \tag{398}$$

Here, we used:

$$\begin{aligned} \chi_{\mathbf{b}}(\mathbf{r}) &= \mathbf{b} \cdot \mathbf{A}_0(\mathbf{r}) + \varphi(\mathbf{r} - \mathbf{b}) - \varphi(\mathbf{r}) \\ \chi_{\mathbf{a}}(\mathbf{r} - \mathbf{b}) &= \mathbf{a} \cdot \mathbf{A}_0(\mathbf{r} - \mathbf{b}) + \varphi(\mathbf{r} - \mathbf{a} - \mathbf{b}) - \varphi(\mathbf{r} - \mathbf{b}) \\ &= \mathbf{a} \cdot \mathbf{A}_0(\mathbf{r}) - \frac{1}{2}\mathbf{a} \cdot (\mathbf{B} \times \mathbf{b}) + \varphi(\mathbf{r} - \mathbf{a} - \mathbf{b}) - \varphi(\mathbf{r} - \mathbf{b}). \end{aligned}$$

The result

$$\chi_{\mathbf{a}}(\mathbf{r}) + \chi_{\mathbf{b}}(\mathbf{r} - \mathbf{a}) = \chi_{\mathbf{a}+\mathbf{b}}(\mathbf{r}) - \frac{1}{2}\mathbf{B} \cdot (\mathbf{a} \times \mathbf{b}) \tag{399}$$

follows immediately by switching $\mathbf{a}$ and $\mathbf{b}$. Combining the two terms we obtain

$$\begin{aligned} \chi_{\mathbf{b}}(\mathbf{r}) + \chi_{\mathbf{a}}(\mathbf{r} - \mathbf{b}) - \chi_{\mathbf{a}}(\mathbf{r}) - \chi_{\mathbf{b}}(\mathbf{r} - \mathbf{a}) &= \frac{1}{2}\mathbf{B} \cdot (\mathbf{a} \times \mathbf{b}) - \frac{1}{2}\mathbf{B} \cdot (\mathbf{b} \times \mathbf{a}) \\ &= \mathbf{B} \cdot (\mathbf{a} \times \mathbf{b}), \end{aligned} \tag{400}$$

which is independent on the position $\mathbf{r}$. Our condition for the above phases can therefore be written as:

$$\frac{e}{\hbar c}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b})=2\pi n, \tag{401}$$

where n is an integer.

The displacement vectors $\mathbf{a}$ and $\mathbf{b}$ are arbitrary. Thus, we can continuously vary the vectors $\mathbf{a}$ and $\mathbf{b}$ on the left hand side. On the other hand, since n is an integer, we cannot continuously vary the right hand side. The only acceptable uniform field is therefore

$$\mathbf{B}=0. \tag{402}$$

This is the Meissner effect of charged bosons with ODLRO. A system with ODLRO cannot support a uniform magnetic field.

This derivation of the Meissner effects makes very evident the importance of macroscopic condensation. Without condensation, we could still perform a similar analysis for the density operator and obtain the condition

$$\begin{aligned} 2\pi n\frac{\hbar c}{e} &= \chi_{\mathbf{b}}(\mathbf{r})+\chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b})-\chi_{\mathbf{a}}(\mathbf{r})-\chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}) \\ &- \left(\chi_{\mathbf{b}}(\mathbf{r}')+\chi_{\mathbf{a}}(\mathbf{r}'-\mathbf{b})-\chi_{\mathbf{a}}(\mathbf{r}')-\chi_{\mathbf{b}}(\mathbf{r}'-\mathbf{a})\right). \end{aligned} \tag{403}$$

Inserting our above expression for the sum of the phases the right hand side gives a zero, i.e. we merely obtain the condition $n=0$, without restriction on $\mathbf{B}$. In other words, as long as the density matrix is determined by a sum over many eigenstates, no Meissner effect occurs. Only the condensation in one state and a density matrix

$$\rho^{(1)}(\mathbf{r},\mathbf{r}')\to n_0\phi_0^*(\mathbf{r}')\,\phi_0(\mathbf{r}). \tag{404}$$

for large $|\mathbf{r}-\mathbf{r}'|$ yields a vanishing $\mathbf{B}$-field. We conclude, that macroscopic condensation and Meissner effect are closely related.

The analysis of ODLRO in fermionic systems proceeds in close analogy to the bosonic case discussed in the previous section[**?**]. It is, however, based upon the two-particle density matrix

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')=\left\langle\psi_\alpha^\dagger(\mathbf{r}_1)\,\psi_\beta^\dagger(\mathbf{r}_2)\,\psi_{\beta'}(\mathbf{r}_2')\,\psi_{\alpha'}(\mathbf{r}_1')\right\rangle.$$

We consider the combined index $(\mathbf{r}_1\alpha,\mathbf{r}_2\beta)$ that describes the two-particle matrix. Expanding $\rho^{(2)}$ with respect to its eigenfunctions

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')=\sum_p n_p\phi_p^*(\mathbf{r}_1\alpha,\mathbf{r}_2\beta)\,\phi_p(\mathbf{r}_1'\alpha',\mathbf{r}_2'\beta'), \tag{405}$$

with eigenvalues n_p. ODLRO is again a state where the largest eigenvalue n_0 is of the order of the particle number N. In this case holds

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')\to n_0\phi_0^*(\mathbf{r}_1\alpha,\mathbf{r}_2\beta)\,\phi_0(\mathbf{r}_1'\alpha',\mathbf{r}_2'\beta') \tag{406}$$

in the limit where $|\mathbf{r}_i-\mathbf{r}_i'|\to\infty$ while $|\mathbf{r}_1-\mathbf{r}_2|$ and $|\mathbf{r}_1'-\mathbf{r}_2'|$ remain finite.

From the antisymmetry of the fermionic wave function follows

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2\right) &= -\rho^{(2)}_{\beta\alpha\alpha'\beta'}\left(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}'_1,\mathbf{r}'_2\right)\\ &= -\rho^{(2)}_{\alpha\beta\beta'\alpha'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_2,\mathbf{r}'_1\right). \end{aligned} \tag{407}$$

This implies for the eigenfunction

$$\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) = -\phi_0\left(\mathbf{r}_2\beta,\mathbf{r}_1\alpha\right) \tag{408}$$

as expected for a genuine two particle wave function.

