Kapitel 5

Green's function formalism

5.1 Introduction

Green's functions appear naturally as response functions, *i.e.* as answers to the function how a quantum mechanical system responds to an external perturbation, like for example electrical or magnetic fields; the corresponding response functions would then describe the electrical conductivity or the magnetic susceptibility of a system. Here we will be concerned with small perturbations and thus only the linear response of the system. We describe the system by a Hamiltonian

$$H = H_0 + V_t \tag{5.1}$$

where V_t represents the interaction with an external field. H_0 describes the system with the external field switched off; due to interactions H_0 is not necessarily exactly solvable. The external field F_t couples to the observable $\hat{B}$ of the system:

$$V_t = \hat{B} F_t \tag{5.2}$$

Here, $\hat{B}$ is an operator and F_t is a complex number. We now consider an observable $\hat{A}$ of the system that is not explicitly time dependent and ask how the dynamic expectation value $\langle \hat{A} \rangle$ reacts to the perturbation V_t. Without field we have

$$\langle \hat{A} \rangle_0 = \mathrm{Tr}(\rho_0 \hat{A}) \tag{5.3}$$

where ρ_0 is the density matrix of the system without external fields:

$$\rho_0 = \frac{e^{-\beta \mathcal{H}}}{\mathrm{Tr} e^{-\beta \mathcal{H}}} \tag{5.4}$$

in the grand canonical ensemble $\mathcal{H} = H - \mu \hat{N}$ (with chemical potential μ, particle number operator $\hat{N}$). The density matrix will change if we switch on the field:

$$\rho_0 \to \rho_t \tag{5.5}$$

This means for the expectation value of $\hat{A}$

$$\langle \hat{A} \rangle_t = \mathrm{Tr}(\rho_t \hat{A}) \tag{5.6}$$

In the Schrödinger picture, the equation of motion of the density matrix (the statistical operator) is determined by the von Neumann equation

$$i\hbar\frac{\partial\rho_t}{\partial t} = \big[\mathcal{H} + V_t, \rho_t\big] \tag{5.7}$$

We consider a perturbation that is switched on at some time so that the boundary condition for our first order differential equation is an unperturbed system for $t \to -\infty$

$$\lim_{t\to-\infty}\rho_t = \rho_0\,. \tag{5.8}$$

We now switch to the Dirac picture where we have

$$\rho_t^D(t) = e^{\frac{i}{\hbar}\mathcal{H}_0 t}\rho_t e^{-\frac{i}{\hbar}\mathcal{H}_0 t} \tag{5.9}$$

with the equation of motion

$$\frac{d}{dt}\rho_t^D(t) = \frac{i}{\hbar}\big[\rho_t^D, V_t^D\big]_-(t)\,. \tag{5.10}$$

Integrating with the boundary condition

$$\lim_{t\to-\infty}\rho_t^D(t) = \rho_0 \tag{5.11}$$

leads to

$$\rho_t^D(t) = \rho_0 - \frac{i}{\hbar}\int_{-\infty}^t dt'\big[V_{t'}^D(t'), \rho_{t'}^D(t')\big]_- \tag{5.12}$$

This equation can be solved by iteration (by substituting $\rho_t^D(t)$ repeatedly on the right hand side):

$$\begin{aligned}\rho_t^D(t) &= \rho_0 + \sum_{n=1}^{\infty}\rho_t^{D(n)}(t) \qquad \text{with}\\ \rho_t^{D(n)}(t) &= \Big(-\frac{i}{\hbar}\Big)^n\int_{-\infty}^t dt_1\int_{-\infty}^{t_1} dt_2\cdots\int_{-\infty}^{t_{n-1}} dt_n\\ &\quad\times\big[V_{t_1}^D(t_1), \big[V_{t_2}^D(t_2), \big[\cdots\big[V_{t_n}^D(t_n), \rho_0\big]\cdots\big]_-\big]_-\big]_-\end{aligned} \tag{5.13}$$

While this formula is exact, it is not practical. For sufficiently small external perturbations, we can restrict to linear terms in the perturbation V_t which is called **linear response**:

$$\rho_t^D \approx \rho_0 - \frac{i}{\hbar}\int_{-\infty}^t dt'\,\big[V_{t'}^D(t'), \rho_0\big]_- \tag{5.14}$$

We can use this result to determine the perturbed expectation value of (5.6):

$$\begin{aligned}\langle\hat{A}\rangle_t = \mathrm{Tr}(\rho_t^D\hat{A}^D) &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^t dt'\,\mathrm{Tr}\Big\{\big[V_{t'}^D(t'), \rho_0\big]_-\hat{A}^D\Big\}\\ &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^t dt'\,F_{t'}\mathrm{Tr}\underbrace{\Big\{\big[\hat{B}^D(t'), \rho_0\big]_-\hat{A}^D(t)\Big\}}_{=\hat{B}\rho_0\hat{A}-\rho_0\hat{B}\hat{A}=\rho_0\hat{A}\hat{B}-\rho_0\hat{B}\hat{A}}\\ &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^t dt'\,F_{t'}\mathrm{Tr}\Big\{\rho_0\big[\hat{A}^D(t), \hat{B}^D(t')\big]_-\Big\}\end{aligned} \tag{5.15}$$

Here, cyclic invariance of the trace was exploited. This shows how the system reacts to the external perturbation, as measured from the observable $\hat{A}$:

$$\Delta A_t = \langle \hat{A} \rangle_t - \langle \hat{A} \rangle_0 = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \, F_{t'} \langle [\hat{A}^D(t), \hat{B}^D(t')]_- \rangle_0 \tag{5.16}$$

This response is determined by an expectation value of the unperturbed system. The Dirac representation of the operators $\hat{A}^D(t)$, $\hat{B}^D(t')$ corresponds to the Heisenberg representation when the field is switched off.
Now we define the retarded two-time greens function

$$G^r_{AB}(t,t') = \langle\langle A(t); B(t') \rangle\rangle = -i\Theta(t-t') \big\langle \big[A(t), B(t')\big]_- \big\rangle_0 \tag{5.17}$$

The operators are to be taken in Heisenberg representation of the field free system. The retarded Green's function describes the response of a system as manifested in observable $\hat{A}$ when the perturbation couples to observable $\hat{B}$:

$$\Delta A_t = -\frac{1}{\hbar} \int_{-\infty}^{\infty} dt' \, F_{t'} G^r_{AB}(t,t') \tag{5.18}$$

It is called retarded because due to the Heaviside function, only perturbations for $t < t'$ contribute.
With the Fourier transform $F(\omega)$ of the perturbation

$$F_t = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, F(\omega) e^{-i(\omega + i\delta)t} \tag{5.19}$$

where $\delta > 0$ is infinitesimally small and using the later result that with a Hamiltonian that is not explicitly time dependent the Green's function depends only on time differences $t - t'$, we can rewrite (5.18) in the form of the **Kubo formula**

$$\Delta A_t = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d\omega \, F(\omega) G^r_{AB}(\omega + i\delta) e^{-i(\omega+i\delta)t} \tag{5.20}$$

The $\delta > 0$ in the exponent enforces the boundary condition (5.8).
We will now look into two applications of response functions.

Magnetic Susceptibility

The perturbation is a spatially homogeneous magnetic field that oscillates in time:

$$B_t = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, B(\omega) e^{-i(\omega+i\delta)t} , \tag{5.21}$$

which couples to the magnetic moment

$$\vec{m} = \sum_i m_i = \frac{g\mu_B}{\hbar} \sum_i \vec{S}_i \, . \tag{5.22}$$

Thus, the perturbing potential term in the Hamiltonian becomes

$$V_t = -\vec{m} \cdot \vec{B}_t = -\frac{1}{2\pi} \sum_\alpha \int_{-\infty}^{\infty} d\omega \, m^\alpha B^\alpha(\omega) e^{-i(\omega+i\delta)t} \tag{5.23}$$

where $\alpha = x, y, z$ are Cartesian directions. An interesting quantity is now the magnetization in response to the applied field. As it is

$$\vec{M} = \frac{1}{V}\langle\vec{m}\rangle = \frac{g\mu_B}{\hbar V}\sum_i \langle\vec{S}_i\rangle\,, \tag{5.24}$$

we have to choose the magnetic momentum operator for both $\hat{A}$ and $\hat{B}$ operators in the Kubo formula:

$$M_t^\beta - M_0^\beta \;=\; -\frac{1}{V}\sum_\alpha \int_{-\infty}^{\infty} dt'\, B_{t'}^\alpha \langle\!\langle m^\beta(t); m^\alpha(t')\rangle\!\rangle\,. \tag{5.25}$$

Only in a ferromagnet there is a finite magnetization M_0^β without a field. Eq. (5.25) defines the **magnetic susceptibility tensor**

$$\chi_{ij}^{\beta\alpha}(t,t') \;=\; -\frac{\mu_0}{V}\frac{g^2\mu_B^2}{\hbar^2}\langle\!\langle S_i^\beta(t); S_j^\alpha(t')\rangle\!\rangle \tag{5.26}$$

as a retarded Green's function. Thus

$$\Delta M_t^\beta \;=\frac{1}{\mu_0}\sum_{ij}\int_{-\infty}^{\infty} dt'\, B_{t'}^\alpha \chi_{ij}^{\beta\alpha}(t,t') \tag{5.27}$$

or in terms of frequency

$$\Delta M_t^\beta \;= \frac{1}{2\pi\mu_0}\sum_{ij}\sum_\alpha \int_{-\infty}^{\infty} d\omega\, e^{-i(\omega+i\delta)t}\chi_{ij}^{\beta\alpha}(\omega)B^\alpha(\omega) \tag{5.28}$$

We have implicitly assumed that the system we consider has permanent localized moments.
Two types of susceptibilities are interesting: The **longitudinal susceptibility**

$$\chi_{ij}^{zz}(\omega) = \frac{\mu_0}{V}\frac{g^2\mu_B^2}{\hbar^2}\langle\!\langle S_i^z; S_j^z\rangle\!\rangle_\omega \tag{5.29}$$

where the index indicates the Fourier transform of the retarded Green's function. This can be used to obtain information about the stability of magnetic orderings. For the paramagnetic phase, one calculates the spatial Fourier transform

$$\chi_{\vec{q}}^{zz}(\omega) = \frac{1}{N}\sum_{ij}\chi_{ij}^{zz}(\omega)e^{i\vec{q}\cdot\left(\vec{R}_i-\vec{R}_j\right)} \tag{5.30}$$

At the singularities of this response function, an infinitesimally small field is sufficient to create a finite magnetization, *i.e.* a spontaneous ordering of the moments. For that purpose, the conditions under which

$$\left\{\lim_{(\vec{q},\omega)\to 0}\chi_{\vec{q}}^{zz}(\omega)\right\}^{-1} = 0 \tag{5.31}$$

are studied; they indicate the paramagnetic $\leftrightarrow$ ferromagnetic transition.

