Lecture Notes*, Theory of Condensed Matter II

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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 $\rho_{\text{eq}} = \frac{1}{Z_g} e^{-\beta(H-\mu N)}$, 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

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

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

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

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

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

where the density matrix obeys the von Neuman equation

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

Note, in case of $\rho\left(t\right)$ and $W\left(t\right)$ 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 $\rho\left(t\right) = \sum_i \left|\Psi_{\mathrm{tot},i}\left(t\right)\right\rangle p_i \left\langle\Psi_{\mathrm{tot},i}\left(t\right)\right|$ from the Schrödinger equation of the many body wave function $\left|\Psi_{\mathrm{tot},i}\left(t\right)\right\rangle$ 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 $t \to -\infty$:

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

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

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

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

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

We can now determine the expectation value of A:

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

One can cyclically change the order under the trace operation:

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

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:

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

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.

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

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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $B = A^\dagger$)

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

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 $\left|\Psi_m^N\right\rangle = |m\rangle$ where we explicitly denote that we are considering a system with N particles. Let the final state be given as $\left|\Psi_f^N\right\rangle$. The corresponding energies are E_m^N and E_f^N. The transition probability per unit time between the two states is then given by Fermi's golden rule

$$w = 2\pi \left|\left\langle \Psi_f^N \left| V \right| \Psi_m^N \right\rangle\right|^2 \delta\left(\omega - E_f^N + E_m^N\right). \tag{69}$$

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:

$$V = \sum_{\mathbf{k},\mathbf{k}'\alpha\alpha'} d_{\mathbf{k},\mathbf{k}'}^{\alpha,\alpha'} \psi_{\mathbf{k}\alpha}^\dagger \psi_{\mathbf{k}'\alpha'}, \tag{71}$$

where $\psi_{\mathbf{k}\alpha}^\dagger$ is the creation operator of an electron with momentum $\mathbf{k}$ and spin α and $d_{\mathbf{k},\mathbf{k}'}^{\alpha,\alpha'} = -\left\langle \mathbf{k}\alpha \left| \mathbf{P} \right| \mathbf{k}'\alpha' \right\rangle \cdot \mathbf{E}_0$ 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

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

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

$$\begin{aligned} A &= \sum_{\mathbf{k},\alpha} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}}\psi_{\mathbf{k}\alpha} \\ B &= A^\dagger \end{aligned} \quad (76)$$

If we recall our earlier result that $J(\omega) = -2n_\eta(\omega)\,\mathrm{Im}G^r_{AA^\dagger}(\omega)$ 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

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

such that

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$H = \sum_{ij}h_{ij}c^\dagger_i c_j, \tag{87}$$

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]

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

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

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

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

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

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

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

$\hat{G}(\omega)$ 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

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

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

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

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

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

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

For the Hamiltonian of a free electron system

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

follows accordingly

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

Another relevant quantity to be Fourier transformed is the density

$$\rho\left(\mathbf{r}\right) = \sum_{\alpha} \psi^{\dagger}_{\alpha}\left(\mathbf{r}\right)\psi_{a}\left(\mathbf{r}\right). \tag{115}$$

It follows

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

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

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

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

$$\rho^{\mathrm{el}}\left(\mathbf{r}\right) = -e\sum_{\alpha}\psi^{\dagger}_{\alpha}\left(\mathbf{r}\right)\psi_{a}\left(\mathbf{r}\right). \tag{119}$$

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. $\rho^{\mathrm{el}}\left(\mathbf{r}\right) = -e\rho\left(\mathbf{r}\right)$.

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

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

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

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

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 $\left\langle\rho^{\mathrm{el}}(\mathbf{r})\right\rangle = \rho_0^{\mathrm{el}}$ becomes independent on $\mathbf{r}$. It follows

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

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 ρ_{ion} of the ions that is, on the time scale of the electrons, fixed. Charge neutrality implies that $\rho^{\mathrm{ion}} + \rho_0^{\mathrm{el}} = 0$. The total induced charge

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

in our solid is then related to the external potential via

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

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

The above relation between $\rho^{\mathrm{ind}}(\mathbf{r},t)$ and $\varphi^{\mathrm{ext}}(\mathbf{r}',t')$ 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

With this relation we obtain

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

Comparing this with Eq.(126) yields

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

Thus, the retarded density-density Green's function $\chi \left(\mathbf{q}, \omega\right)$ 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