A displacement $\mathbf{a}$ can again be thought of as a gauge transformation[**?**, **?**]. Thus, one can use either the wave functions $\Psi_\nu\left(\mathbf{r}_j,\gamma_j\right)$ (here γ_j stands for the spin and other quantum numbers) or the alternative functions

$$\Psi'_\nu\left(\mathbf{r}_j,\gamma_j\right) = e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}(\mathbf{r}_j)}\Psi_\nu\left(\mathbf{r}_j-\mathbf{a},\gamma_j\right).$$

As our magnetic field is assumed to be homogeneous, the displacement will not affect the coupling of the magnetic field to the spin. Expressing $\rho^{(2)}$ in terms of both sets of wave functions, we find the relationship

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2\right) &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r_2})-\chi_{\mathbf{a}}\left(\mathbf{r}'_1\right)-\chi_{\mathbf{a}}\left(\mathbf{r}'_2\right)\right)}\\ &\times\ \rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1-\mathbf{a},\mathbf{r}_2-\mathbf{a},\mathbf{r}'_1-\mathbf{a},\mathbf{r}'_2-\mathbf{a}\right). \end{aligned} \tag{409}$$

For the eigenfunction follows from Eq.409 that

$$\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) = f_{\mathbf{a}}e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r}_2)\right)}\phi_0\left(\mathbf{r}_1-\mathbf{a}\alpha,\mathbf{r}_2-\mathbf{a}\beta\right). \tag{410}$$

This is the two particle generalization of our earlier result Eq.394 for bosons. Meissner effect and flux quantization followed rather directly from this result. The Meissner effect follows from two consecutive displacements in alternate order:

$$\begin{aligned}\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{b}}(\mathbf{r}_1)+\chi_{\mathbf{b}}(\mathbf{r}_2)\right)}e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}_1-\mathbf{b})+\chi_{\mathbf{a}}(\mathbf{r}_2-\mathbf{b})\right)}\\ &\times\ f_{\mathbf{a}}f_{\mathbf{b}}\phi_0\left(\mathbf{r}_1-\mathbf{a}-\mathbf{b}\alpha,\mathbf{r}_2-\mathbf{a}-\mathbf{b}\beta\right) \end{aligned} \tag{411}$$

and

$$\begin{aligned}\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r}_2)\right)}e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{b}}(\mathbf{r}_1-\mathbf{a})+\chi_{\mathbf{b}}(\mathbf{r}_2-\mathbf{a})\right)}\\ &\times\ f_{\mathbf{a}}f_{\mathbf{b}}\phi_0\left(\mathbf{r}_1-\mathbf{a}-\mathbf{b}\alpha,\mathbf{r}_2-\mathbf{a}-\mathbf{b}\beta\right), \end{aligned} \tag{412}$$

which requires that the two phase factors must be the same. We already found that

$$\chi_{\mathbf{b}}\left(\mathbf{r}\right)+\chi_{\mathbf{a}}\left(\mathbf{r}-\mathbf{b}\right)-\chi_{\mathbf{a}}\left(\mathbf{r}\right)-\chi_{\mathbf{b}}\left(\mathbf{r}-\mathbf{a}\right) = \mathbf{B}\cdot\left(\mathbf{a}\times\mathbf{b}\right). \tag{413}$$

The condition of identical phases then corresponds to

$$\frac{2e}{\hbar c}\mathbf{B}\cdot\left(\mathbf{a}\times\mathbf{b}\right) = 2\pi n. \tag{414}$$

The only difference to the case of single-particle ODLRO is the new factor 2 that is a consequence of the two-particle ODLRO considered here. In case one were to analyze ODLRO in $\rho^{(l)}$ one would have a coefficient $\frac{le}{\hbar c}$. The argumentation which implied that a homogeneous magnetic field must vanish is now the same as before: The left hand side of the above condition can be continuously varied while the right hand side cannot and the only solution is:

$$\mathbf{B} = \mathbf{0}. \tag{415}$$

13.2 the superconducting order parameter

n case of ODLRO, we have

$$\rho^{(1)}(\mathbf{r}, \mathbf{r}', t)\Big|_{|\mathbf{r}-\mathbf{r}'|\to\infty} = n_0(t)\,\phi_0^*(\mathbf{r}', t)\,\phi_0(\mathbf{r}, t), \tag{416}$$

where we allowed for an explicit time dependence of the density matrix, that exists in out-of-equilibrium situations. This suggest to introduce the quantity

$$\Psi(\mathbf{r}, t) \quad = \quad \sqrt{n_0(t)}\phi_0(\mathbf{r}, t). \tag{417}$$

A definition that immediately implies

$$\int d^d r\,|\Psi(\mathbf{r}, t)|^2 = n_0(t), \tag{418}$$

which follows from the normalization to unity of the eigenfunction $\phi_0(\mathbf{r}, t)$. The behavior of the eigenfunction ϕ_0 under gauge transformations, suggests that the function $\Psi(\mathbf{r}, t)$ behaves in many ways like a condensate wave function. Frequently, the order parameter of a Bose condensate is also defined via the expectation value of the field operator

$$\Psi(\mathbf{r}, t) = \langle\psi(\mathbf{r}, t)\rangle. \tag{419}$$

Then, Bose condensation is associated with a spontaneous breaking of the global $U(1)$ symmetry $\psi(\mathbf{r}) \to e^{i\theta}\psi(\mathbf{r})$. At first glance these two statements seem contradictory. $\Psi(\mathbf{r}, t)$ was defined for a system with fixed particle number and, more importantly, for a Hamiltonian with conserved particle number. Breaking the global $U(1)$ symmetry implies that the particle number conservation is spontaneously broken, which seems at first glance rather odd. Notice that merely using a grand-canonical ensemble does not resolve the issue. Particle number conservation implies that the density matrix is block-diagonal with respect to the number of particles. In such a situation it must hold that $\langle\psi(\mathbf{r}, t)\rangle = 0$ even for a grand-canonical description. The two definitions of the order-parameter can, however, be reconciled. This is done by explicitly breaking particle conservation and adding a term

$$H_\eta = -\int d^d r\left(\eta(\mathbf{r})\,\psi^\dagger(\mathbf{r}) + \eta^*(\mathbf{r})\,\psi(\mathbf{r})\right) \tag{420}$$

to the Hamiltonian and taking the limit $\eta \to 0$ after the thermodynamic limit. It turns out that $\langle \psi(\mathbf{r},t)\rangle \neq 0$ when the system establishes ODLRO. The density matrix can be decomposed as

$$\begin{aligned}\rho^{(1)}(\mathbf{r},\mathbf{r}',t) &= \left\langle \psi^{\dagger}(\mathbf{r},t)\right\rangle \langle \psi(\mathbf{r},t)\rangle \\ &+ \left\langle \left(\psi^{\dagger}(\mathbf{r},t)-\left\langle \psi^{\dagger}(\mathbf{r},t)\right\rangle\right)\left(\psi(\mathbf{r}',t)-\langle \psi(\mathbf{r}',t)\rangle\right)\right\rangle, \quad (421)\end{aligned}$$

where the first term remains finite for large $\mathbf{r}-\mathbf{r}'$, while the second one decays. We will not demonstrate this here, but rather perform the corresponding analysis when we discuss fermionic systems.