The other interesting case is the **transversal susceptibility**

$$\chi_{ij}^{+-}(\omega) = -\frac{\mu_0}{V}\frac{g^2\mu_B^2}{\hbar^2}\langle\langle S_i^+; S_j^-\rangle\rangle_\omega \quad \text{where} \quad S_i^\pm = S_i^x \pm iS_i^y \tag{5.32}$$

Poles of this susceptibility correspond to spin wave (magnon) energies:

$$\left\{\chi_{\vec{q}}^{+-}(\omega)\right\}^{-1} = 0 \Longleftrightarrow \omega = \omega(\vec{q})\,. \tag{5.33}$$

The examples show that linear response theory not only treats weak external perturbations but also yields information about the unperturbed system.

Electrical conductivity

Now we consider a spatially homogeneous electrical field that oscillates in time:

$$\vec{E}_t = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \vec{E}(\omega)e^{-i(\omega+i\delta)t}\,. \tag{5.34}$$

The electrical field couples to the electrical dipole moment $\vec{P}$

$$\vec{P} = \int d^3r\, \vec{r}n(\vec{r})\,. \tag{5.35}$$

We consider N point charges q_i at positions $\vec{r}_i(t)$; the charge density is

$$n(\vec{r}) = \sum_{i=1}^{N} q_i\delta(\vec{r}-\vec{r}_i)\,. \tag{5.36}$$

This gives a dipole moment operator

$$\vec{P} = \sum_{i=1}^{N} q_i\vec{r}_i\,. \tag{5.37}$$

The electrical field causes the additional external potential term in the Hamiltonian

$$V_t = -\vec{P}\cdot\vec{E}_t = -\frac{1}{2\pi}\sum_\alpha\int_{-\infty}^{\infty} d\omega\, P^\alpha E^\alpha(\omega)e^{-i(\omega+i\delta)t}\,. \tag{5.38}$$

An interesting quantity is the response of the current density to the external field:

$$\vec{j} = \frac{1}{V}\sum_{i=1}^{N} q_i\frac{d\vec{r}_i}{dt} = \frac{1}{V}\frac{d\vec{P}}{dt}\,. \tag{5.39}$$

Its expectation value without field disappears:

$$\langle\vec{j}\rangle_0 = 0\,. \tag{5.40}$$

After switching the field on, we have

$$\langle j^\beta\rangle_t = -\frac{1}{\hbar}\sum_\alpha\int_{-\infty}^{\infty} dt'\, E_{t'}^\alpha\langle\langle j^\beta(t); P^\alpha(t')\rangle\rangle\,. \tag{5.41}$$

In terms of the Fourier transforms this becomes

$$\langle j^{\beta}\rangle_t = \frac{1}{2\pi}\sum_{\alpha}\int_{-\infty}^{\infty} d\omega\, e^{-i(\omega+i\delta)t}\sigma^{\beta\alpha}(\omega)E^{\alpha}(\omega) \tag{5.42}$$

This is **Ohms law**, defining the **electrical conductivity tensor**

$$\sigma^{\beta\alpha}(\omega) \equiv -\langle\!\langle j^{\beta}; P^{\alpha}\rangle\!\rangle_{\omega} \tag{5.43}$$

that has retarded Green's functions as components. This can be rewritten as

$$\sigma^{\beta\alpha}(\omega) = i\frac{N}{V}\frac{q^2}{m(\omega+i\delta)}\delta_{\alpha\beta} + \frac{i}{\hbar}\frac{\langle\!\langle j^{\beta}; j^{\alpha}\rangle\!\rangle}{\omega+i\delta} \tag{5.44}$$

The first term represents the conductivity of a noninteracting electron system as given by classical Drude theory, and the second one involving a retarded current-current Green's function represents the interaction between the particles.

5.2 Two time Green's functions

The full Green's function formalism has two more Green's functions besides the retarded Green's function:

Retarded Green's function

$$G^{r}_{AB}(t,t') \equiv \langle\!\langle A(t); B(t')\rangle\!\rangle^{r} = -i\Theta(t-t')\big\langle [A(t), B(t')]_{-\varepsilon}\big\rangle \tag{5.45}$$

Advanced Green's function

$$G^{a}_{AB}(t,t') \equiv \langle\!\langle A(t); B(t')\rangle\!\rangle^{a} = i\Theta(t'-t)\big\langle [A(t), B(t')]_{-\varepsilon}\big\rangle \tag{5.46}$$

Causal Green's function

$$G^{c}_{AB}(t,t') \equiv \langle\!\langle A(t); B(t')\rangle\!\rangle^{c} = -i\big\langle T_{\varepsilon}\big(A(t)B(t')\big)\big\rangle \tag{5.47}$$

Again, we have for the operators in Heisenberg representation

$$X(t) = e^{\frac{i}{\hbar}\mathcal{H}t}Xe^{-\frac{i}{\hbar}\mathcal{H}t}, \mathcal{H} = H - \mu\hat{N}, \langle X\rangle = \frac{\mathrm{Tr}(e^{-\beta\mathcal{H}}X)}{\mathrm{Tr}e^{-\beta\mathcal{H}}}, \beta = \frac{1}{k_B T} \tag{5.48}$$

where we omit the index 0 of $\mathcal{H}$ and H as we are not dealing with external perturbations in this chapter. ϵ has the value $\varepsilon = -$ for Fermi operators, $\varepsilon = +$ for Bose operators:

$$\big[A[t], B(t')\big]_{-\varepsilon} = A(t)B(t') - \varepsilon B(t')A(t) \tag{5.49}$$

$\varepsilon = -$ yields the anticommutator, $\varepsilon = +$ the commutator.
The **Wick time ordering operator** T_{ε} sorts operators in a product according to their time arguments:

$$T_{\varepsilon}(A(t)B(t')) = \Theta(t-t')A(t)B(t') + \varepsilon\Theta(t'-t)B(t')A(t) \tag{5.50}$$

The ε makes it distinct from the Dirac time ordering operator.

The **spectral density** is another very important function of manybody theory:

$$S_{AB}(t,t') = \frac{1}{2\pi}\big\langle [A(t), B(t')]_{-\varepsilon}\big\rangle \tag{5.51}$$

It contains the same information as the Green's function.
We now prove the fact that Green's function and spectral density are homogeneous in time if the Hamiltonian is not explicitly time dependent:

$$\begin{aligned}\frac{\partial \mathcal{H}}{\partial t} = 0 \to G^{\alpha}_{AB}(t,t') &= G^{\alpha}_{AB}(t-t')\,, \quad (\alpha = r, a, c)\\ S_{AB}(t,t') &= S_{AB}(t-t')\end{aligned} \tag{5.52}$$

We only need to prove that for the so called **correlation functions**

$$\langle A(t)B(t')\rangle\,, \quad \langle B(t')A(t)\rangle \tag{5.53}$$

The proof is based on cyclic invariance of the trace:

$$\begin{aligned}\mathrm{Tr}\big\{e^{-\beta\mathcal{H}}A(t), B(t')\big\} &= \mathrm{Tr}\big\{e^{-\beta\mathcal{H}}e^{\frac{i}{\hbar}\mathcal{H}t}Ae^{-\frac{i}{\hbar}\mathcal{H}(t-t')}Be^{-\frac{i}{\hbar}\mathcal{H}t'}\big\}\\ &= \mathrm{Tr}\big\{e^{-\beta\mathcal{H}}e^{\frac{i}{\hbar}\mathcal{H}(t-t')}Ae^{-\frac{i}{\hbar}\mathcal{H}(t-t')}B\big\}\\ &= \mathrm{Tr}\big\{e^{-\beta H}A(t-t')B(0)\big\}\end{aligned} \tag{5.54}$$

Thus,

$$\langle A(t)B(t')\rangle = \langle A(t-t')B(0)\rangle\,, \tag{5.55}$$

and analogously

$$\langle B(t')A(t)\rangle = \langle B(0)A(t-t')\rangle\,. \tag{5.56}$$

Actually calculating the Green's function can be done via the general equation of motion for Heisenberg operators

$$i\hbar\frac{d}{dt}A_H(t) = \big[A_H, H_H\big]_{-}(t) + i\hbar\frac{\partial A_H}{\partial t} \tag{5.57}$$

We also have

$$\frac{d}{dt}\Theta(t-t') = \delta(t-t') = -\frac{d}{dt'}\Theta(t-t') \tag{5.58}$$

Then, all three Green's functions formally have the same equation of motion:

$$i\hbar\frac{\partial}{\partial t}G^{\alpha}_{AB}(t,t') = \hbar\delta(t-t')\big\langle\big[A,B\big]_{-\varepsilon}\big\rangle + \big\langle\!\big\langle\big[A,\mathcal{H}\big]_{-}(t);B(t')\big\rangle\!\big\rangle^{\alpha} \tag{5.59}$$

But the solutions have to obey different boundary conditions:

$$\begin{aligned}G^{r}_{AB}(t,t') &= 0 \quad \text{for} \quad t < t'\\ G^{a}_{AB}(t,t') &= 0 \quad \text{for} \quad t > t'\\ G^{c}_{AB}(t,t') &= \begin{cases}-i\langle A(t-t'), B(0)\rangle & \text{for} \quad t > t'\\ -i\varepsilon\langle B(0), A(t-t')\rangle & \text{for} \quad t < t'\end{cases}\end{aligned} \tag{5.60}$$

