Lecture Notes[1], Theory of Condensed Matter II, Karlsruhe Institute of Technology

Jörg Schmalian

April 21, 2018

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. Next we will introduce the Feynman-diagram technique of thermal Green's functions and apply these techniques to problems such as itinerant ferromagnetism, superconductivity, and dynamical screening of the Coulomb interaction. 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 to be 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 a statement as possible. In fact, the beauty of condensed matter theory is to make predictions about new states of matter and universal behavior that are emergent, i.e. that are 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, synnetry arguments and, of course, by good physical intuition. This is the same, regardless of 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

Chapter 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

$$\langle A \rangle = \mathrm{tr}\left(\rho \mathrm{A}\right), \tag{1.1}$$

with density operator (often called density matrix)

$$\rho = \frac{1}{Z} e^{-\beta H}. \tag{1.2}$$

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

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

$$H_{\mathrm{tot}} = H + W(t) \tag{1.3}$$

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

$$W(t) = -\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{B}(t) \tag{1.4}$$

of an external magnetic field to the electron spins

$$\mathbf{S}_i = \frac{\hbar}{2} \sum_{\alpha\beta} c^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta} \tag{1.5}$$

of a magnetic system. Another example is the interaction

$$W(t) = -\sum_i \mathbf{P}_i \cdot \mathbf{E}(t) \tag{1.6}$$

between the electrical polarization

$$\mathbf{P}_i = e \sum_\alpha c^\dagger_{i\alpha} \mathbf{R}_i c_{i\alpha} \tag{1.7}$$

of electrons at lattice sites i and an external electrical field.

As for the time dependence of $W(t)$, we 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

$$\begin{aligned} \mathbf{E}(t) &= \lim_{\delta \to 0^+} \mathbf{E}_0 \exp\left(-i(\omega + i\delta)t\right) \\ \mathbf{B}(t) &= \lim_{\delta \to 0^+} \mathbf{B}_0 \exp\left(-i(\omega + i\delta)t\right), \end{aligned} \tag{1.8}$$

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

$$W(t) = \lim_{\delta \to 0^+} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} W(\omega) e^{-i(\omega + i\delta)t}. \tag{1.9}$$

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

$$\langle A \rangle_t = \mathrm{tr}\left(\rho(\mathrm{t})\,\mathrm{A}\right), \tag{1.10}$$

where the density matrix obeys the von Neuman equation

$$i\hbar \frac{\partial}{\partial t} \rho(t) = \left[H + W(t), \rho(t)\right]. \tag{1.11}$$

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

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

$$\rho(t \to -\infty) = \rho = \frac{1}{Z} e^{-\beta H}. \tag{1.12}$$

In most cases the external perturbation is small and we can confine ourselves to changes in $\langle A \rangle_t$ that are linear in $W(t)$. This regime is referred to as *linear response*. The subsequent formalism can be (and has been) extended to include higher order non-linearities. Here we will, however, only consider the leading order, linear effects.

To proceed we go to the interaction representation

$$\rho(t) = e^{-iHt/\hbar} \rho^{(I)}(t)\, e^{iHt/\hbar}. \tag{1.13}$$

Note, $\rho^{(I)}(t)$ corresponds to the interaction picture of the Hamiltonian H_{tot}. The Hamiltonian of our system of interest is of course H ($W(t)$ is only used to probe this system). If considered with regards to H, $\rho^{(I)}(t)$ 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

$$i\hbar \frac{\partial \rho(t)}{\partial t} = \left[H, \rho(t)\right] + e^{-iHt/\hbar} i\hbar \frac{\partial \rho^{(I)}(t)}{\partial t} e^{iHt/\hbar}. \tag{1.14}$$

Inserting the von Neuman equation yields

$$i\hbar \frac{\partial \rho^{(I)}(t)}{\partial t} = \left[W^{(I)}(t), \rho^{(I)}(t)\right], \tag{1.15}$$

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

$$\rho^{(I)}(t) = \rho - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \left[W^{(I)}(t'), \rho^{(I)}(t')\right]. \tag{1.16}$$

If we return to the Schrödinger picture, it follows

$$\rho(t) = \rho - \frac{i}{\hbar}\int_{-\infty}^{t} dt' e^{-iH(t-t')/\hbar}\left[W(t'), \rho(t')\right] e^{iH(t-t')/\hbar}. \tag{1.17}$$

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

$$\rho(t) = \rho - \frac{i}{\hbar}\int_{-\infty}^{t} dt' e^{-iH(t-t')/\hbar}\left[W(t), \rho\right] e^{iH(t-t')/\hbar}. \tag{1.18}$$

We can now determine the expectation value of A:

$$\langle A\rangle_t = \langle A\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \mathrm{tr}\left(\left[\mathrm{W^{(I)}(t'), \rho}\right]\mathrm{A^{(I)}(t)}\right). \tag{1.19}$$

One can cyclically change the order under the trace operation:

$$\mathrm{tr}\left[(\mathrm{W}\rho - \rho\mathrm{W})\,\mathrm{A}\right] = \mathrm{tr}\left[(\mathrm{AW} - \mathrm{WA})\,\rho\right], \tag{1.20}$$

which gives

$$\langle A\rangle_t = \langle A\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \left\langle\left[A^{(I)}(t), W^{(I)}(t')\right]\right\rangle. \tag{1.21}$$

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

$$\left\langle\left\langle A^{(I)}(t); B^{(I)}(t')\right\rangle\right\rangle = -\frac{i}{\hbar}\theta(t-t')\left\langle\left[A^{(I)}(t), B^{(I)}(t')\right]\right\rangle \tag{1.22}$$

such that

$$\boxed{\langle A\rangle_t = \langle A\rangle + \int_{-\infty}^{\infty} dt' \left\langle\left\langle A^{(I)}(t); W^{(I)}(t')\right\rangle\right\rangle.} \tag{1.23}$$

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 offers 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:

$$W^{(I)}(t) = -\sum_i \mathbf{P}_i^{(I)} \cdot \mathbf{E}(t). \tag{1.24}$$

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

$$\mathbf{E}(t) = \mathbf{E}_0 \exp\left(-i\left(\omega + i0^+\right)t\right). \tag{1.25}$$

If we are interested in the electrical current it follows

$$\langle j_\alpha\rangle_t = -\sum_i \int_{-\infty}^{\infty} dt' \left\langle\left\langle j_\alpha^{(I)}(t); P_{\beta,i}^{(I)}(t')\right\rangle\right\rangle E_{0,\beta} e^{-i(\omega+i\delta)t'} \tag{1.26}$$

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.