While the definition $\Psi(\mathbf{r},t)$ in terms of the condensate eigenfunctions of the density matrix is conceptually more satisfying, the usage of $\langle \psi(\mathbf{r},t)\rangle$ is very convenient in mean-field theories like the Bogoliubov theory of dilute or weakly interacting condensed bosons.

In full analogy to the case of charged bosons, the natural choice of the order parameter of a fermionic system with ODLRO is the condensate wave function

$$\Psi(\mathbf{R},\mathbf{r},\alpha,\beta,t) = \sqrt{n_0(t)}\phi_0(\mathbf{r}_1\alpha,\mathbf{r}_2\beta), \quad (422)$$

where we use instead of the individual particle coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ the relative coordinate $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ and the center of gravity coordinate $\mathbf{R}=\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$, respectively. An alternative approach is motivated by the theory of magnetism.

Consider a magnet with global $SU(2)$ spin-rotation invariance. Applying a finite magnetic field $\mathbf{B}(\mathbf{r})$, the symmetry is spontaneously broken if the expectation value

$$\mathbf{s_0}(\mathbf{r}) = \frac{1}{2}\lim_{\mathbf{B}\to 0}\lim_{N,V\to\infty}\sum_{\alpha\beta}\left\langle \psi_{\alpha}^{\dagger}(\mathbf{r})\,\boldsymbol{\sigma}_{\alpha\beta}\psi_{\beta}(\mathbf{r})\right\rangle \quad (423)$$

is finite. Without the external magnetic field, multiple degenerate configurations would cancel each other, leading to a zero magnetization. The same is true if one performs the limit $\mathbf{B}\to 0$ for a finite system as there is still a finite macroscopic tunneling probability between degenerate states. This is the reason why the zero field limit must be performed after the thermodynamic limit.

In the context of superconductivity, spontaneous symmetry breaking can be analyzed if we add to the Hamiltonian a source term

$$H = -\int d^d r_1 d^d r_2 \sum_{\alpha\beta}\left(\eta_{\alpha\beta}(\mathbf{r}_1,\mathbf{r}_2)\,\psi_{\alpha}^{\dagger}(\mathbf{r}_1)\,\psi_{\beta}^{\dagger}(\mathbf{r}_2)+h.c.\right). \quad (424)$$

A physical realization of the source field $\eta_{\alpha\beta}(\mathbf{r}_1,\mathbf{r}_2)$ is the coupling to another superconductor via a weak Josephson junction (see below). Just like in case of a magnet, we perform the limit $\eta\to 0$ after the thermodynamic limit. One expects ODLRO to be identical to a finite expectation value

$$\Psi(\mathbf{R},\mathbf{r},\alpha,\beta,t) = \lim_{\eta\to 0}\lim_{N,V\to\infty}\langle \psi_{\beta}(\mathbf{r}_2)\,\psi_{\alpha}(\mathbf{r}_1)\rangle. \quad (425)$$

While a general proof for the equivalence between these two definitions does not seem to exist, we will later show that they are identical within the BCS

theory. This formulation makes evident the statement that at a superconducting transition the global $U(1)$ symmetry

$$\psi_\alpha(\mathbf{r}) \to e^{i\theta}\psi_\alpha(\mathbf{r}) \tag{426}$$

is spontaneously broken. Breaking the global $U(1)$ symmetry implies that the particle number conservation is spontaneously broken. While one frequently encounters the notion that at the superconducting transition the electromagnetic gauge symmetry is spontaneously broken, it seems more adequate to simply refer to a global $U(1)$ symmetry as the same symmetry is also broken in neutral fermionic superfluids. What is unique about charged superfluids is however associated with the condensed matter realization of the Higgs mechanism in superconductors that we will discuss later. For a lucid discussion of the issue of gauge symmetry breaking at the superconducting transition, see Ref.[**?**].

The source field $\eta_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2)$ has well defined behavior upon exchanging particles. Fermi statistics implies that

$$\psi^\dagger_\alpha(\mathbf{r}_1)\,\psi^\dagger_\beta(\mathbf{r}_2) = -\psi^\dagger_\beta(\mathbf{r}_2)\,\psi^\dagger_\alpha(\mathbf{r}_1)\,. \tag{427}$$

If we now relabel the indices $\mathbf{r}_1\alpha \longleftrightarrow \mathbf{r}_2\beta$ the source field must compensate for the minus sign to recover the original Hamiltonian, i.e.

$$\eta_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = -\eta_{\beta\alpha}(\mathbf{r}_2, \mathbf{r}_1)\,. \tag{428}$$

The (2×2) matrix form of η suggests an expansion in terms of Pauli matrices $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ and the unit matrix σ^0. Out of those for matrices. σ^y is the only one that is antisymmetric ($\sigma^y_{\alpha\beta} = -\sigma^y_{\beta\alpha}$). All other are symmetric. This suggests an expansion (the additional factor i is for convenience):

$$\eta_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = \eta_s(\mathbf{r}_1, \mathbf{r}_2)\,(i\sigma^y)_{\alpha\beta} + \boldsymbol{\eta}_t(\mathbf{r}_1, \mathbf{r}_2)\cdot(i\sigma^y\boldsymbol{\sigma})_{\alpha\beta}\,. \tag{429}$$

The first term behaves like a singlet two particle wave function; it is antisymmetric with respect to the spin indices, i.e. it must be symmetric with respect to the spatial indices. The opposite is the case for the second term that describes the triplet part of the source field.