On the right hand side of (5.59) a new Green's functions appears as $[A, \mathcal{H}]_-$ is again an operator. Usually this leads to a higher order Green's function, *i.e.* one that contains more operators than the original $G^{\alpha}_{AB}(t, t')$. For this higher order Green's function, another equation of motion of type (5.59) can be written. This leads to an infinite chain of equations of motion. The system of equations can only be solved if the chain is stopped at some point by decoupling, *i.e.* by making physically motivated approximations to some higher order Green's functions.
Often it is more practical to work in the frequency domain rather than in the time domain:

$$G^{\alpha}_{AB}(\omega) \equiv \langle\langle A; B\rangle\rangle^{\alpha}_{\omega} = \int_{-\infty}^{\infty} d(t-t') G^{\alpha}_{AB}(t-t') e^{i\omega(t-t')}$$
$$G^{\alpha}_{AB}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, G^{\alpha}_{AB}(\omega) e^{-i\omega(t-t')} \tag{5.61}$$

The spectral density transforms in the same way. If we use the exponential definition of the Delta function:

$$2\pi\delta(x) = \int_{-\infty}^{\infty} dy e^{ixy} \tag{5.62}$$

or equivalently

$$2\pi\delta(x) = \int_{-\infty}^{\infty} dy e^{-ixy} \tag{5.63}$$

we have for our case:

$$\delta(\omega-\omega') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')\, e^{\pm i(\omega-\omega')(t-t')}$$
$$\delta(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{\pm i\omega(t-t')} \tag{5.64}$$

the equation of motion (5.59) becomes

$$\omega\langle\langle A; B\rangle\rangle^{\alpha}_{\omega} = \left\langle \left[A, B\right]_{-\varepsilon}\right\rangle + \frac{1}{\hbar}\left\langle\left\langle \left[A, \mathcal{H}\right]_{-}; B\right\rangle\right\rangle^{\alpha}_{\omega} \tag{5.65}$$

This is now an algebraic equation, not a differential equation any more. Meanwhile, the difficulty that an infinite chain of such equations is produced remains.

Spectral representation

Spectral representations of the Green's functions are important in order to find boundary conditions for the Eq. (5.65).
We take E_n and $|E_n\rangle$ to be eigenenergies and eigenvectors of the Hamiltonian $\mathcal{H}$ of the system we consider:

$$\mathcal{H}|E_n\rangle = E_n|E_n\rangle \tag{5.66}$$

We assume the states $|E_n\rangle$ to form a complete orthonormal system

$$\sum_n |E_n\rangle\langle E_n| = \mathbb{1}\,; \qquad \langle E_n|E_m\rangle = \delta_{nm} \tag{5.67}$$

First we consider the correlation functions $\langle A(t)B(t')\rangle$ and $\langle B(t')A(t)\rangle$ ($\Omega = \mathrm{Tr} e^{-\beta\mathcal{H}}$):

$$\begin{aligned}
\Omega\langle A(t)B(t')\rangle &= \mathrm{Tr}\big\{e^{-\beta\mathcal{H}}A(t)B(t')\big\} = \sum_n \langle E_n|e^{-\beta\mathcal{H}}A(t)B(t')|E_n\rangle \\
&= \sum_{n,m}\langle E_n|A(t)|E_m\rangle\langle E_m|B(t')|E_n\rangle e^{-\beta E_n} \\
&= \sum_{n,m}\langle E_n|A|E_m\rangle\langle E_m|B|E_n\rangle e^{-\beta E_n} e^{\frac{i}{\hbar}(E_n-E_m)(t-t')} \\
&= \sum_{n,m}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} e^{-\beta(Em-E_n)} e^{-\frac{i}{\hbar}(E_n-E_m)(t-t')}
\end{aligned} \tag{5.68}$$

Introducing a unit operator $\mathbb{1}$ has significantly simplified the time dependence of the Heisenberg operators. In the last step we have exchanged n and m indices. Analogously we find for the other correlation function

$$\Omega\langle B(t')A(t)\rangle = \sum_{n,m}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} e^{-\frac{i}{\hbar}(E_n-E_m)(t-t')} \tag{5.69}$$

If we now substitute (5.68) and (5.69) into the definition of the spectral density (5.51) or rather its Fourier transform

$$\begin{aligned}
S_{AB}(\omega) &= \int_{-\infty}^{\infty} d(t-t')S_{AB}(t-t')e^{i\omega(t-t')} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}\big(\langle A(t)B(t')\rangle - \varepsilon\langle B(t'),A(t)\rangle\big) \\
&= \frac{1}{\Omega}\frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{i(t-t')\left(\omega-\frac{E_n-E_m}{\hbar}\right)} e^{-\beta E_n}\big(e^{-\beta(E_m-E_n)}-\varepsilon\big)\times \\
&\qquad \times\sum_{nm}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle
\end{aligned} \tag{5.70}$$

and with the definition of the delta function (5.64)

$$S_{AB}(\omega) = \frac{1}{\Omega}\sum_{nm}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle(e^{\beta\hbar\omega}-\varepsilon)e^{-\beta E_n}\delta\Big(\omega-\frac{E_n-E_m}{\hbar}\Big) \tag{5.71}$$

The argument of the delta function contains the possible excitation energies of the system. Now we will express the Green's functions with the help of the spectral density. We use the following representation of the step function:

$$\Theta(t-t') = \frac{i}{2\pi}\int_{-\infty}^{\infty} dx\frac{e^{ix(t-t')}}{x+i0^+} \tag{5.72}$$

This can be proven using the residue theorem (see below). Using this relation, we can transform the retarded Green's function

$$\begin{aligned}
G^r_{AB}(\omega) &= \int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}\big(-i\Theta(t-t')\big)\big(2\pi S_{AB}(t-t')\big) \\
&= \int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}\big(-i\Theta(t-t')\big)\int_{-\infty}^{\infty} d\omega' S_{AB}(\omega')e^{-i\omega'(t-t')} \\
&= \int_{-\infty}^{\infty} d\omega'\int_{-\infty}^{\infty} dx\frac{S_{AB}(\omega')}{x+i0^+}\frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{-i(x-\omega+\omega')(t-t')} \\
&= \int_{-\infty}^{\infty} d\omega'\int_{-\infty}^{\infty} dx\frac{S_{AB}(\omega')}{x+i0^+}\delta\big(x-(\omega-\omega')\big)
\end{aligned} \tag{5.73}$$

This leads to the **spectral representation of the retarded Green's function**

$$G^r_{AB}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{S_{AB}(\omega')}{\omega - \omega' + i0^+} \tag{5.74}$$

Analogous treatment of the advanced Green's function yields the **spectral representation of the advanced Green's function**

$$G^a_{AB}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{S_{AB}(\omega')}{\omega - \omega' - i0^+} \tag{5.75}$$

The only (but significant) difference between G^r_{AB} and G^a_{AB} is the sign of $i0^+$; it determines the analytic properties of retarded and advanced functions, G^r_{AB} can be continued analytically into the upper, G^a_{AB} into the lower complex plane. Neither is true for the causal function G^c_{AB}. Substituting the spectral representation (5.71) of the spectral density into (5.74) and (5.75) yields the important expression

$$G^{\substack{r\\a}}_{AB} = \frac{1}{\Omega} \sum_{nm} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} \frac{e^{\beta(E_n - E_m)} - \varepsilon}{\omega - \frac{(E_n - E_m)}{\hbar} \pm i0^+} \tag{5.76}$$

Both functions are meromorphic in the complex plane (holomorphic except for a set of isolated points) with singularities at the exact excitation energies of the interacting system. As retarded and advanced Green's functions have the same physical content, they are sometimes joined into one function $G_{AB}(\omega)$; G^r_{AB} and G^a_{AB} are considered the two branches of a single function in the complex ω plane (obtained by considering $\omega + i\eta$ or $\omega - i\eta$ a complex variable and calling it again ω):

$$G_{AB}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{S_{AB}(\omega')}{\omega - \omega'} = \begin{cases} G^r_{AB}(\omega) & \text{if} \quad \mathrm{Im}\,\omega > 0 \\ G^a_{AB}(\omega) & \text{if} \quad \mathrm{Im}\,\omega < 0 \end{cases} \tag{5.77}$$

The singularities are on the real axis. In text books, r and a indices are often omitted, and interpretation of Green's functions written like in Eq. (5.77) in terms of retarded or advanced Green's functions is left to the reader.
We still need the spectral representation of the causal Green's functions. Using the definition (5.47), we have

$$G^c_{AB}(\omega) = -i \int_{-\infty}^{\infty} d(t-t') e^{-i\omega(t-t')} \big\{\Theta(t-t')\langle A(t)B(t')\rangle + \varepsilon\Theta(t'-t)\langle B(t')A(t)\rangle\big\} \tag{5.78}$$

Using results (5.68), (5.69) and (5.72), we obtain

$$\begin{aligned} G^c_{AB}(\omega) &= \frac{1}{\Omega} \sum_{nm} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} \frac{1}{2\pi} \int_{-\infty}^{\infty} dt'' \int_{-\infty}^{\infty} dx \frac{1}{x + i0^+} \\ &\quad \Big\{ e^{\beta(E_n - E_m)} e^{i\left(\omega - \frac{E_n - E_m}{\hbar} - x\right)t''} + \varepsilon e^{i\left(\omega - \frac{E_n - E_m}{\hbar} + x\right)t''} \Big\} \\ &= \frac{1}{\Omega} \sum_{nm} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} \int_{-\infty}^{\infty} dx \frac{1}{x + i0^+} \\ &\quad \Big\{ e^{\beta(E_n - E_m)} \delta\Big(\omega - \frac{E_n - E_m}{\hbar} - x\Big) + \varepsilon\delta\Big(\omega - \frac{E_n - E_m}{\hbar} + x\Big) \Big\} \end{aligned} \tag{5.79}$$

This yields the spectral representation of the causal Green's function

$$G^c_{AB}(\omega) = \frac{1}{\Omega}\sum_{nm}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n}\Big\{\frac{e^{\beta(E_n-E_m)}}{\omega - \frac{E_n-E_m}{\hbar}+i0^+} - \frac{\varepsilon}{\omega - \frac{E_n-E_m}{\hbar}-i0^+}\Big\} \quad (5.80)$$