1.1 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:

$$\begin{aligned} G^r_{A,B}(t,t') &= \langle\langle A(t); B(t')\rangle\rangle^r \\ &\equiv -i\theta(t-t')\left\langle [A(t), B(t')]_\eta \right\rangle . \end{aligned} \tag{1.27}$$

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 the Heisenberg picture if we refer to the Hamiltonian H of the system we are interested in:

$$A(t) = e^{iHt} A e^{-iHt}. \tag{1.28}$$

Finally, we introduce

$$[A, B]_\eta = AB + \eta BA \tag{1.29}$$

to simultaneously analyze the commutator for $\eta = -1$ and the anti-commutator for $\eta = +1$. We will see very soon that the generalization to anti-commutators is sometimes a very sensible thing to do if one considers 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 $W(t')$ for $t' < t$. It is however possible, at least formally, to introduce other Green's functions. Important examples are advanced Green's functions:

$$\begin{aligned} G^a_{A,B}(t,t') &= \langle\langle A(t); B(t')\rangle\rangle^r \\ &\equiv i\theta(t'-t)\left\langle [A(t), B(t')]_\eta \right\rangle \end{aligned} \tag{1.30}$$

and the time-ordered (sometimes called causal) Green's functions:

$$\begin{aligned} G^c_{A,B}(t,t') &= \langle\langle A(t); B(t')\rangle\rangle^c \\ &\equiv -i\left\langle T_\eta A(t) B(t')\right\rangle , \end{aligned} \tag{1.31}$$

with time ordering operator

$$T_\eta A(t) B(t') = \theta(t-t') A(t) B(t') - \eta\theta(t'-t) B(t') A(t) . \tag{1.32}$$

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 knowing one of these functions allows to determine the others. They contain the same information.

1.1.1 Homogeneity of time

An important property of all of those Green's functions is that they are only functions of the difference $t - t'$. To demonstrate that this is the case we start from the definition:

$$\begin{aligned} G^r_{A,B}(t,t') &= -i\theta(t-t')\left\langle [A(t), B(t')]_\eta \right\rangle \\ &= -i\theta(t-t')\left(\langle A(t) B(t')\rangle + \eta\langle B(t') A(t)\rangle\right) \end{aligned} \tag{1.33}$$

The correlation functions are explicitly given as

$$\begin{aligned} \langle A(t) B(t')\rangle &= \frac{1}{Z}\mathrm{tr}\left(e^{-\beta H} e^{iHt} A e^{-iHt} e^{iHt'} B e^{-iHt'}\right) \\ &= \frac{1}{Z}\mathrm{tr}\left(e^{-\beta H} e^{iH(t-t')} A e^{-iH(t-t')} B\right) \\ &= \langle A(t-t') B(0)\rangle \end{aligned} \tag{1.34}$$

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

$$\boxed{G^r_{A,B}(t,t') = G^r_{A,B}(t-t').} \tag{1.35}$$

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 $[H, X_i] = 0$.

1.1.2 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]:

$$i\partial_t A(t) = [A(t), H]_- . \tag{1.36}$$

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

We start from

$$\begin{aligned} i\partial_t G^r_{A,B}(t) &= \partial_t \left\{ \theta(t) \left\langle [A(t), B(0)]_\eta \right\rangle \right\} \\ &= \delta(t) \left\langle [A,B]_\eta \right\rangle + \theta(t) \left\langle [\partial_t A(t), B(0)]_\eta \right\rangle \\ &= \delta(t) \left\langle [A,B]_\eta \right\rangle - i\theta(t) \left\langle \left[[A(t),H]_-, B(0) \right]_\eta \right\rangle, \end{aligned} \tag{1.37}$$

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.

$$\boxed{i\partial_t G^r_{A,B}(t) = \delta(t) \left\langle [A,B]_\eta \right\rangle + G^r_{[A,H]_-,B}(t).} \tag{1.38}$$

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 can be expressed in terms of the initial one, 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 if 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.(1.35) follows that we can Fourier transform the Green's function

$$G^r_{AB}(\omega) = \int_{-\infty}^{\infty} dt G^r_{AB}(t) e^{i\omega t}. \tag{1.39}$$

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

$$\omega G^r_{A,B}(\omega) = \left\langle [A,B]_\eta \right\rangle + G^r_{[A,H]_-,B}(\omega). \tag{1.40}$$

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.(1.38) and (1.40). On the other hand, the detailed time dependence of $G^r(t)$, $G^a(t)$, and

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

$G^c(t)$ 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 implies that the Fourier transform in Eq.(1.39) 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.

1.1.3 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.

$$H|l\rangle = E_l|l\rangle. \tag{1.41}$$

Then, we can write a thermal expectation value as

$$\langle A\rangle = \mathrm{tr}(\rho \mathrm{A}) = \frac{1}{Z}\sum_l e^{-\beta E_l}\langle l|A|l\rangle. \tag{1.42}$$

For a correlation function follows accordingly

$$\begin{aligned}\langle A(t)B(0)\rangle &= \frac{1}{Z}\sum_l e^{-\beta E_l}\langle l|A(t)B(0)|l\rangle \\ &= \frac{1}{Z}\sum_l e^{-\beta E_l}\left\langle l\left|e^{iHt}Ae^{-iHt}B\right|l\right\rangle \\ &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_l}e^{it(E_l-E_m)}\langle l|A|m\rangle\langle m|B|l\rangle\end{aligned} \tag{1.43}$$

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

$$\begin{aligned}\langle B(0)A(t)\rangle &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_l}e^{-it(E_l-E_m)}\langle l|B|m\rangle\langle m|A|l\rangle \\ &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_m}e^{it(E_l-E_m)}\langle l|A|m\rangle\langle m|B|l\rangle\end{aligned} \tag{1.44}$$

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

$$\langle B(0)A(t)\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}J(\omega)e^{-i\omega t}. \tag{1.45}$$

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

$$\begin{aligned}J(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}\langle B(0)A(t)\rangle \\ &= \frac{1}{Z}\sum_{l.m} e^{-\beta E_m}\langle l|A|m\rangle\langle m|B|l\rangle\int_{-\infty}^{\infty} dt e^{it(\omega+E_l-E_m)}.\end{aligned} \tag{1.46}$$

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

$$\boxed{J(\omega) = \frac{2\pi}{Z}\sum_{l.m} e^{-\beta E_m}\langle l|A|m\rangle\langle m|B|l\rangle\,\delta(\omega+E_l-E_m).} \tag{1.47}$$