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

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

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

If we consider for example a single point-charge as source, we have $\rho^{\text{ext}}(\mathbf{r},t) = e\delta(\mathbf{r})$, which yields $\rho^{\text{ext}}(\mathbf{q},\omega) = 2\pi e\delta(\omega)$ and finally $\varphi^{\text{ext}}(\mathbf{q},\omega) = 2\pi e\delta(\omega)\frac{4\pi}{q^2}$. 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):

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

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

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

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

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

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

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

The equation of motion requires the analysis of the commutator

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

This yields with

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

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

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

This can be solved and leads to

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

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

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

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

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

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

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

with so called Lindhard function $L(Q,\nu)$ 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 $\chi^r_{\mathbf{q}}(\omega)$ of Eq.(149). First, we notice the general property

$$\chi^r_{\mathbf{q}=\mathbf{0}}(\omega \neq 0) = 0. \tag{151}$$

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

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

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

$$\chi^r_{\mathbf{q}\to\mathbf{0}}(\omega=0) = \rho_F \tag{153}$$

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

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 $L_0\left(Q\gg 1\right)\sim\frac{1}{3Q^2}$ while for small momenta holds $L_0\left(Q\ll 1\right)\sim 1-\frac{1}{3}Q^2$. For $Q\to 1$ 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.

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

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

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

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

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

We can analytically perform this Fourier transformation

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

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

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

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 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

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

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

After analogous steps as for the real part we obtain

$$\begin{aligned}\mathrm{Im}\chi_{\mathbf{q}}^{r}\left(\omega\right) &= -\frac{m}{2\pi q}\int_{0}^{k_F} kdk\int_{-1}^{1} d\mu\left(\delta\left(\frac{m\omega}{kq}+\frac{q}{2k}-\mu\right)\right.\\ &- \left.\delta\left(\frac{m\omega}{kq}-\frac{q}{2k}-\mu\right)\right). \end{aligned} \tag{176}$$

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

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

with

$$\begin{aligned}L''\left(Q,\nu\right) &= \frac{\pi}{2Q}\int_{0}^{1} pdp\left[\theta\left(p+\frac{\nu}{Q}-Q\right)\theta\left(p-\frac{\nu}{Q}+Q\right)\right.\\ &- \left.\theta\left(p+\frac{\nu}{Q}+Q\right)\theta\left(p-\frac{\nu}{Q}-Q\right)\right] \end{aligned} \tag{178}$$

The integration over p finally yields

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

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

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

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

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

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

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

Fourier transformation to momentum space yields

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

with interaction matrix element

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

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

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

Thus, our first step is to determine the commutator

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

which gives rise to the equation of motion

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

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

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

which yields

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

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

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

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 $B = \psi_j^\dagger \psi_k^\dagger \psi_l$, we found

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \psi_{\mathbf{k}\alpha}^\dagger \psi_{\mathbf{k}_1\alpha_1}^\dagger \psi_{\mathbf{k}_1-\mathbf{q}_1\alpha_1} \psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha} &\approx \langle n_{\mathbf{k}_1\alpha_1} \rangle \delta_{\mathbf{q}_1,0} \psi_{\mathbf{k}\alpha}^\dagger \psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha} \\ &+ \langle n_{\mathbf{k}\alpha} \rangle \delta_{\mathbf{q}_1,-\mathbf{q}} \psi_{\mathbf{k}_1\alpha_1}^\dagger \psi_{\mathbf{k}_1-\mathbf{q}_1\alpha_1} \\ &- \langle n_{\mathbf{k}\alpha} \rangle \delta_{\mathbf{k},\mathbf{k}_1-\mathbf{q}_1} \delta_{\alpha\alpha_1} \psi_{\mathbf{k}_1\alpha_1}^\dagger \psi_{\mathbf{k}+\mathbf{q}+\mathbf{q}_1\alpha} \\ &- \langle n_{\mathbf{k}_1\alpha_1} \rangle \delta_{\mathbf{k}_1,\mathbf{k}+\mathbf{q}+\mathbf{q}_1} \delta_{\alpha\alpha_1} \psi_{\mathbf{k}\alpha}^\dagger \psi_{\mathbf{k}_1-\mathbf{q}_1\alpha} \end{aligned} \tag{202}$$

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

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.