We have expressed the retarded and advanced Green's functions by the spectral density. Using the Dirac identity

$$\frac{1}{x\pm i0^+} = \mathrm{P}\frac{1}{x} \pm i\pi\delta(x) \quad (5.81)$$

that should be interpreted as

$$\lim_{\delta\to 0^+}\int dx\frac{f(x)}{x\pm i\delta} = \mathrm{P}\int dx\frac{f(x)}{x} \pm i\pi f(0) \quad (5.82)$$

with the Cauchy principal value denoted by P, we can write the spectral density in terms of the Green's functions:

$$\begin{aligned} &G_{AB}(\omega+i0^+) - G_{AB}(\omega-i0^+) \\ &\quad = \int_{-\infty}^{\infty} d\omega S_{AB}(\omega')\Big\{\frac{1}{\omega-\omega'+i0^+} - \frac{1}{\omega-\omega'-i0^+}\Big\} \\ &\quad = \int_{-\infty}^{\infty} d\omega S_{AB}(\omega')\big\{-2\pi i\delta(\omega-\omega')\big\} = \frac{2\pi}{i}S_{AB}(\omega)\,, \end{aligned} \quad (5.83)$$

and thus

$$S_{AB}(\omega) = \frac{i}{2\pi}\big\{G_{AB}(\omega+i0^+) - G_{AB}(\omega-i0^+)\big\} \quad (5.84)$$

Assuming the spectral density to be real, this means

$$S_{AB}(\omega) = \mp\frac{1}{\pi}\,\mathrm{Im}\,G^{\substack{r\\a}}_{AB}(\omega) \quad (5.85)$$

We now prove the formula

$$\theta(t) = \lim_{\delta\to 0^+}\frac{i}{2\pi}\int_{-\infty}^{\infty} dx\frac{e^{-ixt}}{x+i\delta} \quad (5.86)$$

that was essential for arriving at the spectral representation of the Green's functions (5.74) and (5.75). We first consider the case $t>0$. For these t values we can obtain a closed integration contour by adding a semicircle of radius R in the lower complex plane for the integral (5.86) (see Fig. 5.1); the factor e^{-ixt} ensures that in the limit $R\to\infty$, the contribution of the semicircle to the integral vanishes (Jordan's lemma). To see that, we consider the argument $-ixt$ of the exponential function:

$$-ixt = -i(x'+ix'')t = -ix't + x''t \quad (5.87)$$

In order to have a vanishing exponential function in the limit $R=|x|\to\infty$, we need $x''t\to-\infty$ and thus a contour in the lower complex plane $x''<0$ for $t>0$. Thus the integral (5.86) can be written as

$$\lim_{\delta\to 0^+}\frac{i}{2\pi}\int_{-\infty}^{\infty} dx\frac{e^{-ixt}}{x+i\delta} = \lim_{\delta\to 0^+}\frac{i}{2\pi}\int_{C<} dx\frac{e^{-ixt}}{x+i\delta} \quad (5.88)$$

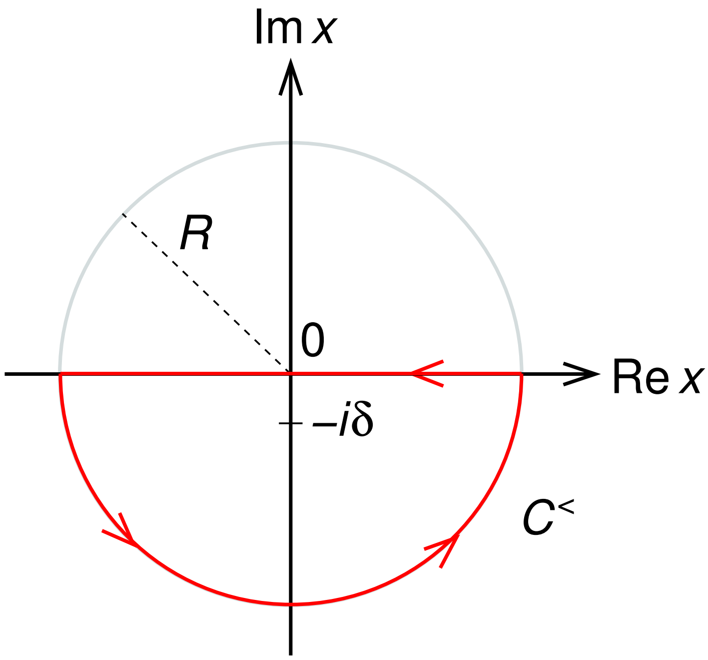

Abbildung 5.1: Integration contour for the case $t > 0$.

This can be evaluated with the residue theorem

$$\oint_{\partial D} dx\, f(x) = 2\pi i \sum_{x_i \in D} \mathrm{Res}\,\{f(x_i)\} \tag{5.89}$$

where D is a domain in the complex plane with outline ∂D. The contour integration needs to be done in the mathematically positive sense which is counterclockwise. The sum runs over all poles x_i of $f(x)$ in D. $Resf(x_i)$ is the residue of $f(x)$ at x_i; if the Laurent series of $f(x)$ at x_i has the form

$$f(x) = \frac{a_{-1}}{x - x_i} + \sum_{n=0}^{\infty} a_n (x - x_i)^n \tag{5.90}$$

then $a_{-1} = \mathrm{Res}\,\{f(x_i)\}$. For a simple pole at x_0 the residue can be calculated as

$$\mathrm{Res}\,\{f(x_0)\} = \lim_{x \to x_0} (x - x_0) f(x) \tag{5.91}$$

Alternatively if $f(x) = \frac{p(x)}{q(x)}$ and $q(x)$ has a simple zero at $x = x_0$

$$\mathrm{Res}\,\{f(x_0)\} = \frac{p(x_0)}{q'(x_0)} \tag{5.92}$$

For a pole of order $m > 1$

$$\mathrm{Res}\,\{f(x_0)\} = \frac{1}{(m-1)!} \lim_{x \to x_0} \left\{ \frac{d^{m-1}}{dx^{m-1}} \left[(x - x_0)^m f(x) \right] \right\} \tag{5.93}$$

Here,

$$a_{-1} = \lim_{x \to -i\delta} \frac{x + i\delta}{x + i\delta} e^{-ixt} = e^{-\delta t} = 1 \quad \text{for} \quad \delta \to 0 \tag{5.94}$$

Thus,

$$\lim_{\delta\to 0^+} \frac{i}{2\pi} \int_{C^<} dx \frac{e^{-ixt}}{x+i\delta} = 2\pi i \frac{i}{2\pi} a_{-1} = -1 \tag{5.95}$$

For the second case, $t < 0$, we have to close the integration contour $C^>$ in the upper half

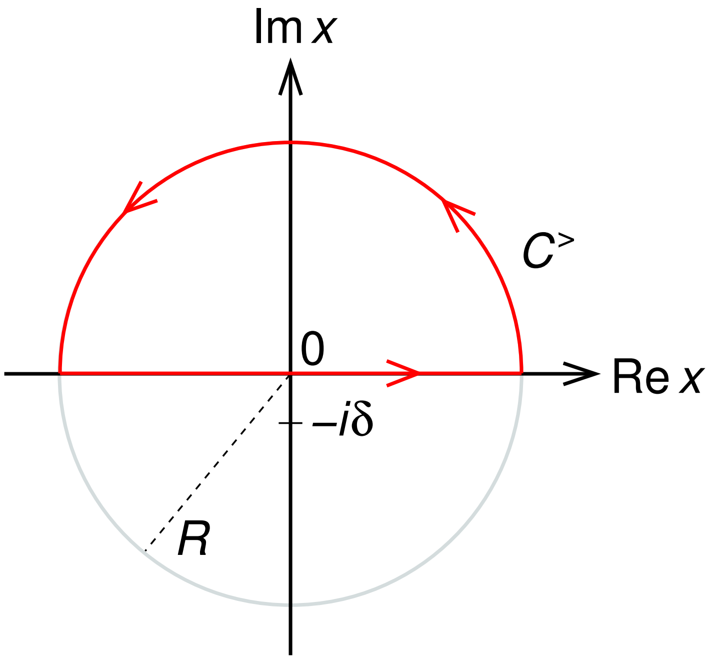

Abbildung 5.2: Integration contour for the case $t < 0$.

plane (see Fig. 5.2). Then we can write

$$\lim_{\delta\to 0^+} \frac{i}{2\pi} \int_{-\infty}^{\infty} dx \frac{e^{-ixt}}{x+i\delta} = \lim_{\delta\to 0^+} \frac{i}{2\pi} \int_{C^>} dx \frac{e^{-ixt}}{x+i\delta} \tag{5.96}$$

As the contour doesn't contain a singularity of the integrand the value of the integral is zero according to Cauchy's integral theorem. Combining the cases for $t > 0$ and $t < 0$, we find

$$\lim_{\delta\to 0} \frac{i}{2\pi} \int_{-\infty}^{\infty} dx \frac{e^{-ixt}}{x+i\delta} = \Theta(t) \tag{5.97}$$

Now we can discuss the analytical properties of the Green's functions, *i.e.* their analyticity in the complex ω plane. First we defined the Green's functions $G^{\alpha}_{AB}(\omega)$ via (5.61) only for real frequencies ω, but the spectral representations (5.74) and (5.75) offer an analytic continuation in the complex ω plane. Meanwhile, Eq. (5.80) for the causal Green's function indicates that analytic continuation is not possible as $G^{c}_{AB}(\omega)$ has singularities in the upper and in the lower complex plane.
For retarded and advanced Green's functions one can show that the continuation doesn't only exist but is analytic – for the retarded Green's function in the upper complex plane and for the advanced function in the lower complex plane. To see that we reconsider the definition

$$G^{\alpha}_{AB}(\omega) = \int dt\, G^{\alpha}_{AB}(t) e^{i\omega t} \tag{5.98}$$

and separate real and imaginary parts of ω:

$$\omega = \omega' + i\omega'' \tag{5.99}$$

Then, because of

$$e^{i\omega t} = e^{i\omega' t - \omega'' t} \tag{5.100}$$

an analytic continuation in the complex plane is possible if only positive values of t are accepted for $\omega'' > 0$ and if only negative values of t are admitted for $\omega'' < 0$ because under these conditions $e^{-\omega'' t}$ guarantees the convergence of the integral (5.98) and its ω derivatives for a large class of functions $G^{\alpha}_{AB}(\omega)$. As the retarded Green's function is only nonzero for $t > 0$ and the advanced function only for $t < 0$, the convergence conditions are fulfilled and thus the retarded Green's function is analytic in the upper complex ω plane and the advanced function in the lower. The casual function generally doesn't permit analytic continuation as $\omega'' > 0$ as well as $\omega'' < 0$ would lead to divergencies. This makes retarded and advanced functions better suited for many applications.