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 contributes and we obtain

$$J_{T=0}(\omega) = 2\pi \sum_l \langle 0|B|l\rangle \langle l|A|0\rangle \delta(\omega + E_l - E_0). \tag{1.48}$$

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 for all T real and positive definite: $J(\omega) \geq 0$. With our above results for the two correlation functions follows immediately

$$\langle A(t) B(0)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\beta\omega} J(\omega) e^{-i\omega t}. \tag{1.49}$$

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

$$\begin{aligned} G^r_{AB}(\omega) &= -i\int_{-\infty}^{\infty} dt e^{i\omega t}\theta(t)\left(\langle A(t) B\rangle + \eta\langle BA(t)\rangle\right) \\ &= -i\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\left(e^{\beta\omega'} + \eta\right) J(\omega') \int_{-\infty}^{\infty} dt e^{i(\omega-\omega')t}\theta(t) \end{aligned} \tag{1.50}$$

To proceed we need to analyze the integral

$$\begin{aligned} f(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}\theta(t) \\ &= \int_0^{\infty} dt e^{i\omega t} \\ &= \lim_{\delta\to 0^+} \int_0^{\infty} dt e^{i(\omega+i\delta)t} \\ &= \frac{i}{\omega + i0^+}. \end{aligned} \tag{1.51}$$

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

$$F(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{ie^{-i\omega t}}{\omega + i0^+}. \tag{1.52}$$

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

$$G^r_{AB}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\left(e^{\beta\omega'} + \eta\right) J(\omega')}{\omega - \omega' + i0^+}. \tag{1.53}$$

Inserting the spectral function yields the so called Lehmann representation:

$$G^r_{AB}(\omega) = \frac{1}{Z}\sum_{l.m} \frac{\left(e^{-\beta E_l} + \eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{\omega + E_l - E_m + i0^+} \tag{1.54}$$

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

$$\boxed{G_{AB}(z) = \frac{1}{Z}\sum_{l.m} \frac{\left(e^{-\beta E_l} + \eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{z + E_l - E_m},} \tag{1.55}$$

with complex argument z and the retarded function is given by

$$G^r_{AB}(\omega) = G_{AB}\left(\omega + i0^+\right). \tag{1.56}$$

Repeating our analysis for the advanced Green's function yields

$$G^a_{AB}(\omega) = G_{AB}\left(\omega - i0^+\right). \tag{1.57}$$

If one keeps in mind that under the integral holds

$$\frac{1}{\omega + i0^+} = \mathcal{P}\frac{1}{\omega} - i\pi\delta(\omega), \tag{1.58}$$

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

$$\begin{aligned} G^r_{AB}(\omega) - G^a_{AB}(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(e^{\beta\omega'}+\eta\right)J(\omega') \\ &\times \left(\frac{1}{\omega-\omega'+i0^+} - \frac{1}{\omega-\omega'-i0^+}\right) \\ &= -i\left(e^{\beta\omega}+\eta\right)J(\omega) \end{aligned} \tag{1.59}$$

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

$$J(\omega) = -2n_\eta(\omega)\,\mathrm{Im}G^r_{AA^\dagger}(\omega), \tag{1.60}$$

where

$$n_\eta(\omega) = \frac{1}{e^{\beta\omega}+\eta} \tag{1.61}$$

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

$$\boxed{G^r_{AA^\dagger}(\omega) = -\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\mathrm{Im}G^r_{AA^\dagger}(\omega')}{\omega-\omega'+i0^+},} \tag{1.62}$$

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

$$G_{AA^\dagger}(z) = -\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\mathrm{Im}G^r_{AA^\dagger}(\omega')}{z-\omega'}. \tag{1.63}$$

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

$$\begin{aligned} \langle BA(t)\rangle &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}J(\omega)\,e^{-i\omega t} \\ &= -\int_{-\infty}^{\infty}\frac{d\omega}{\pi}n_\eta(\omega)\,\frac{G^r_{AB}(\omega)-G^a_{AB}(\omega)}{2i}e^{-i\omega t}. \end{aligned} \tag{1.64}$$

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

$$\boxed{\left(\omega + i0^+\right) G^r_{A,B}(\omega) = \left\langle [A,B]_\eta \right\rangle + G^r_{[A,H]_-,B}(\omega).} \tag{1.65}$$

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

$$\int_{-\infty}^{\infty} d\omega G^r_{A,B}(\omega) = -i\pi \left\langle [A,B]_\eta \right\rangle. \tag{1.66}$$

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

$$H = \sum_{\mathbf{k}\alpha} (\varepsilon_{\mathbf{k}} - \mu) \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}\alpha}. \tag{1.67}$$

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

$$[\psi_{\mathbf{k}\alpha}, H]_- = (\varepsilon_{\mathbf{k}} - \mu) \psi_{\mathbf{k}\alpha} \tag{1.68}$$

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

$$\left(\omega + i0^+\right) G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \left\langle \left[\psi_{\mathbf{k}\alpha}, \psi^\dagger_{\mathbf{k}'\alpha'}\right]_+ \right\rangle + (\varepsilon_{\mathbf{k}} - \mu) G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) \tag{1.69}$$

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

$$G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \delta_{\alpha\alpha'}\delta_{\mathbf{k}\mathbf{k}'} G^r_{\mathbf{k}}(\omega), \tag{1.70}$$

with

$$\boxed{G^r_{\mathbf{k}}(\omega) = \frac{1}{\omega + i0^+ - \varepsilon_{\mathbf{k}} + \mu}.} \tag{1.71}$$

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

$$-\frac{1}{\pi} \mathrm{Im} G^r_{\mathbf{k}}(\omega) = \delta(\omega - \varepsilon_{\mathbf{k}} + \mu). \tag{1.72}$$

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

$$\begin{aligned} \left\langle \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}\alpha} \right\rangle &= -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} n_+(\omega) \mathrm{Im} G^r_{\mathbf{k}}(\omega). \\ &= \int_{-\infty}^{\infty} d\omega f(\omega) \delta(\omega - \varepsilon_{\mathbf{k}} + \mu) \\ &= f(\varepsilon_{\mathbf{k}} - \mu). \end{aligned} \tag{1.73}$$

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.