The same is of course true for the order parameter itself, i.e. we expand

$$\Psi(\mathbf{R}, \mathbf{r}, \alpha, \beta) = \Psi_s(\mathbf{R}, \mathbf{r})\,(i\sigma^y)_{\alpha\beta} + \boldsymbol{\Psi}_t(\mathbf{R}, \mathbf{r})\cdot(i\sigma^y\boldsymbol{\sigma})_{\alpha\beta}\,, \tag{430}$$

where the singlet and triplet part obey:

$$\begin{aligned} \Psi_s(\mathbf{R}, \mathbf{r}) &= \Psi_s(\mathbf{R}, -\mathbf{r})\,, \\ \boldsymbol{\Psi}_t(\mathbf{R}, \mathbf{r}) &= -\boldsymbol{\Psi}_t(\mathbf{R}, -\mathbf{r})\,. \end{aligned} \tag{431}$$

Consider now a three dimensional system with inversion symmetry. Then each operator should either be even or odd under $\mathbf{r} \to -\mathbf{r}$. The spin is a pseudovector, i.e. it does not change under parity. Thus, it must hold that

$$\Psi(\mathbf{R}, \mathbf{r}, \alpha, \beta) = \pm\Psi(\mathbf{R}, -\mathbf{r}, \alpha, \beta)\,. \tag{432}$$

It follows that a superconducting state with inversion symmetry must either form ODLRO of triplets or of singlets. For a combination of the singlet and triplet pairing, the total wave function would have no well defined parity eigenvalue. It is interesting that our proof is valid even if one includes spin orbit interaction. In crystals without inversion symmetry or on the surface of a three dimensional crystal, both pairing states can of course exist simultaneously.

The two-particle density matrix $\rho^{(2)}$ is an equal-time correlation function. Using the fluctuation-dissipation theorem we can therefore relate it to a retarded Green's function (we use the abbreviation $\{\mathbf{r}_i\} = (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2)$

$$\begin{aligned} \rho^{(2)}_{\alpha\beta\alpha'\beta'}(\{\mathbf{r}_i\}) &= \left\langle \psi^\dagger_\alpha(\mathbf{r}_1)\,\psi^\dagger_\beta(\mathbf{r}_2)\,\psi_{\beta'}(\mathbf{r}'_2)\,\psi_{\alpha'}(\mathbf{r}'_1)\right\rangle \\ &= -\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\mathrm{Im}\chi_{\alpha\beta\alpha'\beta'}(\{\mathbf{r}_i\},\omega+i0^+)}{e^{\beta\omega}-1}, \end{aligned}$$

where χ us the Fourier transform ($\chi(\omega) = \int_{-\infty}^{\infty} dt\chi(t)\,e^{i\omega t}$) of the retarded function

$$\chi_{\alpha\beta\alpha'\beta'}(\{\mathbf{r}_i\},t) = -i\theta(t)\left\langle\left[\psi^\dagger_\alpha(\mathbf{r}_1,t)\,\psi^\dagger_\beta(\mathbf{r}_2,t),\psi_{\beta'}(\mathbf{r}'_2,0)\,\psi_{\alpha'}(\mathbf{r}'_1,0)\right]_-\right\rangle,$$

where the operators are now in the Heisenberg picture. χ is the pair-susceptibility of the system, i.e. the change of the expectation value $\left\langle \psi^\dagger_\beta(\mathbf{r}_2,t)\,\psi^\dagger_\alpha(\mathbf{r}_1,t)\right\rangle$ with respect to a rime dependent source field $\eta_{\alpha'\beta'}(\mathbf{r}'_1,\mathbf{r}'_2,t')$:

$$\chi_{\alpha\beta\alpha'\beta'}(\{\mathbf{r}_i\},t-t') = \left.\frac{\delta\left\langle\psi^\dagger_\beta(\mathbf{r}_2,t)\,\psi^\dagger_\alpha(\mathbf{r}_1,t)\right\rangle}{\delta\eta^*_{\alpha'\beta'}(\mathbf{r}'_1,\mathbf{r}'_2,t')}\right|_{\eta,\eta^*\to 0}. \tag{433}$$

As before, the limit of vanishing source fields must be taken after the thermodynamic limit.

13.3 The pairing instability

The analysis of the previous section revealed that there seems to be an instability of the Fermi surface with respect to a weak attractive interaction between fermions. For simplicity, we consider a model with weak attraction governed by the model Hamiltonian

$$\begin{aligned} H &= \sum_\alpha \int d^d r\psi^\dagger_\alpha(\mathbf{r})\left(-\frac{\nabla^2}{2m}-\mu\right)\psi_\alpha(\mathbf{r}) \\ &+ V\int d^d r\psi^\dagger_\uparrow(\mathbf{r})\,\psi^\dagger_\downarrow(\mathbf{r})\,\psi_\downarrow(\mathbf{r})\,\psi_\uparrow(\mathbf{r}). \end{aligned} \tag{434}$$

We will see that the analysis of this continuum's model is ill defined without proper regularization. Therefore we consider a model where we restricts ourselves to an effective low energy theory, i.e. we consider a system where the

fermionic excitations are confined to an energy scale $\pm\Lambda$ around the Fermi energy. We explore the behavior of this toy model.

In our Hamiltonian it suffices to consider a singlet wave function and to focus on $\mathbf{r}_1 = \mathbf{r}_2$ and $\mathbf{r}_1' = \mathbf{r}_2'$, i.e. we analyze the pairing susceptibility.

$$\chi\left(\mathbf{r},\mathbf{r}',t\right) = -i\theta\left(t\right)\left\langle \left[\psi_\uparrow^\dagger\left(\mathbf{r},t\right)\psi_\downarrow^\dagger\left(\mathbf{r},t\right),\psi_\downarrow\left(\mathbf{r}',0\right)\psi_\uparrow\left(\mathbf{r}',0\right)\right]_- \right\rangle . \tag{435}$$

Fourier transformation and Wick rotation to the imaginary time axis yields

$$\chi\left(\mathbf{r},\mathbf{r}',\tau\right) = -\left\langle T_\tau \psi_\uparrow^\dagger\left(\mathbf{r},\tau\right)\psi_\downarrow^\dagger\left(\mathbf{r},\tau\right)\psi_\downarrow\left(\mathbf{r}',0\right)\psi_\uparrow\left(\mathbf{r}',0\right)\right\rangle . \tag{436}$$

In what follows we analyze this pairing susceptibility.