Spectral theorem

We saw that Green's functions and spectral density contain microscopic information about the excitation energies of the considered system. We will now find that also the macroscopic thermodynamic properties are available from suitably defined Green's functions. We start with the correlation function $\langle B(t'), A(t)\rangle$ because its spectral representation (5.69) is similar to the corresponding representation of the spectral density (5.71). Combining (5.69) and (5.71) yields

$$\langle B(t')A(t)\rangle = \int_{-\infty}^{\infty} d\omega \frac{S^{(-)}_{AB}(\omega)}{e^{\beta\hbar\omega} + 1} e^{-i\omega(t-t')} \tag{5.101}$$

where we have chosen the anticommutator spectral density with $\varepsilon = -1$. When using commutator spectral densities ($\varepsilon = +1$) a constant D needs to be added to this expression

$$\langle B(t')A(t)\rangle = \int_{-\infty}^{\infty} d\omega \frac{S^{(\varepsilon)}_{AB}(\omega)}{e^{\beta\hbar\omega} - \varepsilon} e^{-i\omega(t-t')} + \frac{1}{2}(1+\varepsilon)D \tag{5.102}$$

This is due to the fact that the commutator spectral density doesn't determine the correlation function completely. We can see that by separating diagonal (in ω) and offdiagonal parts of $S_{AB}(\omega)$ (Eq. (5.71))

$$S^{(\varepsilon)}_{AB}(\omega) = \hat{S}^{(\varepsilon)}_{AB}(\omega) + (1-\varepsilon)D\delta(\omega) \tag{5.103}$$

where

$$\begin{aligned} \hat{S}^{(\varepsilon)}_{AB}(\omega) &= \frac{1}{\Omega} \sum_{n,m}^{E_n \neq E_m} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n}\left(e^{\beta\hbar\omega} - \varepsilon\right)\delta\Big(\omega - \frac{E_n - E_m}{\hbar}\Big) \\ D &= \frac{1}{\Omega} \sum_{n,m}^{E_n = E_m} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} \end{aligned} \tag{5.104}$$

The diagonal terms contained in D fall out of the commutator spectral density even though they are needed for determining the correlations. We have

$$\begin{aligned}\langle B(t')A(t)\rangle &= D + \int_{-\infty}^{\infty} d\omega \frac{\hat{S}^{(\varepsilon)}_{AB}(\omega)}{e^{\beta\hbar\omega} - \varepsilon} e^{-i\omega(t-t')} \\ \langle A(t)B(t')\rangle &= D + \int_{-\infty}^{\infty} d\omega \frac{\hat{S}^{(\varepsilon)}_{AB}(\omega)e^{\beta\hbar\omega}}{e^{\beta\hbar\omega} - \varepsilon} e^{-i\omega(t-t')}\end{aligned} \tag{5.105}$$

as can be read off from the spectral representations (5.68) and (5.69).

Exact relations

There are a number of symmetry relations and sum rules for Green's functions that are useful as soon as approximations for calculating Green's functions need to be developed.

1.

$$G^r_{AB}(t,t') = \varepsilon G^a_{BA}(t',t) \tag{5.106}$$

follows from the definitions because

$$\begin{aligned}\langle\langle A(t); B(t')\rangle\rangle^r &= -i\Theta(t-t')\langle[A(t), B(t')]_{-\varepsilon}\rangle \\ &= i\varepsilon\Theta(t-t')\langle[B(t'), A(t)]_{-\varepsilon}\rangle = \varepsilon\langle\langle B(t'); A(t)\rangle\rangle^a\end{aligned} \tag{5.107}$$

2.

$$G^r_{AB}(\omega) = \varepsilon G^a_{BA}(-\omega) \quad \text{for real} \quad \omega \tag{5.108}$$

follows by Fourier transforming Eq. (5.106). From the combined Green's functions for complex ω (Eq. (5.83)) we have

$$G_{AB}(\omega) = \varepsilon G_{BA}(-\omega) \quad \text{for complex} \quad \omega \tag{5.109}$$

3.

$$\left(G^{r,a}_{AB}(t,t')\right)^* = \varepsilon G^{r,a}_{A^\dagger B^\dagger}(t',t) \tag{5.110}$$

4. Another important relation follows from the equation of motion:

$$\begin{aligned}\int_{-\infty}^{\infty} d\omega \left\{\omega\langle\langle A;B\rangle\rangle^r_\omega - \hbar\big\langle[A,B]_{-\varepsilon}\big\rangle\right\} &= \int_{-\infty}^{\infty} d\omega\, \langle\langle[A,\mathcal{H}]_-;B\rangle\rangle^r_\omega \\ &= \int_{-\infty}^{\infty} d\omega\,(-i)\int_0^{\infty} dt\,\big\langle\big[[A,\mathcal{H}]_-(t), B(0)\big]_{-\varepsilon}\big\rangle e^{i\omega t} \\ &= \hbar\int_0^{\infty} dt\,\big\langle[\dot{A}(t), B(0)]_{-\varepsilon}\big\rangle \int_{-\infty}^{\infty} d\omega\, e^{i\omega t} = 2\pi\hbar\int_0^{\infty} dt\,\big\langle[\dot{A}(t), B(0)]_{-\varepsilon}\big\rangle\delta(t)\end{aligned} \tag{5.111}$$

Using $\int_0^\infty dx\, f(x)\delta(x) = \frac{1}{2}f(0)$ we find

$$\int_{-\infty}^{\infty} d\omega \left\{\omega G^r_{AB}(\omega) - \hbar\langle[A,B]_{-\varepsilon}\rangle\right\} = \pi\hbar\big\langle[\dot{A}(0), B(0)]_{-\varepsilon}\big\rangle \tag{5.112}$$

and analogously for the other two Green's functions

$$\int_{-\infty}^{\infty} d\omega \left\{\omega G^{a}_{AB}(\omega) - \hbar\big\langle [A,B]_{-\varepsilon}\big\rangle\right\} = -\pi\hbar\big\langle [\dot{A}(0), B(0)]_{-\varepsilon}\big\rangle$$
$$\int_{-\infty}^{\infty} d\omega \left\{\omega G^{c}_{AB}(\omega) - \hbar\big\langle [A,B]_{-\varepsilon}\big\rangle\right\} = \pi\hbar\left\{\big\langle \dot{A}(0), B(0)\big\rangle + \varepsilon\big\langle B(0), \dot{A}(0)\big\rangle\right\} \quad (5.113)$$

The importance for these relations arises from the following argument: The right hand sides, being expectation values of products of operators (observables) are finite; thus, the integrals on the left hand side need to converge. This leads to the requirement for the integrands:

$$\lim_{\omega\to\infty} G^{\alpha}_{AB}(\omega) = \frac{\hbar}{\omega}\big\langle [A,B]_{-\varepsilon}\big\rangle \quad (5.114)$$

The expectation value on the right can usually be calculated directly so that this relation determined the high frequency behavior of the Green's function; they fall off as $\frac{1}{\omega}$. In case the (anti)commutator on the right hand side of (5.114) vanishes, the Green's function will go to zero with a higher power of $\frac{1}{\omega}$ for $\omega \to \infty$.

Kramers Kronig relations

We have seen that G^{r}_{AB} and G^{a}_{AB} are completely defined by the spectral density S_{AB}. But S_{AB} can be obtained solely from the imaginary part of these functions. Thus, real and imaginary parts of the Green's functions are not independent. We consider the integral

$$I_c(\omega) = \int_c d\omega' \frac{G^{r}_{AB}(\omega')}{\omega - \omega' - i0^{+}} \quad (5.115)$$

$G^{r}_{AB}(\omega)$ is analytic in the complete upper frequency plane. If we take ω to be real, this

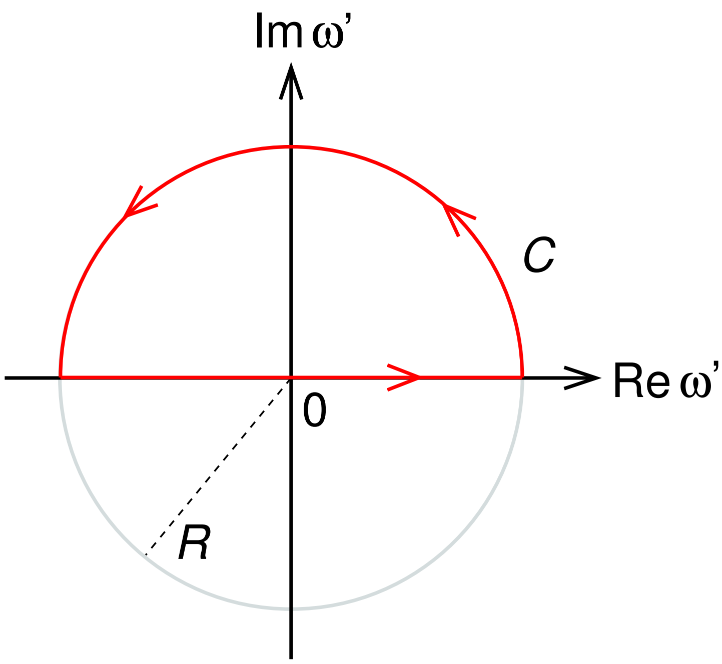

Abbildung 5.3: Integration contour in the complex ω' plane for the Kramers Kronig relations.

is true for the entire integrand; then the integral along the contour C of Fig. 5.3 becomes

$$I_c(\omega) = 0 \tag{5.116}$$

Letting the radius R of the semicircle go to infinity, the part of the contour integral along the semicircle disappears because of (5.114), and using the Dirac identity (5.81) we find

$$0 = \int_{-\infty}^{\infty} d\omega' \, \frac{G^r_{AB}(\omega')}{\omega - \omega' - i0^+} = P\int_{-\infty}^{\infty} d\omega' \, \frac{G^r_{AB}(\omega')}{\omega - \omega'} + i\pi G^r_{AB}(\omega) \tag{5.117}$$