1.2 Green's function for free particles

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

$$H = \sum_{ij} h_{ij} c_i^\dagger c_j, \tag{1.74}$$

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

$$\begin{aligned} \left[c_i, c_j^\dagger\right]_\eta &= \delta_{ij}, \\ \left[c_i, c_j\right]_\eta &= \left[c_i^\dagger, c_j^\dagger\right]_\eta = 0, \end{aligned} \tag{1.75}$$

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

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

$$G_{ij}^r(t) = -i\theta(t) \left\langle \left[c_i(t), c_j^\dagger\right]_\eta \right\rangle. \tag{1.76}$$

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

$$\left[c_i, H\right]_- = \sum_{lm} h_{lm} \left[c_i, c_l^\dagger c_m\right]_- \tag{1.77}$$

It holds

$$\begin{aligned} \left[c_i, c_l^\dagger c_m\right]_- &= c_i c_l^\dagger c_m - c_l^\dagger c_m c_i \\ &= -\eta c_l^\dagger c_i c_m + \delta_{il} c_m - c_l^\dagger c_m c_i \\ &= \eta^2 c_l^\dagger c_m c_i + \delta_{il} c_m - c_l^\dagger c_m c_i \\ &= \delta_{il} c_m, \end{aligned} \tag{1.78}$$

which yields

$$\left[c_i, H\right]_- = \sum_m h_{im} c_m, \tag{1.79}$$

regardless of whether we consider bosons or fermions.

For our equation of motion follows then

$$\left(\omega + i0^+\right) G_{ij}^r(\omega) = \delta_{ij} + \sum_m h_{im} G_{mj}^r(\omega). \tag{1.80}$$

We see that the equation of motion closes in the sense that only Green's functions of the type defined in Eq.(1.76) are needed. It is also natural to introduce a matrix $\hat{G}(\omega)$ with matrix elements $G_{ij}(\omega)$ and similarly $\hat{h}$ for the matrix representation of the Hamiltonian with elements h_{ij}. Then follows[3]

$$\omega \hat{G}(\omega) = \hat{1} + \hat{h} \cdot \hat{G}(\omega), \tag{1.81}$$

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

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

or

$$\left(\omega - \hat{h}\right) \hat{G}(\omega) = \hat{1}. \tag{1.82}$$

This leads to

$$\boxed{\hat{G}(\omega) = \left(\omega - \hat{h}\right)^{-1}.} \tag{1.83}$$

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

$$G^r_{\mathbf{k}}(\omega) = \frac{1}{\omega + i0^+ - \varepsilon_{\mathbf{k}}}, \tag{1.84}$$

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

1.2.1 Perturbation theory and Dyson equation

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

$$h_{ij} = \varepsilon^0_i \delta_{ij} + V_{ij}, \tag{1.85}$$

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

This suggests to write

$$\begin{aligned} \hat{G}^{-1} &= \omega - \hat{h}^0 - \hat{V} \\ &= \hat{G_0}^{-1} - \hat{V}, \end{aligned} \tag{1.86}$$

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

$$G_{0,ij}(\omega) = \frac{\delta_{ij}}{\omega - \varepsilon^0_i}. \tag{1.87}$$

Eq.(1.86) is called the Dyson equation for single particle systems, i.e. for systems without interactions. We can multiply Eq.(1.86) from the left with $\hat{G}_0$ and from the right with $\hat{G}$ and obtain

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}. \tag{1.88}$$

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

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 \hat{V} \hat{G}_0 \cdots. \tag{1.89}$$

1.2.2 Higher order correlation functions

The knowledge of $G^r_{ij}(\omega)$ yields immediate information about expectation values of the form $\left\langle c^\dagger_i c_j \right\rangle$. Suppose we want to know something about a more complicated expectation value, such as $\left\langle c^\dagger_j c^\dagger_k c_l c_i \right\rangle$, 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 $B = c^\dagger_j c^\dagger_k c_l$.

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

$$\omega G_{i,jkl}(\omega) = \left\langle \left[c_i, c_j^\dagger c_k^\dagger c_l \right]_\eta \right\rangle + \sum_m h_{im} G_{m,jkl}(\omega). \tag{1.90}$$

The remaining commutator or anticommutator is easily calculated as:

$$\begin{aligned} \left[c_i, c_j^\dagger c_k^\dagger c_l \right]_\eta &= c_i c_j^\dagger c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= -\eta c_j^\dagger c_i c_k^\dagger c_l + \delta_{ij} c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= c_j^\dagger c_k^\dagger c_i c_l - \eta \delta_{ik} c_j^\dagger c_l + \delta_{ij} c_k^\dagger c_l + \eta c_j^\dagger c_k^\dagger c_l c_i \\ &= \delta_{ij} c_k^\dagger c_l - \eta \delta_{ik} c_j^\dagger c_l. \end{aligned} \tag{1.91}$$

This yields for the equation of motion the result:

$$\omega G_{i,jkl}(\omega) = \delta_{ij} \left\langle c_k^\dagger c_l \right\rangle - \eta \delta_{ik} \left\langle c_j^\dagger c_l \right\rangle + \sum_m h_{im} G_{m,jkl}(\omega). \tag{1.92}$$

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

$$\sum_m \left(\hat{G}(\omega)^{-1} \right)_{im} G_{m,jkl}(\omega) = \delta_{ij} \left\langle c_k^\dagger c_l \right\rangle - \eta \delta_{ik} \left\langle c_j^\dagger c_l \right\rangle, \tag{1.93}$$

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

$$G_{i,jkl}(\omega) = G_{ij}(\omega) \left\langle c_k^\dagger c_l \right\rangle - \eta G_{ik}(\omega) \left\langle c_j^\dagger c_l \right\rangle \tag{1.94}$$

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

$$\boxed{\left\langle c_j^\dagger c_k^\dagger c_l c_i \right\rangle = \left\langle c_j^\dagger c_i \right\rangle \left\langle c_k^\dagger c_l \right\rangle - \eta \left\langle c_j^\dagger c_l \right\rangle \left\langle c_k^\dagger c_i \right\rangle.} \tag{1.95}$$

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.