We first analyze the pair susceptibility of non-interacting electrons. The Fourier transform in momentum and frequency space is then given as

$$\chi_0\left(\mathbf{q},i\nu_m\right) = T\sum_n \int \frac{d^dk}{\left(2\pi\right)^d} G_{\mathbf{k}}\left(i\omega_n\right) G_{-\mathbf{k}+\mathbf{q}}\left(-i\omega_n + i\nu_m\right), \tag{437}$$

where $\nu_m = 2m\pi T$ and $\omega_n = \left(2n+1\right)\pi T$ are bosonic and fermionic Matsubara frequencies, respectively.

$$G_{\mathbf{k}}\left(i\omega_n\right) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} \tag{438}$$

is the bare fermionic Green's function and $\epsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu$. Since we suspect that superconductivity is a homogeneous instability, without spatial and temporal modulations, we consider the limit $\mathbf{q} = 0$ and $\omega_n = 0$. It follows

$$\begin{aligned} \chi_0\left(T\right) &= T\sum_m \int \frac{d^dk}{\left(2\pi\right)^d} \frac{1}{\omega_n^2 + \epsilon_{\mathbf{k}}^2} \\ &= T\sum_m \int d\epsilon \frac{\rho\left(\epsilon\right)}{\omega_n^2 + \epsilon^2}, \end{aligned} \tag{439}$$

with density of states

$$\rho\left(\omega\right) = \int \frac{d^dk}{\left(2\pi\right)^d} \delta\left(\omega - \epsilon_{\mathbf{k}}\right). \tag{440}$$

We perform the Matsubara frequency sum and obtain

$$\chi_0\left(T\right) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho\left(\epsilon\right)}{2\epsilon} \tanh\left(\frac{\epsilon}{2T}\right). \tag{441}$$

This expression makes evident that some appropriate cut off procedure is required to analyze the pairing susceptibility. While the above integral is well defined for any lattice model of a solid, where the density of states of individual bands has some upper and lower cut off, the continuum's theory diverges at the

upper cut off. As mentioned above, an appropriate approach is to define the theory in an energy window $[\mu - \Lambda, \mu + \Lambda]$ around the Fermi energy and assume that the density of states is constant in this window. Then we have to evaluate:

$$\chi_0(T) = \rho_F \int_{-\Lambda}^{\Lambda} d\epsilon \frac{1}{2\epsilon} \tanh\left(\frac{\epsilon}{2T}\right). \tag{442}$$

We perform the integration to leading logarithmic accuracy:

$$\begin{aligned}
\int_{-\Lambda}^{\Lambda} \frac{\tanh\left(\frac{\varepsilon}{2T}\right)}{2\varepsilon} d\varepsilon &= \int_0^{\beta\Lambda/2} \frac{\tanh(x)}{x} dx \\
&= -\int_0^{\beta\Lambda/2} \frac{\log(x)}{\cosh^2(x)} dx + \tanh(x) \log x \Big|_0^{\beta\Lambda/2} \\
&= \gamma_E - \log\frac{\pi}{4} + \log\left(\frac{\Lambda}{2T}\right) + \mathcal{O}\left(\frac{T}{\Lambda}\right) \\
&= \log\left(\frac{2\Lambda e^{\gamma_E}}{\pi T}\right) + \mathcal{O}\left(\frac{T}{\Lambda}\right).
\end{aligned} \tag{443}$$

We obtain for the pairing susceptibility of a free electron gas

$$\chi_0(T) = \rho_F \log\left(\frac{2\Lambda e^{\gamma_E}}{\pi T}\right).$$

For any finite temperature the free electron pairing-susceptibility is finite. However the logarithmic increase of $\chi_0(T)$ for $T \to 0$ already indicates that a Fermi gas becomes increasingly susceptible if one adds an external pairing source $\eta_{\alpha\beta} = \eta_s i\sigma^y_{\alpha\beta}$.

Next we include electron-electron interactions. To this extend we sum ladder diagrams for the pairing susceptibility. We obtain:

$$\begin{aligned}
\chi_0(\mathbf{q}, i\nu_m) &= \chi_0(\mathbf{q}, i\nu_m) - V\chi_0(\mathbf{q}, i\nu_m)^2 + V^2\chi_0(\mathbf{q}, i\nu_m)^2 \cdots \\
&= \frac{\chi_0(\mathbf{q}, i\nu_m)}{1 + V\chi_0(\mathbf{q}, i\nu_m)}.
\end{aligned} \tag{444}$$

In case of a negative (attractive) interaction $V < 0$, follows that the $\mathbf{q} = \mathbf{0}$ and $\nu_m = 0$ susceptibility diverges at the transition temperature when

$$|V|\chi_0(T_c) = 1. \tag{445}$$

With dimensionless coupling constant $\lambda = \rho_F |V|$ follows

$$T_c = \frac{2e^{\gamma_E}}{\pi}\Lambda e^{-\frac{1}{\lambda}}. \tag{446}$$

13.4 The BCS theory

The BCS theory gives an answer to the open question that emerges as consequence of the Cooper instability: What happens with an entire Fermi-sea of

attractively interacting electrons? Based on the insight that the leading instability occurs at zero center-of-mass momentum we model the attractive interaction between electrons, mediated by phonons via he BCS or pairing Hamiltonian:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V_0}{N} \sum_{\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \tag{447}$$

It consists of the usual kinetic energy with band dispersion

$$\varepsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu \tag{448}$$

and an interaction term. The choice of the parabolic spectrum is in fact not necessary. The subsequent analysis will reveal that it is trivial to generalize the approach to different dispersions as long as it is spin-independent and $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$. The sign in front of the interaction V_0 was chosen such that $V_0 > 0$ corresponds to an attractive coupling. The matrix element

$$\gamma_{\mathbf{k},\mathbf{k}'} = \begin{cases} 1 & |\varepsilon_{\mathbf{k}}|, |\varepsilon_{\mathbf{k}'}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

takes into account that only fermionic states that have energies relative to the Fermi energy below the phonon frequency interact.

To find an approximate solution of this problem we perform the Hartree-Fock decoupling

$$AB = (A - \langle A \rangle)(B - \langle B \rangle) + A\langle B \rangle + B\langle A \rangle - \langle A \rangle \langle B \rangle \tag{449}$$

with

$$\begin{aligned} A &= c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} \\ B &= c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}. \end{aligned} \tag{450}$$

This choice for A and B is motivated by the expectation, that $\langle A \rangle \neq 0$ and $\langle B \rangle \neq 0$ amount to pairing of electrons, as discussed earlier. Performing the mean field decoupling yields:

$$H^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left(\Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right) + N \frac{|\Delta|^2}{V_0}, \tag{451}$$

where we introduced the abbreviation

$$\Delta_{\mathbf{k}} = -\frac{V_0}{N} \sum_{\mathbf{k}} \gamma_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle. \tag{452}$$

Δ is the value of $\Delta_{\mathbf{k}}$ for momenta with $|\varepsilon_{\mathbf{k}}| < \omega_D$. The last term is a consequence of the $\langle A \rangle \langle B \rangle$ expectation value, where we used

$$\Delta^2 = \frac{V_0^2}{N} \sum_{\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle \langle c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} \rangle \tag{453}$$

since $\gamma_{\mathbf{k},\mathbf{k}'} = \gamma^2_{\mathbf{k},\mathbf{k}'}$.