This gives

$$G^r_{AB}(\omega) = \frac{i}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{G^r_{AB}(\omega')}{\omega - \omega'} \tag{5.118}$$

Analogously we find for the advanced Green's function if we close the semicircle in the lower complex ω' plane where $G^a_{AB}(\omega')$ is analytic and by replacing $-i0^+$ by $+i0^+$:

$$G^a_{AB}(\omega) = -\frac{i}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{G^a_{AB}(\omega')}{\omega - \omega'} \tag{5.119}$$

This means that we don't need to know the entire Green's functions; it is enough to know the real or the imaginary part, and the other part is given by the **Kramers Kronig relations** which we read off from (5.118) and (5.119):

$$\begin{aligned}
\operatorname{Re} G^{\overset{r}{a}}_{AB}(\omega) &= \mp \frac{1}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{\operatorname{Im} G^{\overset{r}{a}}_{AB}(\omega')}{\omega - \omega'} \\
\operatorname{Im} G^{\overset{r}{a}}_{AB}(\omega) &= \pm \frac{1}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{\operatorname{Re} G^{\overset{r}{a}}_{AB}(\omega')}{\omega - \omega'}
\end{aligned} \tag{5.120}$$

Assuming the spectral density to be real, (Eq. (5.85)) is valid and thus

$$\begin{aligned}
\operatorname{Re} G^r_{AB}(\omega) = \operatorname{Re} G^a_{AB}(\omega) &= P\int_{-\infty}^{\infty} d\omega' \, \frac{S_{AB}(\omega')}{\omega - \omega'} \\
\operatorname{Im} G^r_{AB}(\omega) = -\operatorname{Im} G^a_{AB}(\omega) &= -\pi S_{AB}(\omega)
\end{aligned} \tag{5.121}$$

Eqs. (5.71) and (5.72) provide a connection to the causal Green's function:

$$\begin{aligned}
\operatorname{Im} G^c_{AB}(\omega) &= -\pi S_{AB}(\omega) \frac{e^{\beta\hbar\omega} + \varepsilon}{e^{\beta\hbar\omega} - \varepsilon} \\
\operatorname{Re} G^c_{AB}(\omega) &= \operatorname{Re} G^{r,a}_{AB}(\omega) \, .
\end{aligned} \tag{5.122}$$

While the Kramers Kronig relations (5.120) are generally valid, the following relations require the spectral density to be real as it often is; in this case, the different types of Green's functions can be converted by these equations; this can be useful as equations of motion methods determine $G^{r,a}_{AB}$ while diagrammatic techniques are used to calculate G^c_{AB}.

5.3 Application to noninteracting electrons

We will get to know the properties of Green's functions for the simple example of noninteracting electrons. The advantage of using the Green's function formalism is not obvious in this case as all results could have been obtained with other methods, but the real strength of the new formalism will become clear in the case of interacting electrons.
We first consider Bloch electrons that don't interact with another but are subject to the periodic potential of the lattice. The Hamiltonian is

$$\mathcal{H} = H_0 - \mu\hat{N}\,, \quad H_0 = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\,, \quad \hat{N} = \sum_{\vec{k}\sigma} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} \tag{5.123}$$

All properties we are interested in can be obtained from the socalled one-electron Green's function

$$G^\alpha_{\vec{k}\sigma}(\omega) = \langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle^\alpha_\omega\,, \quad \alpha = r, a, c\,; \quad \varepsilon = \,-1 \tag{5.124}$$

The choice of $\varepsilon = -1$ is plausible as we deal with a purely Fermionic system but it is not necessary. We now proceed in the same way in which more complicated problems would be tackled: The first step is writing and solving the equation of motion:

$$\omega G^\alpha_{\vec{k}\sigma}(\omega) = \left\langle \left[a_{\vec{k}\sigma}, a^\dagger_{\vec{k}\sigma}\right]_+\right\rangle + \left\langle\!\left\langle \left[a_{\vec{k}\sigma}, \mathcal{H}\right]_-; a^\dagger_{\vec{k}\sigma}\right\rangle\!\right\rangle^\alpha \tag{5.125}$$

Using the commutation relations

$$\left[a_{\vec{k}\sigma'}, a_{\vec{k}'\sigma'}\right]_+ = \left[a^\dagger_{\vec{k}\sigma} a^\dagger_{\vec{k}'\sigma'}\right]_+ = 0, \left[a_{\vec{k}\sigma} a^\dagger_{\vec{k}'\sigma'}\right]_+ = \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'} \tag{5.126}$$

we find

$$\begin{aligned} \left[a_{\vec{k}\sigma}, \mathcal{H}\right]_- &= \sum_{\vec{k}'\sigma'} \left(\varepsilon(\vec{k}') - \mu\right) \left[a_{\vec{k}\sigma}, a^\dagger_{\vec{k}'\sigma'} a_{\vec{k}'\sigma'}\right]_- \\ = \sum_{\vec{k}'\sigma'} (\varepsilon(\vec{k}') - \mu) \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'} a_{\vec{k}'\sigma'} &= \left(\varepsilon(\vec{k}) - \mu\right) a_{\vec{k}\sigma} \end{aligned} \tag{5.127}$$

Substituting in (5.125) leads to

$$\omega G^\alpha_{\vec{k}\sigma}(\omega) = 1 + \left(\varepsilon(\vec{k}) - \mu\right) G^\alpha_{\vec{k}\sigma}(\omega) \tag{5.128}$$

solving for $G^\alpha_{\vec{k}\sigma}$ and fulfilling the boundary conditions with $+i0^+$ or $-i0^+$ yields

$$G^{\substack{r\\a}}_{\vec{k}\sigma}(\omega) = \frac{1}{\omega - \varepsilon(\vec{k}) + \mu \pm i0^+} \tag{5.129}$$

We will use the convention $\hbar = 1$ from now on. The singularities of this function correspond to the possible excitation energies of the system. With complex argument ω we have the combined function

$$G_{\vec{k}\sigma}(\omega) = \frac{1}{\omega - \varepsilon(\vec{k}) + \mu} \tag{5.130}$$

The one electron spectral density is

$$S_{\vec{k}\sigma}(\omega) = \delta\big(\omega - \varepsilon(\vec{k}) + \mu\big) \tag{5.131}$$

From the frequency domain we can now change to the time domain. The retarded Green's function is

$$G^r_{\vec{k}\sigma}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \, \frac{e^{-i\omega(t-t')}}{\omega - \varepsilon(\vec{k}) + \mu + i0^+} \tag{5.132}$$

Substitution of ω by $\omega' = \omega - \varepsilon(\vec{k}) + \mu$ leads to

$$G^r_{\vec{k}\sigma}(t-t') = e^{-i\left(\varepsilon(\vec{k})-\mu\right)(t-t')}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{e^{-i\omega'(t-t')}}{\omega' + i0^+} \tag{5.133}$$

Using Eq. (5.72) gives

$$G^r_{\vec{k}\sigma}(t-t') = \, -i\Theta(t-t')e^{-i\left(\varepsilon(\vec{k})-\mu\right)(t-t')} \tag{5.134}$$

This shows how indeed the introduction of $+i0^+$ has fulfilled the boundary condition. Analogously we find for the advanced function:

$$G^a_{\vec{k}\sigma}(t-t') = \, -i\Theta(t'-t)e^{-i\left(\varepsilon(\vec{k})-\mu\right)(t-t')} \tag{5.135}$$

In the noninteracting system, the time dependent Green's functions show an oscillatory behavior with a frequency that corresponds to an exact excitation energy. We will see later that this remains true for interacting systems, but they will additionally have a damping factor that corresponds to a finite lifetime of the quasiparticles. The time dependent spectral density is easily found from (5.131):

$$S_{\vec{k}\sigma}(t-t') = \frac{1}{2\pi}e^{-i\left(\varepsilon(\vec{k})-\mu\right)(t-t')} \tag{5.136}$$

The average occupation number $\langle n_{\vec{k}\sigma}\rangle$ of the level $(\vec{k}\sigma)$ can be found by substituting (5.131) into the spectral theorem (5.102)

$$\langle a^\dagger_{\vec{k}\sigma}(t)a_{\vec{k}\sigma}(t)\rangle = \langle n_{\vec{k}\sigma}\rangle = \int_{-\infty}^{\infty} d\omega \, \frac{\delta(\omega - \varepsilon(\vec{k}) + \mu)}{e^{\beta\omega}+1} = \frac{1}{e^{\beta\left(\varepsilon(\vec{k})-\mu\right)}+1} \tag{5.137}$$

This is the result known from quantum statistics, the Fermi function

$$f_-(\omega) = \frac{1}{e^{\beta(\omega-\mu)}+1} \tag{5.138}$$

evaluated for $\omega = \varepsilon(\vec{k})$. Using $\langle n_{\vec{k}\sigma}\rangle$ we can fix the total electron number N_e by summing over wave vector and spin:

$$N_e = \sum_{\vec{k}\sigma}\int_{-\infty}^{\infty} d\omega \, S_{\vec{k}\sigma}(\omega)\frac{1}{e^{\beta\omega}+1} = \sum_{\vec{k}\sigma}\int_{-\infty}^{\infty} d\omega \, f_-(\omega)S_{\vec{k}\sigma}(\omega-\mu) \tag{5.139}$$

If we denote with $\rho_\sigma(\omega)$ the density of states per spin for the free Fermion system (for which $\rho_\sigma(\omega) = \rho_{-\sigma}(\omega)$), we can write N_e as

$$N_e = N \sum_\sigma \int_{-\infty}^{\infty} d\omega\, f_-(\omega)\rho_\sigma(\omega) \tag{5.140}$$

N is the number of lattice sites if we consider a one band model; $\rho_\sigma(\omega)$ is normalized to 1. Comparing (5.139) and (5.140) leads to the definition of **quasiparticle density of states**

$$\rho_\sigma(\omega) = \frac{1}{N} \sum_{\vec{k}} S_{\vec{k}\sigma}(\omega - \mu) \tag{5.141}$$

These considerations are not only true for the free system but are generally valid. We will see that (5.141) represents the general definition of the quasiparticle density of states for any interacting electron system. For noninteracting systems we can enter $S_{\vec{k}\sigma}(\omega)$:

$$\rho_\sigma(\omega) = \frac{1}{N} \sum_{\vec{k}} \delta(\omega - \varepsilon(\vec{k})) \tag{5.142}$$