1.3 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

$$w = 2\pi \left| \left\langle \Psi_f^N \left| V \right| \Psi_m^N \right\rangle \right|^2 \delta\left(\omega - E_f^N + E_m^N\right). \tag{1.96}$$

The perturbation caused by the irradiation is of the form

$$V = -\mathbf{P} \cdot \mathbf{E}_0. \tag{1.97}$$

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

$$V = \sum_{\mathbf{k},\mathbf{k}'\alpha\alpha'} d^{\alpha,\alpha'}_{\mathbf{k},\mathbf{k}'} \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}'\alpha'}, \tag{1.98}$$

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

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

$$\left| \Psi^N_f \right\rangle = \psi^\dagger_{\mathbf{k}_f\beta} \left| \Psi^{N-1}_l \right\rangle \tag{1.99}$$

is the photoelectron added to one of the eigenstates of the $N-1$-particle system. At the same time we assume $\psi_{\mathbf{k}_f\beta} \left| \Psi^N_m \right\rangle = 0$, 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

$$w = 2\pi \left| \left\langle \Psi^{N-1}_l \left| \psi_{\mathbf{k}_f\beta} \sum_{\mathbf{k},\mathbf{k}'\alpha\alpha'} d^{\alpha,\alpha'}_{\mathbf{k},\mathbf{k}'} \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}'\alpha'} \right| \Psi^N_m \right\rangle \right|^2 \delta\left(\omega - E^N_f + E^N_m\right) \tag{1.100}$$

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

It follows

$$w = 2\pi \left| \left\langle \Psi^{N-1}_l \left| \sum_{\mathbf{k},\alpha} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \psi_{\mathbf{k}\alpha} \right| \Psi^N_m \right\rangle \right|^2 \delta\left(\omega - E^N_f + E^N_m\right) \tag{1.101}$$

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

$$I_{\mathbf{k}_f\beta}(\omega) = \frac{2\pi}{Z} \sum_{lm} e^{-\beta E_m} \left| \left\langle l \left| \sum_{\mathbf{k},\alpha} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \psi_{\mathbf{k}\alpha} \right| m \right\rangle \right|^2 \delta\left(\omega - \epsilon_{\mathbf{k}_f} - E_l + E_m\right) \tag{1.102}$$

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

$$\begin{aligned} A &= \sum_{\mathbf{k},\alpha} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \psi_{\mathbf{k}\alpha} \\ B &= A^\dagger \end{aligned} \tag{1.103}$$

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

$$\boxed{G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = -i\theta(t - t')(t) \left\langle \left[\psi_{\mathbf{k}\alpha}(t), \psi^\dagger_{\mathbf{k}'\alpha'}(0) \right]_+ \right\rangle,} \tag{1.104}$$

such that

$$I_{\mathbf{k}_f\beta}(\omega) = -2f\left(\omega - \epsilon_{\mathbf{k}_f}\right) \sum_{\mathbf{k}\mathbf{k}',\alpha\alpha'} d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \operatorname{Im} G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}\left(\omega - \epsilon_{\mathbf{k}_f}\right) d^{\alpha',\beta*}_{\mathbf{k}',\mathbf{k}_f}. \tag{1.105}$$

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

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

$$H = \sum_{\mathbf{k}\alpha} \left(\varepsilon_{\mathbf{k}} - \mu\right) \psi^{\dagger}_{\mathbf{k}\alpha} \psi_{\mathbf{k}\alpha}. \tag{1.106}$$

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

$$\left[\psi_{\mathbf{k}\alpha}, H\right]_- = \left(\varepsilon_{\mathbf{k}} - \mu\right) \psi_{\mathbf{k}\alpha} \tag{1.107}$$

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

$$\left(\omega + i0^+\right) G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \left\langle \left[\psi_{\mathbf{k}\alpha}, \psi^{\dagger}_{\mathbf{k}'\alpha'}\right]_+ \right\rangle + \left(\varepsilon_{\mathbf{k}} - \mu\right) G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) \tag{1.108}$$

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

$$G^r_{\mathbf{k},\mathbf{k}'\alpha\alpha'}(\omega) = \delta_{\alpha\alpha'}\delta_{\mathbf{k}\mathbf{k}'} G^r_{\mathbf{k}}(\omega), \tag{1.109}$$

with

$$\boxed{G^r_{\mathbf{k}}(\omega) = \frac{1}{\omega + i0^+ - \varepsilon_{\mathbf{k}} + \mu}.} \tag{1.110}$$

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

$$-\frac{1}{\pi}\mathrm{Im}G^r_{\mathbf{k}}(\omega) = \delta\left(\omega - \varepsilon_{\mathbf{k}} + \mu\right). \tag{1.111}$$

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

$$\begin{aligned}
\left\langle \psi^{\dagger}_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha} \right\rangle &= -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} n_+(\omega)\, \mathrm{Im}G^r_{\mathbf{k}}(\omega). \\
&= \int_{-\infty}^{\infty} d\omega f(\omega)\, \delta\left(\omega - \varepsilon_{\mathbf{k}} + \mu\right) \\
&= f\left(\varepsilon_{\mathbf{k}} - \mu\right).
\end{aligned} \tag{1.112}$$

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:

$$I_{\mathbf{k}_f\beta}(\omega) = \frac{2}{\pi} f\left(\omega - \epsilon_{\mathbf{k}_f}\right) \sum_{\mathbf{k},\alpha} \left| d^{\beta,\alpha}_{\mathbf{k}_f,\mathbf{k}} \right|^2 \delta\left(\omega - \epsilon_{\mathbf{k}_f} - \varepsilon_{\mathbf{k}\alpha} + \mu\right). \tag{1.113}$$

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

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

Chapter 2

The Kubo identity

We consider a system characterized by Hamiltonian H with additional external and time-dependent perturbation

$$W = -\sum_j A_j F_j(t) \tag{2.1}$$

characterized by operators A_j and time dependent functions $F_j(t)$. The usual linear response analysis yields for the time dependence of the expectation value $\langle A_i \rangle_t$ of A_i to linear order in the perturbation:

$$\langle A_i \rangle_t = \langle A_i \rangle + \int_{-\infty}^{\infty} dt \sum_j G_{ij}(t - t') F_j(t'), \tag{2.2}$$

with retarded Green's function

$$G_{ij}(t) = -i\theta(t) \langle [A_i(t), A_j(0)] \rangle. \tag{2.3}$$

Here time-dependent operators are in the Heisenberg representation of H.

Next we prove the so called Kubo identity

$$i[A(t), \rho] = \rho \int_0^{\beta} d\tau \dot{A}(t - i\tau). \tag{2.4}$$

Here, we used

$$A(t - i\tau) = e^{iH(t-i\tau)} A e^{-iH(t-i\tau)}.$$

To prove the identity we write

$$\begin{aligned} \rho \int_0^{\beta} d\tau \dot{A}(t - i\tau) &= i\rho \int_0^{\beta} d\tau \frac{d}{d\tau} A(t - i\tau) \\ &= i\rho (A(t - i\beta) - A(t)) \\ &= i\frac{e^{-\beta H}}{Z} \left(e^{\beta H} A(t) e^{-\beta H} - A(t) \right) \\ &= i(A(t)\rho - \rho A(t)), \end{aligned} \tag{2.5}$$

which proves the Kubo identity.