The form of this Hamiltonian is similar to an effective free-electron problem in the sense that it only contains terms that are products of two operators $c^\dagger_{\mathbf{k}\sigma}$ or $c_{\mathbf{k}\sigma}$, respectively. However, the appearance terms like $\Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ and $\Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$ has no analog in the free-electron limit. An expectation value $\left\langle c^\dagger_{\mathbf{k}',\uparrow}\, c^\dagger_{-\mathbf{k}',\downarrow} \right\rangle \neq 0$ must be understood as consequence of an external source field that couples to the operators A and B and is switched off after the thermodynamic limit has been taken. Within a mean field theory such source field would only be an infinitesimal addition to the mean field anyway. Thus, we never actually have to include the mentioned source field since we are breaking the symmetry "by hand" anyway. Those anomalous terms are obviously the ones that explicitly violate charge conservation at the mean field level. In order to bring this Hamiltonian into the desired form, we introduce the Nambu spinor

$$c_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}, \tag{454}$$

which allows us to express $H^{\mathrm{MF}}_{\mathrm{BCS}}$ in a form that resembles more the usual free fermion problem:

$$H^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} h_{\mathbf{k}} c_{\mathbf{k}} + N \frac{\Delta^2}{V_0} + \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}, \tag{455}$$

with 2×2-matrix

$$h_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & -\varepsilon_{\mathbf{k}} \end{pmatrix}. \tag{456}$$

The eigenvalues of $h_{\mathbf{k}}$ are determined by $(E - \varepsilon_{\mathbf{k}})(E + \varepsilon_{\mathbf{k}}) - |\Delta_{\mathbf{k}}|^2 = 0$, which yields

$$E_{\mathbf{k}\pm} = \pm E_{\mathbf{k}} \tag{457}$$

with

$$E_{\mathbf{k}} = \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} > 0. \tag{458}$$

$h_{\mathbf{k}}$ is diagonalized by a unitary transformation $U_{\mathbf{k}}$. The columns of $U_{\mathbf{k}}$ are the eigenvectors $\mathbf{u}^{(i)}_{\mathbf{k}}$ of $h_{\mathbf{k}}$. Interestingly there is some nontrivial structure in the matrix $h_{\mathbf{k}}$ that is worth exploring as it can be very helpful for more complex systems such as multi-band superconductors or inhomogeneous systems. It holds with $\gamma = i\sigma^y$ (note $\gamma^2 = -1$) that

$$\gamma h^*_{\mathbf{k}} \gamma^{-1} = -h_{\mathbf{k}}. \tag{459}$$

Suppose one eigenvector of $h_{\mathbf{k}}$ is $\mathbf{u}^{(1)}_{\mathbf{k}} = (u_{\mathbf{k}}, v_{\mathbf{k}})^T$ and it corresponds to the eigenvalue $+E_{\mathbf{k}}$, i.e. $h_{\mathbf{k}} \mathbf{u}^{(1)}_{\mathbf{k}} = E_{\mathbf{k}} \mathbf{u}^{(1)}_{\mathbf{k}}$. We can now construct the another vector

$$\mathbf{u}^{(2)}_{\mathbf{k}} = -\gamma \mathbf{u}^{(1)*}_{\mathbf{k}} = (-v^*_{\mathbf{k}}, u^*_{\mathbf{k}})^T \tag{460}$$

which obeys

$$\gamma \mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma^2 \mathbf{u}_{\mathbf{k}}^{(1)} = \mathbf{u}_{\mathbf{k}}^{(1)} \tag{461}$$

$\mathbf{u}_{\mathbf{k}}^{(2)}$ is also an eigenvector but with eigenvalue $-E_{\mathbf{k}}$. To show that this is the case, we take the complex conjugate of the second eigenvalue equation $h_{\mathbf{k}}^* \mathbf{u}_{\mathbf{k}}^{(2)*} = -E_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(2)*}$ and write it as $\gamma h_{\mathbf{k}}^* \gamma^{-1} \gamma \mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma E_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(2)*}$ which yields $-h_{\mathbf{k}} \gamma \mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma E_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(2)*}$ amd leads to the first eigenvalue equation $h_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(1)} = E_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(1)}$, proving our assertion. Thus, the eigenvalues of the mean field Hamiltonian occur in a pair of opposite sign and with eigenvalues related by the unimodular transformation γ. The unitary transformation that diagonalizes the above 2×2 matrix is

$$U_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}}^* \\ v_{\mathbf{k}} & u_{\mathbf{k}}^* \end{pmatrix} \tag{462}$$

and it follows $U_{\mathbf{k}}^{-1} h_{\mathbf{k}} U_{\mathbf{k}} = \mathrm{diag}\,(E_{\mathbf{k}}, -E_{\mathbf{k}})$. It is straightforward to determine $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ from the eigenvalue equations. Unitarity, i.e. normalization of the eigenvectors implies $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ and it follows

$$u_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}} - \varepsilon_{\mathbf{k}}} v_{\mathbf{k}}. \tag{463}$$

This leads to:

$$\begin{aligned} u_{\mathbf{k}}^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \\ v_{\mathbf{k}}^2 &= 1 - u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right). \end{aligned} \tag{464}$$

as well as $u_{\mathbf{k}} v_{\mathbf{k}}^* = -\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$.

The unitary transformation transforms the Nambu spinor $c_{\mathbf{k}}$ according to $a_{\mathbf{k}} = U_{\mathbf{k}}^{-1} c_{\mathbf{k}}$ with $a_{\mathbf{k}} = \left(a_{\mathbf{k}\uparrow}, a_{-\mathbf{k}\downarrow}^\dagger\right)^T$ and it follows

$$\begin{aligned} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger h_{\mathbf{k}} c_{\mathbf{k}} &= \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger U_{\mathbf{k}} \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} U_{\mathbf{k}}^{-1} c_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} a_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} E_{\mathbf{k}} \left(a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow} a_{-\mathbf{k}\downarrow}^\dagger\right) \\ &= \sum_{\mathbf{k}} E_{\mathbf{k}} \left(a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} + a_{-\mathbf{k}\downarrow} a_{-\mathbf{k}\downarrow}^\dagger - 1\right) \\ &= \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} E_{\mathbf{k}} \end{aligned} \tag{465}$$

The mean field Hamiltonian is then given as:

$$H_{\mathrm{BCS}}^{\mathrm{MF}} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + N\frac{\Delta^2}{V_0} + \sum_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} \right). \tag{466}$$

Now, we managed to bring the Hamiltonian into the desired form of a free Fermi gas. In particular, it holds $\left\langle a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \right\rangle = f(E_{\mathbf{k}})$, where $f(\varepsilon) = \frac{1}{\exp(\beta\varepsilon)+1}$ is the usual Fermi function. Since $E_{\mathbf{k}} > 0$, we obtain $\left\langle a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \right\rangle = 0$ at $T = 0$. The ground state energy is then given by the constant term in

$$E_0 = N\frac{\Delta^2}{V_0} + \sum_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} \right). \tag{467}$$

The fermionic excitations only describe excitations above the ground state.