The **internal energy** U is the thermodynamic expectation value of the Hamiltonian and therefore determined in a simple way by $\langle n_{\vec{k}\sigma} \rangle$:

$$U = \langle H_0 \rangle = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) \langle n_{\vec{k}\sigma} \rangle = \frac{1}{2} \sum_{\vec{k}\sigma} \int_{-\infty}^{\infty} d\omega\, \big(\omega + \varepsilon(\vec{k})\big) f_-(\omega) S_{\vec{k}\sigma}(\omega - \mu) \tag{5.143}$$

The last expression will turn out to be generally valid for interacting systems. From U we obtain the free energy F and thus the entire thermodynamics by considering that

$$F(T,V) = U(T,V) - T\,S(T,V) = U(T,V) + T\left(\frac{\partial F}{\partial T}\right)_V \tag{5.144}$$

which leads to

$$U(T,V) = -T^2 \left[\frac{\partial}{\partial T}\left(\frac{1}{T} F(T,V)\right)\right]_V \tag{5.145}$$

Using the third law of thermodynamics

$$\lim_{T \to 0} \left[\frac{1}{T}(F(T) - F(0))\right] = \left(\frac{\partial F}{\partial T}\right)_V (T = 0) = -S(T = 0, V) = 0 \tag{5.146}$$

and $F(0,V) = U(0,V)$ we can integrate (5.145) and obtain

$$F(T,V) = U(0,V) - T \int_0^T dT' \,\frac{U(T',V) - U(0,V)}{T'^2} \tag{5.147}$$

All other properties of equilibrium thermodynamics can be derived from $F(T,V)$. Here we considered Green's functions $G^\alpha_{\vec{k}\sigma}(\omega)$ corresponding to Bloch electrons; we could also have worked in Wannier representation. For the Green's function

$$G^\alpha_{ij\sigma}(\omega) = \langle\langle a_{i\sigma}; a^\dagger_{j\sigma} \rangle\rangle^\alpha_\omega \tag{5.148}$$

one finds the equation of motion

$$\omega G^{\alpha}_{ij\sigma}(\omega) = \delta_{ij} + \sum_m (t_{im} - \mu\delta_{im}) G^{\alpha}_{mj\sigma}(\omega) \tag{5.149}$$

that doesn't directly decouple but can be solved by Fourier transformation:

$$G^{\substack{r\\a}}_{ij\sigma}(\omega) = \frac{1}{N}\sum_{\vec{k}} \frac{e^{i\vec{k}(\vec{R}_i - \vec{R}_j)}}{\omega - (\varepsilon(\vec{k}) - \mu) \pm i0^+} \tag{5.150}$$

5.4 Quasiparticles

We will now investigate how to extract information about interacting electron systems using Green's functions. We consider the Hamiltonian in Bloch representation

$$H = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} + \frac{1}{2}\sum_{\vec{k}\vec{p}\vec{q}\sigma'\sigma} v_{\vec{k}\vec{p}}(\vec{q}) a^{\dagger}_{\vec{k}+\vec{q}\sigma} a^{\dagger}_{\vec{p}-\vec{q}\sigma'} a_{\vec{p}\sigma'} a_{\vec{k}\sigma} \tag{5.151}$$

where we consider a one band problem so that we can suppress band indices. The Bloch energies are:

$$\varepsilon(\vec{k}) = \int d^3r\, \psi^*_{\vec{k}}(\vec{r}) \left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r}) \right] \psi_{\vec{k}}(\vec{r}) \tag{5.152}$$

where $\psi_{\vec{k}}(\vec{r})$ is a Bloch function and $V(\vec{r})$ is the periodic lattice potential. The $\varepsilon(\vec{k})$ are given once the model that we study is specified. The Coulomb matrix element is

$$v_{\vec{k}\vec{p}}(\vec{q}) = \frac{e^2}{4\pi\varepsilon_0} \int d^3r_1 d^3r_2 \frac{\psi^*_{\vec{k}+\vec{q}}(\vec{r}_1)\psi^*_{\vec{p}-\vec{q}}(\vec{r}_2)\psi_{\vec{p}}(\vec{r}_2)\psi_{\vec{k}}(\vec{r}_1)}{|\vec{r}_1 - \vec{r}_2|} \tag{5.153}$$

For a constant lattice potential $V(\vec{r}) = \text{const}$ this becomes

$$v_{\vec{k}\vec{p}}(\vec{q}) \xrightarrow{V(\vec{r})=\text{const}} v_0(\vec{q}) = \frac{e^2}{\varepsilon_0 V q^2} \tag{5.154}$$

We will also use the Hamiltonian in Wannier representation

$$H = \sum_{ij\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{1}{2}\sum_{ijkl\sigma\sigma'} v(ij;kl) a^{\dagger}_{i\sigma} a^{\dagger}_{j\sigma'} a_{l\sigma'} a_{k\sigma} \tag{5.155}$$

The hopping integrals t_{ij} are connected to the Bloch energies $\varepsilon(\vec{k})$ by Fourier transform. We will now see that the one electron Green's functions

$$\begin{aligned} G^{\alpha}_{\vec{k}\sigma}(\omega) &\equiv \langle\langle a_{\vec{k}\sigma}; a^{\dagger}_{\vec{k}\sigma} \rangle\rangle^{\alpha}_{\omega}\,, \\ G^{\alpha}_{ij\sigma}(\omega) &\equiv \langle\langle a_{i\sigma}; a^{\dagger}_{j\sigma} \rangle\rangle^{\alpha}_{\omega}\,, \quad \alpha = r, a, c\,; \quad \varepsilon = -1 \end{aligned} \tag{5.156}$$

and the corresponding one electron spectral density

$$S_{\vec{k}\sigma}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{-i\omega(t-t')}\big\langle\big[a_{\vec{k}\sigma}(t), a^\dagger_{\vec{k}\sigma}(t')\big]_+\big\rangle$$
$$S_{ij\sigma}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{-i\omega(t-t')}\big\langle\big[a_{i\sigma}(t), a^\dagger_{j\sigma}(t')\big]_+\big\rangle \tag{5.157}$$

determine the full equilibrium thermodynamics also for interacting electron systems. To calculate them, we write down the equation of motion of the $\vec{k}$-dependent Green's function, we need the commutator

$$\big[a_{\vec{k}\sigma}, \mathcal{H}\big]_- = (\varepsilon(\vec{k}) - \mu)a^\dagger_{\vec{k}\sigma} + \sum_{\vec{p}\vec{q}\sigma'} v_{\vec{p},\vec{k}+\vec{q}}(\vec{q})a^\dagger_{\vec{p}-\vec{q}\sigma}a_{\vec{p}\sigma'}a_{\vec{k}+\vec{q}\sigma} \tag{5.158}$$

using the higher order Green's function

$${}^\alpha\Gamma^{\sigma'\sigma}_{\vec{p}\vec{k};\vec{q}}(\omega) \equiv \langle\langle a^\dagger_{\vec{p}-\vec{q}\sigma}a_{\vec{p}\sigma'}a_{\vec{k}+\vec{q}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle^\alpha_\omega \tag{5.159}$$

we have the equation of motion

$$\big(\omega - \varepsilon(\vec{k}) + \mu\big)G^\alpha_{\vec{k}\sigma}(\omega) = 1 + \sum_{\vec{p}\vec{q}\sigma'} v_{\vec{p},\vec{k}+\vec{q}}(\vec{q})\,{}^\alpha\Gamma^{\sigma'\sigma}_{\vec{p}\vec{k};\vec{q}}(\omega) \tag{5.160}$$

The unknown function Γ prevents us from directly solving for $G^\alpha_{\vec{k}\sigma}$. But we postulate that the following decomposition is possible:

$$\langle\langle[a_{\vec{k}\sigma}, \mathcal{H}-\mathcal{H}_0]_-; a^\dagger_{\vec{k}\sigma}\rangle\rangle^\alpha_\omega = \sum_{\vec{p}\vec{q}\sigma'} v_{\vec{p},\vec{k}+\vec{q}}(\vec{q})\,{}^\alpha\Gamma^{\sigma'\sigma}_{\vec{p}\vec{k};\vec{q}} \equiv \Sigma^\alpha_\sigma(\vec{k},\omega)G^\alpha_{\vec{k}\sigma}(\omega) \tag{5.161}$$

This equation defines the **self energy** $\Sigma^\alpha_\sigma(\vec{k},\omega)$. It allows us to solve Eq. (5.160) for $G^\alpha_{\vec{k}\sigma}$:

$$G^\alpha_{\vec{k}\sigma}(\omega) = \frac{1}{\omega - \varepsilon(\vec{k}) + \mu - \Sigma^\alpha_\sigma(\vec{k},\omega)} \tag{5.162}$$

Comparison with the corresponding expression for noninteracting electrons shows that the entire effect of the particle interactions is contained in the selfenergy. Usually it is a complex function of $(\vec{k},\omega)$; the real part determines the energy of the quasiparticles, and the imaginary part their lifetime.
We can rearrange (5.162) a bit; writing $G^{(0)}_{\vec{k}\sigma}$ for the one electron Green's function of noninteracting electrons, we have (suppressing the index α)

$$G_{\vec{k}\sigma}(\omega) = \Big\{\big[G^{(0)}_{\vec{k}\sigma}(\omega)\big]^{-1} - \Sigma_\sigma(\vec{k},\omega)\Big\}^{-1}$$
$$\Big\{\big[G^{(0)}_{\vec{k}\sigma}(\omega)\big]^{-1} - \Sigma_\sigma(\vec{k},\omega)\Big\}G_{\vec{k}\sigma}(\omega) = 1 \tag{5.163}$$

This gives us the socalled **Dyson equation**

$$G_{\vec{k}\sigma}(\omega) = G^{(0)}_{\vec{k}\sigma}(\omega) + G^{(0)}_{\vec{k}\sigma}(\omega)\Sigma_\sigma(\vec{k},\omega)G_{\vec{k}\sigma}(\omega) \tag{5.164}$$

Electronic self energy

We will now investigate the general structure of self energy, Green's function and spectral density. The self energy corresponding to Eq. (5.162) is in general a complex quantity.