Using this identity, it follows

$$\begin{aligned} G_{ij}(t - t') &= -i\theta(t - t') \frac{1}{Z} \mathrm{tr}([A_j(t'), \rho] A_i(t)) \\ &= -\theta(t - t') \int_0^{\beta} d\tau \left\langle \dot{A}_j(t' - i\tau) A_i(t) \right\rangle \end{aligned} \tag{2.6}$$

We can write this as

$$G_{ij}(t) = -\theta(t) \int_0^{\beta} d\tau \left\langle \dot{A}_j(-t - i\tau) A_i \right\rangle. \tag{2.7}$$

The Fourier transform $G_{ij}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega_+ t} G_{ij}(t)$ with $\omega_+ = \omega + i0^+$ is given as

$$G_{ij}(\omega) = -\int_0^{\infty} dt \int_0^{\beta} d\tau e^{i\omega_+ t} \left\langle \dot{A}_j(-t - i\tau) A_i \right\rangle \tag{2.8}$$

Let us perform a partial integration

$$\begin{aligned} u'(t) &= -e^{i\omega_+ t} \\ v(t) &= \int_0^{\beta} d\tau \left\langle \dot{A}_j(-t - i\tau) A_i \right\rangle \end{aligned}$$

such that $u(t) = \frac{i}{\omega_+} e^{i\omega_+ t}$ and $v'(t) = \int_0^{\beta} d\tau \left\langle \frac{d}{dt} \dot{A}_j(-t - i\tau) A_i \right\rangle$

$$\begin{aligned} G_{ij}(\omega) &= -\frac{i}{\omega_+} \int_0^{\infty} dt e^{i\omega_+ t} \int_0^{\beta} d\tau \left\langle \frac{d}{dt} \dot{A}_j(-t - i\tau) A_i \right\rangle \\ &+ \frac{i}{\omega_+} e^{i\omega_+ t} \int_0^{\beta} d\tau \left\langle \dot{A}_j(-t - i\tau) A_i \right\rangle \Big|_0^{\infty} \end{aligned} \tag{2.9}$$

The first term can be analyzed using the Kubo identity and be expressed in terms of the Fourier transform $\chi_{ij}(\omega)$ of the retarded Green's function

$$\chi_{ij}(t - t') = -i\theta(t - t') \left\langle \left[A_i(t), \dot{A}_j(t') \right] \right\rangle \tag{2.10}$$

that contains the time derivative of one of the operators. For the last term we use that it vanishes at the upper limit due to the convergence factor in ω_+. Thus, it follows

$$G_{ij}(\omega) = \frac{i}{\omega_+} \left(\chi_{ij}(\omega) - \chi_{ij}^T \right), \tag{2.11}$$

with the isothermal susceptibility

$$\begin{aligned} \chi_{ij}^T &= \int_0^{\beta} d\tau \left\langle \dot{A}_j(-i\tau) A_i \right\rangle \\ &= \left. \frac{d\langle A_i \rangle}{d\widetilde{F}_j} \right|_{\widetilde{F}_j = 0} \end{aligned} \tag{2.12}$$

is the change of the observable $\langle A_i \rangle$ due to an external static field $\widetilde{F}_j$ that couples to $\dot{A}_j$ in the Hamilonian. Notice, this is different from $F_j(t)$ that couples to A_j itself and is in general dynamic. To see that this is the case we expand the statistical factor to linear order in this perturbation:

$$e^{-\beta\left(H - \dot{A}_j \widetilde{F}_j\right)} \approx e^{-\beta H} \left(1 + \int_0^{\beta} \dot{A}_j(-i\tau) \widetilde{F}_j \right). \tag{2.13}$$

Inserting this expression into the change of the expectation value

$$\langle \Delta A_i \rangle = \frac{\mathrm{tr} e^{-\beta\left(H - \dot{A}_j \widetilde{F}_j\right)} A_i}{\mathrm{tr} e^{-\beta\left(H - \dot{A}_j \widetilde{F}_j\right)}} - \frac{\mathrm{tr} e^{-\beta H} A_i}{\mathrm{tr} e^{-\beta H}} \tag{2.14}$$

$$\approx \int_0^{\beta} d\tau \left\langle \dot{A}_j(-i\tau) A_i \right\rangle \widetilde{F}_j \tag{2.15}$$

gives the above result for χ_{ij}^T. An important implication of Eq.2.11 occurs for $D_{ij} = \chi_{ij}(0) - \chi_{ij}^T \neq 0$. In this case follows

$$\mathrm{Re} G_{ij}(\omega) = \pi D_{ij} \delta(\omega) - \frac{\mathrm{Im} \chi_{ij}(\omega)}{\omega}. \tag{2.16}$$

This is a generalized Drude term in the response function.

Let us discuss a few specific examples. If one considers a homogeneous electric field that couples to charges, it can depend on the gauge whether we can even accomplish a coupling of the type in Eq.2.1. We could for example use $\mathbf{p} \to \mathbf{p} - \frac{e}{c}\mathbf{A}$ with time dependent vector potential and vanishing scalar potential. In this case holds for a parabolic spectrum that there are also perturbation quadratic in $\mathbf{A}$. Alternatively, we can use an electrostatic potential $\phi(\mathbf{x}, t) = \mathbf{E}(t) \cdot \mathbf{x}$, i.e. $W = e \int d^d x \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \phi(\mathbf{x}, t)$. Thus we obtain

$$W = \mathbf{p} \cdot \mathbf{E}(t) \tag{2.17}$$

with polarization operator $\mathbf{p} = e \int d^d x \psi^\dagger(\mathbf{x}) \mathbf{x} \psi(\mathbf{x})$. Notice that $\mathbf{j} = \dot{\mathbf{p}} = i[H, \mathbf{p}]$ is the current operator. For the conductivity, the operator to analyze is the α-th component of the current, i.e. $A_i = j_\alpha$. The operators A_j correspond to the components $-p_\beta$ of the polarizaton operator $\mathbf{p}$, i.e. the time derivative corresponds to the current $\dot{A}_j = -j_\beta$. For the conductivity $\sigma_{\alpha\beta}$, defined as,

$$\langle j_\alpha \rangle_t = \int_{-\infty}^{\infty} dt \sum_j \sigma_{\alpha\beta}(t - t') E_\beta(t'), \tag{2.18}$$

follows

$$\begin{aligned} \sigma_{\alpha\beta}(\omega) &= \int_0^\beta d\tau \int_0^\infty e^{i\left(\omega + i0^+\right)t} \langle j_\beta(-t - i\tau) j_\alpha \rangle \\ &= \frac{i}{\omega_+} \left(\chi^T_{\alpha\beta} - \chi_{\alpha\beta}(\omega)\right) \end{aligned} \tag{2.19}$$

with $\chi_{\alpha\beta}(\omega)$ the Fourier transform of $\chi_{\alpha\beta}(t - t') = -i\theta(t - t') \langle [j_\alpha(t), j_\beta(t')] \rangle$ while $\chi^T_{\alpha\beta} = \left.\frac{d\langle j_\alpha \rangle}{da_\beta}\right|_{A_\beta = 0}$, where we added a term $-j_\beta a_\beta$ to the Hamiltonian.