In order to determine Δ at $T = 0$, we minimize E_0 with respect to Δ. We perform the momentum integration via an integration over energy and subtract the value of the energy for $\Delta = 0$, i.e. $\delta E_0(\Delta) = E_0(\Delta) - E_0(\Delta = 0)$. It follows

$$\begin{aligned} \delta E_0 \quad /N = \quad & \frac{\Delta^2}{V_0} + \int_{-\infty}^{\infty} \rho(\epsilon)\, d\varepsilon \left(\varepsilon - \sqrt{\varepsilon^2 + \Delta^2} \right) - 2\int_{-\infty}^{\infty} \rho(\epsilon)\, d\varepsilon \theta(-\varepsilon)\, \varepsilon \\ = \quad & \frac{\Delta^2}{V_0} + 2\rho \int_0^{\omega_D} d\varepsilon \left(\varepsilon - \sqrt{\varepsilon^2 + \Delta^2} \right) \\ = \quad & \frac{\Delta^2}{V_0} + \rho\Delta^2 \log\left(\frac{\Delta}{2\omega_D} \right) - \frac{\rho}{2}\Delta^2 \end{aligned} \tag{468}$$

Minimizing the ground state energy with respect to Δ yields

$$\frac{1}{N}\frac{\partial E_0}{\partial \Delta} = 2\frac{\Delta}{V_0} + 2\rho\Delta \log\left(\frac{\Delta}{2\omega_D} \right) = 0,$$

which has the trivial solution $\Delta = 0$ and the nontrivial solution

$$\Delta(T = 0) = 2\omega_D \exp(-1/\lambda).$$

Inserting the latter into the energy, we find

$$\begin{aligned} E_0 \quad &= \quad E_0(\Delta = 0) - 2N\rho_F \omega_D^2 e^{-2/\lambda}. \\ &= \quad E_0(\Delta = 0) - \frac{N}{2}\rho_F \Delta^2 < E_0(\Delta = 0). \end{aligned} \tag{469}$$

The nontrivial solutions is always energetically lower.

Next we solve the gap equation. From the above unitary transfomation follows:

$$\begin{aligned} c_{\mathbf{k}\uparrow} \quad &= \quad u_{\mathbf{k}}^{*} a_{\mathbf{k}\uparrow} + v_{\mathbf{k}} a_{-\mathbf{k}\downarrow}^{\dagger} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \quad &= \quad -v_{\mathbf{k}} a_{\mathbf{k}\uparrow} + u_{\mathbf{k}} a_{-\mathbf{k}\downarrow}^{\dagger} \end{aligned}$$

which yields

$$c_{-\mathbf{k}\downarrow} = -v_{\mathbf{k}}^* a_{\mathbf{k}\uparrow}^\dagger + u_{\mathbf{k}}^* a_{-\mathbf{k}\downarrow}$$

This can be used to express the operator product $c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}$ that is needed to determine $\Delta_{\mathbf{k}}$. It holds:

$$c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} = \left(u_{\mathbf{k}}^* a_{\mathbf{k}\uparrow} + v_{\mathbf{k}} a_{-\mathbf{k}\downarrow}^\dagger\right)\left(u_{\mathbf{k}}^* a_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}^* a_{\mathbf{k}\uparrow}^\dagger\right)$$

which yields

$$\langle c_{-\mathbf{k},\downarrow}\, c_{\mathbf{k},\uparrow}\rangle = v_{\mathbf{k}} u_{\mathbf{k}}\left(2\left\langle a_{-\mathbf{k}\downarrow}^\dagger a_{-\mathbf{k}\downarrow}\right\rangle - 1\right)$$

and we obtain fo the gap equation:

$$\Delta = -\frac{V_0}{N}\sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}}\left(2f\left(E_{\mathbf{k}}\right) - 1\right). \tag{470}$$

We first analyze the gap quation at $T = 0$. Since $E_{\mathbf{k}} > 0$ follows that $f\left(E_{\mathbf{k}}\right) = 0$ in the limit of $T = 0$ and the gap equation simplifies to

$$\begin{aligned}
\Delta &= V_0 \rho \int_{-\omega_D}^{\omega_D} d\varepsilon \frac{\Delta}{2\sqrt{\varepsilon^2 + \Delta^2}} \\
&= \lambda\Delta \log\left(\frac{\omega_D}{\Delta} + \sqrt{1 + \left(\frac{\omega_D}{\Delta}\right)^2}\right) \\
&\simeq \lambda\Delta \log\left(\frac{2\omega_D}{\Delta}\right).
\end{aligned} \tag{471}$$

This yields the result:$\Delta\left(T = 0\right) = 2\omega_D \exp\left(-1/\lambda\right)$ in full agreement with the one we obtained from the minimization of the ground state energy.

In the vicinity of the transition temperature the gap Δ is small and we can linearize the gap-equation. The linearized gap equation is

$$\Delta = V\sum_{\mathbf{k}} \frac{\Delta}{2\xi_{\mathbf{k}}} \tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) \tag{472}$$

which we write with density of states ρ as

$$\Delta = V\rho\Delta \int_{-\omega_D}^{\omega_D} \frac{\tanh\left(\frac{\beta_c\varepsilon}{2}\right)}{2\varepsilon} d\varepsilon. \tag{473}$$

We perform the integral

$$\begin{aligned}
\int_{-\omega_0}^{\omega_0} \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{2\varepsilon} d\varepsilon &= \int_0^{\beta\omega_D/2} \frac{\tanh\left(x\right)}{x} dx \\
&= -\int_0^{\beta\omega_D/2} \sec h^2\left(x\right)\log\left(x\right) dx + \tanh\left(x\right)\log x\big|_0^{\beta\omega_D/2} \\
&= \gamma_E - \log\frac{\pi}{4} + \log\left(\frac{\omega_D}{2T}\right) = \log\left(\frac{2\omega_D e^{\gamma_E}}{\pi T}\right),
\end{aligned} \tag{474}$$

and obtain

$$\Delta = V\rho\Delta \log\left(\frac{2\omega_D e^{\gamma_E}}{\pi T_c}\right). \tag{475}$$

which yields for the transition temperature:

$$T_c = \frac{2\omega_D e^{\gamma_E}}{\pi} \exp\left(-\frac{1}{\lambda}\right) \simeq 1.134\omega_D \exp\left(-\frac{1}{\lambda}\right) \tag{476}$$

where $\lambda = V\rho$ is the dimensionless coupling constant. If we compare the value of the transition tempeature with the zero temperature gap, it follows

$$\begin{aligned} \frac{2\Delta\left(T=0\right)}{k_B T_c} &= \frac{4\omega_D \exp\left(-\frac{1}{\lambda}\right)}{\frac{2e^{\gamma_E}}{\pi}\omega_D \exp\left(-\frac{1}{\lambda}\right)} \\ &= 2\pi e^{-\gamma_E} \simeq 3.527\,3 \end{aligned} \tag{477}$$

which is in agreement with numerous observations for elementary supeconductors.