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

Inserting these approximate expressions into the equation of motion yields

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

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 $v\left(\mathbf{k}-\mathbf{k}_1\right)$ 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

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

which can be solved and yields

$$\boxed{\chi_{\mathbf{q}}\left(\omega\right) = \frac{\chi^{(0)}_{\mathbf{q}}\left(\omega\right)}{1 + v\left(\mathbf{q}\right)\chi^{(0)}_{\mathbf{q}}\left(\omega\right)},} \quad (205)$$

where

$$\chi^{(0)}_{\mathbf{q}}\left(\omega\right) = \frac{1}{V}\sum_{\alpha\mathbf{k}}\frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\omega + i0^{+} - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}} \quad (206)$$

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

$$\varepsilon\left(\mathbf{q},\omega\right) = 1 + \frac{4\pi e^2}{q^2}\chi^{(0)}_{\mathbf{q}}\left(\omega\right) \quad (207)$$

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

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

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

$$\begin{aligned} G_{A,B}^c\left(t, t'\right) &= \left\langle\left\langle A\left(t\right); B\left(t'\right)\right\rangle\right\rangle^c \\ &\equiv -i\left\langle T A\left(t\right) B\left(t'\right)\right\rangle, \end{aligned} \tag{221}$$

with time ordering operator

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

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

$$e^{-iH\left(t-t'\right)} = e^{-iH_0 t} S\left(t,t'\right) e^{iH_0 t'} \tag{224}$$

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

$$\begin{aligned} A\left(t\right) &= e^{iHt} A e^{-iHt} \\ &= S^{\dagger}\left(t,0\right) e^{-iH_0 t} A e^{-iH_0 t} S\left(t,0\right) \\ &= S^{\dagger}\left(t,0\right) \tilde{A}\left(t\right) S\left(t,0\right) \end{aligned} \tag{225}$$

where

$$\tilde{A}\left(t\right) = e^{-iH_0 t} A e^{-iH_0 t}. \tag{226}$$

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

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

It holds

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

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

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

The solution of the above differential equation is

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

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

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

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

$$\mathcal{G}_{AB}(\tau, \tau') = -\langle T A(\tau) B(\tau') \rangle. \tag{237}$$

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:

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

If $\tau < 0$ holds

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

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

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

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

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

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

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

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

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

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

$$e^{-i\beta\omega_n} = -\eta. \tag{247}$$

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

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

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:

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

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

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

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

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

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

$$\mathcal{S}(\tau,\tau') = Te^{-\int_{\tau'}^{\tau}d\tau''\tilde{V}(\tau'')}.$$

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

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

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:

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

Our goal is to proof that

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

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

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

and write

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

If we look at the second term, we find similarly

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

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

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

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

Next we perform the thermodynamic average

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

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

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

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:

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

and

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

7.3 Wick theorem for time dependent operators

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 Green's functions

$$\mathcal{G}_0^{(n)}(i_1, \cdots i_n; j_1 \cdots j_n) = (-1)^n \left\langle T c_{i_1} \cdots c_{i_n} c_{j_n}^\dagger \cdots c_{j_1} \right\rangle_0 , \tag{302}$$

where now c_{i_1} stands for $c_{i_1}(\tau_{j_1})$ etc., i.e. it also contains a time variable. The corresponding Wick-theorem is

$$\mathcal{G}_0^{(n)}(i_1, \cdots i_n; j_1 \cdots j_n) = \sum_P (-\eta)^P \mathcal{G}_0\left(i_1; j_{P(1)}\right) \cdots \mathcal{G}_0\left(i_n; j_{P(n)}\right) . \tag{303}$$

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).

$$\mathcal{G}_0(i; j) = -\left\langle T c_i c_j^\dagger \right\rangle_0 \tag{304}$$

is the noninteracting single particle Matsubara function. Before we give the proof for this expression, we list an example

$$\mathcal{G}_0^{(2)}(i_1, i_2; j_1 j_2) = \mathcal{G}_0(i_1; j_1)\mathcal{G}_0(i_2; j_2) - \eta \mathcal{G}_0(i_1; j_2)\mathcal{G}_0(i_2; j_1) . \tag{305}$$

Next we prove the above given Wick-theorem.

It holds (it is now more convenient to explicitly list the time arguments)

$$\mathcal{G}_0(i\tau; j) = -\theta(\tau)\left\langle c_i(\tau) c_j^\dagger \right\rangle_0 + \eta\theta(-\tau)\left\langle c_j^\dagger c_i(\tau) \right\rangle_0 \tag{306}$$

We use our results for the time dependence of the Matsubara operators to obtain

$$\mathcal{G}_0(i\tau; j) = -\theta(\tau) e^{-\tau\varepsilon_i}\delta_{ij}\left\langle c_i c_i^\dagger \right\rangle_0 + \eta\theta(-\tau) e^{-\tau\varepsilon_i}\delta_{ij}\left\langle c_i^\dagger c_i \right\rangle_0 . \tag{307}$$

8 Diagrammatic expansion of the partition function

end