Part III

Diagrammatic perturbationtheory at finite T

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

$$\begin{aligned} G^c_{A,B}(t,t') &= \langle\langle A(t);B(t')\rangle\rangle^c \\ &\equiv -i\langle TA(t)B(t')\rangle, \end{aligned} \tag{2.20}$$

with time ordering operator

$$TA(t)B(t') = \theta(t-t')A(t)B(t') - \eta\theta(t'-t)B(t')A(t). \tag{2.21}$$

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

$$H = H_0 + V \tag{2.22}$$

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

$$e^{-iH(t-t')} = e^{-iH_0t}S(t,t')e^{iH_0t'} \tag{2.23}$$

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

$$\begin{aligned} A(t) &= e^{iHt}Ae^{-iHt} \\ &= S^\dagger(t,0)e^{-iH_0t}Ae^{-iH_0t}S(t,0) \\ &= S^\dagger(t,0)\tilde{A}(t)S(t,0) \end{aligned} \tag{2.24}$$

where

$$\tilde{A}(t) = e^{-iH_0t}Ae^{-iH_0t}. \tag{2.25}$$

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

$$S(t,t') = e^{iH_0t}e^{-iH(t-t')}e^{-iH_0t'}. \tag{2.26}$$

It holds

$$\begin{aligned} \partial_t S(t,t') &= iH_0e^{iH_0t}e^{-iH(t-t')}e^{-iH_0t'} \\ &- e^{iH_0t}(iH)e^{-iH(t-t')}e^{-iH_0t'} \\ &= e^{iH_0t}(iH_0 - iH)e^{-iH(t-t')}e^{-iH_0t'} \\ &= -e^{iH_0t}(iV)e^{-iH_0t}e^{iH_0t}e^{-iH(t-t')}e^{-iH_0t'} \\ &= -i\tilde{V}(t)S(t,t') \end{aligned} \tag{2.27}$$

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

$$S(t,t) = 1. \tag{2.28}$$

The solution of the above differential equation is

$$S(t,t') = Te^{-i\int_{t'}^{t}dt''\tilde{V}(t'')}. \tag{2.29}$$

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

$$S(t,t') = \sum_{n=0}^{\infty} S_n(t,t') \tag{2.30}$$

with

$$S_n = \frac{(-i)^n}{n!} T \int_{t'}^{t} dt_n \cdots \int_{t'}^{t} dt_2 \int_{t'}^{t} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{2.31}$$

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

$$S_n = (-i)^n T \int_{t_{n-1}}^{t} dt_n \cdots \int_{t_2}^{t_3} dt_2 \int_{t'}^{t_2} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{2.32}$$

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

$$S_n = (-i)^n \int_{t_{n-1}}^{t} dt_n \cdots \int_{t_2}^{t_3} dt_2 \int_{t'}^{t_2} dt_1 \tilde{V}(t_n) \cdots \tilde{V}(t_2) \tilde{V}(t_1). \tag{2.33}$$

It follows

$$\partial_t S_n(t,t') = -i\tilde{V}(t) S_{n-1}(t,t'), \tag{2.34}$$

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.

2.1 The Matsubara function

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

$$A(\tau) = e^{\tau H} A e^{-\tau H} \tag{2.35}$$

and defines

$$\mathcal{G}_{AB}(\tau,\tau') = -\langle T A(\tau) B(\tau') \rangle. \tag{2.36}$$

with

$$TA(\tau) B(\tau') = \theta(\tau-\tau') A(\tau) B(\tau') - \eta\theta(\tau'-\tau) B(\tau') A(\tau). \tag{2.37}$$

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

$$t \to -i\tau. \tag{2.38}$$

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

$$\mathcal{G}_{AB}(\tau,\tau') = \mathcal{G}_{AB}(\tau-\tau'). \tag{2.39}$$

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

2.1.1 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:

$$m\beta < \tau < (m+1)\beta. \tag{2.40}$$

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:

$$\begin{aligned}
\mathcal{G}_{AB}(\tau - m\beta) &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}e^{(\tau-m\beta)H}Ae^{-(\tau-m\beta)H}B\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{(\tau-(m+1)\beta)H}Ae^{-(\tau-m\beta)H}B\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}Be^{(\tau-(m+1)\beta)H}Ae^{-(\tau-(m+1)\beta)H}\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}BA(\tau-(m+1)\beta)\right)
\end{aligned} \tag{2.41}$$

If $\tau < 0$ holds

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

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

$$\begin{aligned}
\mathcal{G}_{AB}(\tau - m\beta) &= \frac{\eta}{Z}\mathrm{tr}\left(e^{-\beta H}TA(\tau-(m+1)\beta)B\right) \\
&= -\eta\mathcal{G}_{AB}(\tau-(m+1)\beta)
\end{aligned} \tag{2.42}$$

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

$$\mathcal{G}_{AB}(\tau) = -\eta\mathcal{G}_{AB}(\tau+\beta). \tag{2.43}$$

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

$$\mathcal{G}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\mathcal{G}(\omega_n) \tag{2.44}$$

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

$$\mathcal{G}(\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau}. \tag{2.45}$$

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

$$e^{-i\beta\omega_n} = -\eta. \tag{2.46}$$

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

$$\begin{aligned}
\mathcal{G}(\omega_n) &= \frac{1}{2}\int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau} - \frac{\eta}{2}\int_{-\beta}^{0} d\tau\mathcal{G}(\tau+\beta)e^{i\omega_n\tau} \\
&= \frac{1-\eta e^{-i\omega_n\beta}}{2}\int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau} \\
&= \int_0^{\beta} d\tau\mathcal{G}(\tau)e^{i\omega_n\tau}.
\end{aligned} \tag{2.47}$$

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

$$\boxed{\omega_n = \begin{cases} 2n\pi/\beta & \text{for bosons} \\ (2n+1)\,\pi/\beta & \text{for fermions} \end{cases}}. \tag{2.48}$$