Finally, we want to determine the many body wave function that is associated with this new mean field state. To obtain the BCS wave function we use the fact that Eq.466 implies that the ground state wave function is the vacuum state of the Bogoliubov quasiparticles. Thus, it holds

$$a_{\mathbf{k}\sigma} \left|\Phi_{\mathrm{BCS}}\right\rangle = 0 \text{ for all } \mathbf{k}, \sigma. \tag{478}$$

To proceed, we assume

$$\left|\Phi_{\mathrm{BCS}}\right\rangle = C e^{\sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}\downarrow}} \left|0\right\rangle = C \prod_{\mathbf{k}} e^{\phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}} \left|0\right\rangle, \tag{479}$$

Here $\left|0\right\rangle$ is the vacuum state of the original operators, i.e. $c_{i\sigma}\left|0\right\rangle = 0$. We next determine $\phi_{\mathbf{k}}$ from the condition Eq.478. We write explicitly:

$$\begin{aligned} a_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} \\ a_{\mathbf{k}\downarrow} &= v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\uparrow} + u_{\mathbf{k}} c_{\mathbf{k}\downarrow}. \end{aligned} \tag{480}$$

Eq.478 is equivalent to

$$u_{\mathbf{k}} c_{\mathbf{k}\uparrow} \left|\Phi_{\mathrm{BCS}}\right\rangle = v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} \left|\Phi_{\mathrm{BCS}}\right\rangle. \tag{481}$$

We first analyze $c_{\mathbf{k}\uparrow}\left|\Phi_{\mathrm{BCS}}\right\rangle$. It is useful to introduce the operator

$$\theta = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \tag{482}$$

and it follows for the wave function

$$\left|\Phi_{\mathrm{BCS}}\right\rangle \propto \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \left|0\right\rangle. \tag{483}$$

It is easy to show that $[c_{\mathbf{k}\uparrow}, \theta] = b^\dagger_{-\mathbf{k}\downarrow}$with operator $b^\dagger_{-\mathbf{k}\downarrow} = \phi_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}$. Furthermore, it follows that $\left[b^\dagger_{-\mathbf{k}\downarrow}, \theta\right] = 0$. It is now easy to apply $c_{\mathbf{k}\uparrow}$ to each term in the sum of Eq.483 separately. It holds:

$$\begin{aligned} c_{\mathbf{k}\uparrow}\theta\,|0\rangle &= b^\dagger_{-\mathbf{k}\downarrow}\,|0\rangle \\ c_{\mathbf{k}\uparrow}\theta^2\,|0\rangle &= b^\dagger_{-\mathbf{k}\downarrow}\theta\,|0\rangle + \theta c_{\mathbf{k}\uparrow}\theta\,|0\rangle = 2\theta b^\dagger_{-\mathbf{k}\downarrow}\,|0\rangle \\ &\vdots \\ c_{\mathbf{k}\uparrow}\theta^n\,|0\rangle &= n\theta^{n-1} b^\dagger_{-\mathbf{k}\downarrow}\,|0\rangle\,. \end{aligned} \tag{484}$$

This result allows to sum-up the series Eq.483 and we obtain

$$c_{\mathbf{k}\uparrow}\,|\Phi_{\mathrm{BCS}}\rangle = b^\dagger_{-\mathbf{k}\downarrow}\,|\Phi_{\mathrm{BCS}}\rangle \tag{485}$$

The condition $a_{\mathbf{k}\sigma}\,|\Phi_{\mathrm{BCS}}\rangle = 0$ expressed in form of Eq.481 can now be expressed as

$$u_{\mathbf{k}}\phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\downarrow}\,|\Phi_{\mathrm{BCS}}\rangle = v_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}\,|\Phi_{\mathrm{BCS}}\rangle\,. \tag{486}$$

This implies immediately $\phi_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$. It is easy to show that the condition $a_{-\mathbf{k}\downarrow}\,|\Phi_{\mathrm{BCS}}\rangle = 0$ leads to the same condition. It follows with normalization factor:

$$C = \prod_{\mathbf{k}} u_{\mathbf{k}}$$

for the wave function

$$\begin{aligned} |\Phi_{\mathrm{BCS}}\rangle &= \prod_{\mathbf{k}} u_{\mathbf{k}} e^{v_{\mathbf{k}}/u_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}}\,|0\rangle \\ &= \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle\,. \end{aligned}$$

The last step is a consequence of the fact that due to Pauli Principle $\left(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\downarrow}\right)^n = 0$ if $n > 1$. This approach allows to project the BCS-wave function into the space of fixed number of electrons N.

$$|\Psi_{\mathrm{BCS}}, N\rangle = C\left(\sum_{\mathbf{k}} \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\downarrow}\right)^{2N}|0\rangle\,. \tag{487}$$

This projection can alternatively be realized if one starts from the BCS ground state and adds a global phase φ of the function $\phi_{\mathbf{k}}$:

$$|\Psi_{\mathrm{BCS}}, N\rangle = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-iN\varphi/2} \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\varphi} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\downarrow}\right)|0\rangle\,. \tag{488}$$

There exists an interesting relation between the phase φ and the pair number operator $\hat{N}_p$ which should give $2N$ in case of $|\Psi_{\rm BCS}, N\rangle$. With phase φ of $\phi_{\mathbf{k}}$ we have:

$$\begin{aligned} |\Psi_{\rm BCS}, N\rangle &= C\left(e^{i\varphi}\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^{N_p}|0\rangle \\ &= e^{i\varphi N_p}C\left(\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^{N_p}|0\rangle\,. \end{aligned} \tag{489}$$

This demonstrates immediately that

$$\hat{N}_p = -i\frac{\partial}{\partial\varphi}. \tag{490}$$

suggesting that particle number and phase are canonically conjugated variables, i.e. there should be a Heisenberg uncertainty relation between both quantities.
,