2.1.2 Relation to the retarded function

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

$$\begin{aligned} \mathcal{G}_{AB}(\omega_n) &= -\frac{1}{Z}\int_0^\beta d\tau e^{i\omega_n\tau}\mathrm{tr}\left(e^{(\tau-\beta)H}Ae^{-\tau H}B\right) \\ &= -\frac{1}{Z}\sum_{lm}\int_0^\beta d\tau e^{i\omega_n\tau}e^{(\tau-\beta)E_l}e^{-\tau E_m}\langle l|A|m\rangle\langle m|B|l\rangle \\ &= \frac{1}{z}\sum_{lm}\frac{e^{-\beta E_l}-e^{-\beta E_m}e^{i\beta\omega_n}}{i\omega_n+E_l-E_m}\langle l|A|m\rangle\langle m|B|l\rangle \end{aligned} \tag{2.49}$$

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

$$\boxed{\mathcal{G}_{AB}(\omega_n) = \frac{1}{Z}\sum_{l.m}\frac{\left(e^{-\beta E_l}+\eta e^{-\beta E_m}\right)\langle l|A|m\rangle\langle m|B|l\rangle}{i\omega_n+E_l-E_m}} \tag{2.50}$$

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

$$\mathcal{G}_{AB}(\omega_n) = G_{AB}(z = i\omega_n). \tag{2.51}$$

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

$$i\omega_n \to \omega + i0^+. \tag{2.52}$$

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

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

$$H_0 = \sum_\alpha \int \frac{d^dk}{(2\pi)^d}\varepsilon_{\mathbf{k}}\psi^\dagger_{\mathbf{k}\alpha}\psi_{\mathbf{k}\alpha}. \tag{2.53}$$

We obtain for the Fourier transform of

$$\mathcal{G}_{0\mathbf{k}}(\tau) = -\left\langle T\psi_{\mathbf{k}\alpha}(\tau)\,\psi^\dagger_{\mathbf{k}\alpha}\right\rangle_0 \tag{2.54}$$

that

$$\mathcal{G}_{0,\mathbf{k}}(\omega_n) = \frac{1}{i\omega_n-\varepsilon_{\mathbf{k}}}. \tag{2.55}$$

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

2.1.3 Evolution with imaginary time

We already introduced the time dependence introduces

$$A(\tau) = e^{\tau H} A e^{-\tau H} \tag{2.56}$$

which can be used to determine the equation of motion

$$\begin{aligned} \partial_\tau A(\tau) &= HA(\tau) - A(\tau) H \\ &= - [A(\tau), H] \end{aligned} \tag{2.57}$$

For our subsequent analysis we will use

$$e^{\tau H} e^{-\tau H} = 1, \tag{2.58}$$

i.e.

$$\left(e^{\tau H}\right)^{-1} = e^{-\tau H}. \tag{2.59}$$

In full analogy of the S-matrix we can introduce

$$\mathcal{S}(\tau, \tau') = e^{H_0 \tau} e^{-H(\tau - \tau')} e^{-H_0 \tau'}. \tag{2.60}$$

The time evolution of the full Hamiltonian is written as

$$e^{-H(\tau - \tau')} = e^{-H_0 \tau} \mathcal{S}(\tau, \tau') e^{H_0 \tau;}. \tag{2.61}$$

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

$$\mathcal{S}(\tau, \tau) = 1 \tag{2.62}$$

as well as

$$\begin{aligned} \mathcal{S}(\tau_1, \tau_2) \mathcal{S}(\tau_2, \tau_3) &= e^{H_0 \tau_1} e^{-H(\tau_1 - \tau_2)} e^{-H_0 \tau_2} e^{H_0 \tau_2} e^{-H(\tau_2 - \tau_3)} e^{-H_0 \tau_3} \\ &= \mathcal{S}(\tau_1, \tau_3). \end{aligned} \tag{2.63}$$

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

$$\mathcal{S}(\tau_1, \tau_2) = \mathcal{S}(\tau_2, \tau_1)^{-1}. \tag{2.64}$$

The time evolution of the full Hamiltonian is written as

$$\begin{aligned} A(\tau) &= e^{\tau H} e^{-\tau H_0} \tilde{A}(\tau) e^{\tau H_0} e^{-\tau H} \\ &= \mathcal{S}(0, \tau) \tilde{A}(\tau) \mathcal{S}(\tau, 0), \end{aligned} \tag{2.65}$$

where

$$\tilde{A}(\tau) = e^{\tau H_0} A e^{-\tau H_0}. \tag{2.66}$$

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

$$\begin{aligned} -\partial_\tau \mathcal{S}(\tau, \tau') &= -e^{H_0 \tau} (H_0 - H) e^{-H(\tau - \tau')} e^{-H_0 \tau'} \\ &= \tilde{V}(\tau) \mathcal{S}(\tau, \tau'). \end{aligned} \tag{2.67}$$

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

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

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

$$\begin{aligned} Z &= \mathrm{tr} e^{-\beta H} \\ &= \mathrm{tr}\left(e^{-\beta H_0}\mathcal{S}\left(\beta,0\right)\right) \\ &= Z_0\left\langle \mathcal{S}\right\rangle_0 \end{aligned} \tag{2.68}$$

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

$$\mathcal{S}\equiv\mathcal{S}\left(\beta,0\right)=e^{-\int_0^\beta d\tau''\tilde{V}(\tau'')}. \tag{2.69}$$

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

$$\begin{aligned} \mathcal{G}_{\mathbf{k}}\left(\tau\right) &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H}T\psi_{\mathbf{k}\alpha}\left(\tau\right)\psi_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0}\mathcal{S}\left(\beta,0\right)\mathcal{S}\left(0,\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\mathcal{S}\left(\tau,0\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(\tau'\right)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0}T\mathcal{S}\left(\beta,\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\mathcal{S}\left(\tau,0\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0}T\mathcal{S}\left(\beta,\tau\right)\mathcal{S}\left(\tau,0\right)\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\right) \\ &= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta H_0}T\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\mathcal{S}\left(\beta,0\right)\right) \end{aligned} \tag{2.70}$$

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

$$\begin{aligned} \mathcal{G}_{\mathbf{k}}\left(\tau\right) &= -\frac{\left\langle T\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\mathcal{S}\left(\beta,0\right)\right\rangle_0}{\left\langle \mathcal{S}\left(\beta,0\right)\right\rangle_0} \\ &= -\frac{\left\langle T\tilde{\psi}_{\mathbf{k}\alpha}\left(\tau\right)\tilde{\psi}_{\mathbf{k}\alpha}^{\dagger}\left(0\right)\mathcal{S}\right\rangle_0}{\left\langle \mathcal{S}\right\rangle_0} \end{aligned} \tag{2.71}$$

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.