$$\Sigma^{\alpha}_{\sigma}(\vec{k},\omega) = R^{\alpha}_{\sigma}(\vec{k},\omega) + iI^{\alpha}_{\sigma}(\vec{k},\omega)\,, \quad \alpha = r,a,c \tag{5.165}$$

Eq. (5.110) for the Green's function implies

$$\big(\Sigma^{a}_{\sigma}(\vec{k},\omega)\big)^{*} = \Sigma^{r}_{\sigma}(\vec{k},\omega) \tag{5.166}$$

This simple relation allows us to concentrate on the retarded Green's functions, and we will omit the $+i0^{+}$ if $I_\sigma \neq 0$. We can rewrite Eq. (5.162) as

$$G^{r}_{\vec{k}\sigma}(\omega) = \frac{\omega - \varepsilon(\vec{k}) + \mu - R_\sigma(\vec{k},\omega) + iI_\sigma(\vec{k},\omega)}{\big(\omega - \varepsilon(\vec{k}) + \mu - R_\sigma(\vec{k},\omega)\big)^2 + \big(I_\sigma(\vec{k},\omega)\big)^2} \tag{5.167}$$

Thus, the spectral density is

$$S_{\vec{k}\sigma}(\omega) = -\frac{1}{\pi}\frac{I_\sigma(\vec{k},\omega)}{\big(\omega - \varepsilon(\vec{k}) + \mu - R_\sigma(\vec{k},\omega)\big)^2 + \big(I_\sigma(\vec{k},\omega)\big)^2} \tag{5.168}$$

If we compare this to the spectral representation of the spectral density (5.71)

$$S_{\vec{k}\sigma}(\omega) = \frac{1}{\Omega}\sum_{n,m}\big|\langle E_n|a^{\dagger}_{\vec{k}\sigma}|E_m\rangle\big|^2 e^{-\beta E_n}(e^{\beta\omega}+1)\delta\big(\omega - (E_n - E_m)\big) \tag{5.169}$$

which is nonnegative for all $(\vec{k},\sigma,\omega)$, we find for the imaginary part of the retarded self energy

$$I_\sigma(\vec{k},\omega) \leq 0\,. \tag{5.170}$$

We will now investigate (5.168) further. Without explicit knowledge of $R_\sigma(\vec{k},\omega)$ and $I_\sigma(\vec{k},\omega)$ we expect more or less pronounced maxima at the resonances

$$\omega_{i\sigma}(\vec{k}) \equiv \varepsilon(\vec{k}) - \mu + R_\sigma\big(\vec{k},\omega_{i\sigma}(\vec{k})\big)\,, \quad i = 1,2,3,\dots \tag{5.171}$$

We have to distinguish two cases:
Case 1: In a certain energy range containing $\omega_{i\sigma}$,

$$I_\sigma(\vec{k},\omega) \equiv 0 \tag{5.172}$$

Then we have to consider the limit $I_\sigma \to -0^{+}$. Representing the delta function as the limit

$$\delta(\omega - \omega_0) = \frac{1}{\pi}\lim_{x\to 0}\frac{x}{(\omega-\omega_0)^2 + x^2} \tag{5.173}$$

we have

$$S_{\vec{k}\sigma}(\omega) = \delta\big(\omega - \varepsilon(\vec{k}) + \mu - R_\sigma(\vec{k},\omega)\big) \tag{5.174}$$

Using

$$\delta[f(x)] = \sum_i \frac{1}{|f'(x_i)|}\delta(x - x_i)\,; \quad f(x_i) = 0 \tag{5.175}$$

we can write this as

$$\begin{aligned} S_{\vec{k}\sigma}(\omega) &= \sum_{i=1}^{n} \alpha_{i\sigma}(\vec{k})\delta\big(\omega - \omega_{i\sigma}(\vec{k})\big) \\ \alpha_{i\sigma}(\vec{k}) &= \Big|1 - \frac{\partial}{\partial\omega} R_\sigma(\vec{k},\omega)\Big|^{-1}_{\omega\,=\,\omega_{i\sigma}} \end{aligned} \tag{5.176}$$

The sum runs over the resonances $\omega_{i\sigma}$ in the energy range for which Eq. (5.172) holds.
Case 2: We consider

$$I_\sigma(\vec{k},\omega) \neq 0 \tag{5.177}$$

but in a certain energy range around the resonance $\omega_{i\sigma}$

$$\big|I_\sigma(\vec{k},\omega)\big| \ll \big|\varepsilon(\vec{k}) - \mu + R_\sigma(\vec{k},\omega)\big| \tag{5.178}$$

There we expect a pronounced maximum at $\omega = \omega_{i\sigma}$. To see this, we expand the expression

$$F_\sigma(\vec{k},\omega) = \varepsilon(\vec{k}) - \mu + R_\sigma(\vec{k},\omega) \tag{5.179}$$

close to the resonance up to the linear term:

$$\begin{aligned} F_\sigma(\vec{k},\omega) &= F_\sigma(\vec{k},\omega_{i\sigma}) + (\omega - \omega_{i\sigma})\frac{\partial F_\sigma}{\partial\omega}\Big|_{\omega=\omega_{i\sigma}} + \cdots \\ &= \omega_{i\sigma}(\vec{k}) + (\omega - \omega_{i\sigma})\frac{\partial R_\sigma}{\partial\omega}\Big|_{\omega=\omega_{i\sigma}} + \cdots \end{aligned} \tag{5.180}$$

This means

$$\begin{aligned} (\omega - \varepsilon(\vec{k}) + \mu - R_\sigma(\vec{k},\omega))^2 &\simeq (\omega - \omega_{i\sigma})^2\Big(1 - \frac{\partial R_\sigma}{\partial\omega}\Big|_{\omega=\omega_{i\sigma}}\Big)^2 \\ &= \alpha_{i\sigma}^{-2}(\vec{k})\big(\omega - \omega_{i\sigma}(\vec{k})\big)^2 \end{aligned} \tag{5.181}$$

We substitute this expression in (5.168), assuming that $I_\sigma(\vec{k},\omega)$ is only weakly dependent on ω around $\omega_{i\sigma}$ so that

$$I_\sigma(\vec{k},\omega) \approx I_\sigma\big(\vec{k},\omega_{i\sigma}(\vec{k})\big) \equiv I_{i\sigma}(\vec{k}) \tag{5.182}$$

and find the following approximation for the spectral density:

$$S^{(i)}_{\vec{k}\sigma}(\omega) \approx -\frac{1}{\pi}\frac{\alpha^2_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})}{\big(\omega - \omega_{i\sigma}(\vec{k})\big)^2 + \big(\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})\big)^2} \tag{5.183}$$

Under our assumptions, the spectral density has a Lorentzian shape close to the resonance. These considerations show that the spectral density will typically be a linear combination of weighted Lorentzians and delta peaks. The consequence for the time dependence of the spectral density in Case 1 is like in a noninteracting electron system an undamped oscillation:

$$S_{\vec{k}\sigma}(t-t') = \frac{1}{2\pi}\sum_{i=1}^{n} \alpha_{i\sigma}(\vec{k}) e^{-i\omega_{i\sigma}(\vec{k})(t-t')} \tag{5.184}$$

The resonance frequencies $\omega_{i\sigma}(\vec{k})$ determine the oscillation frequencies. In Case 2, the Lorentzians lead to damped oscillations. To see that we assume that (5.183) is approximately valid for the entire energy range. Then we can write

$$\begin{aligned} S^{(i)}_{\vec{k}\sigma}(t-t') \approx &\frac{1}{4\pi^2 i}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega(t-t')}\alpha_{i\sigma}(\vec{k})\times \\ &\times\left\{\frac{1}{\omega-\omega_{i\sigma}(\vec{k})+i\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})} - \frac{1}{\omega-\omega_{i\sigma}(\vec{k})-i\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})}\right\} \end{aligned} \tag{5.185}$$

because

$$\begin{aligned} &\frac{1}{\omega-\omega_{i\sigma}(\vec{k})+i\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})} - \frac{1}{\omega-\omega_{i\sigma}(\vec{k})-i\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})} \\ &\qquad = \frac{-2i\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})}{\left(\omega-\omega_{i\sigma}(\vec{k})\right)^2+\left(\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})\right)^2} \end{aligned} \tag{5.186}$$

The integrals can be solved with the residue theorem. The spectral weights $\alpha_{i\sigma}(\vec{k})$ are positive definite so that because of Eq. (5.170)

$$\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k}) \le 0 \tag{5.187}$$

Thus the first term has a pole in the upper, the second in the lower complex plane. Therefore we choose the integration contours dependent on $t > t'$ as

$$\int_{-\infty}^{\infty} d\omega \ldots = \begin{cases} \int_{C^<} d\omega \ldots & \text{for } t-t' > 0 \\ \int_{C^>} d\omega \ldots & \text{for } t-t' < 0 \end{cases} \tag{5.188}$$

where $C^<$ is a contour closed by a semicircle in the lower complex plane, $C^>$ in the upper complex plane. Then the exponential function in (5.185) suppresses the contribution of the semicircle. This yields (see Eq. (2.87))

$$S^{(i)}_{\vec{k}\sigma}(t-t') \approx \frac{1}{2\pi}\alpha_{i\sigma}(\vec{k})e^{-i\omega_{i\sigma}(\vec{k})(t-t')}e^{-\left|\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})\right||t-t'|} \tag{5.189}$$

This is indeed a damped oscillation, again with the resonance frequency, but now damped with the damping mostly given by the imaginary part of the self energy. Thus we expect for interacting systems a spectral density $S_{\vec{k}\sigma}(t-t')$ that is composed of damped and undamped oscillations.

We will learn more about the significance of the spectral density $S_{\vec{k}\sigma}(t-t')$ by considering the special case $T = 0, |\vec{k}| > k_F, t > t'$ where k_F is the Fermi wave vector; thus, the system is in its ground state $|E_0\rangle$. By addition of a $(\vec{k}, \sigma)$ electron at time t the state

$$|\varphi_0(t)\rangle = a^{\dagger}_{\vec{k}\sigma}(t)|E_0\rangle \tag{5.190}$$

is created which is not necessarily an eigenstate of the Hamiltonian. If we now consider the definition

$$S_{\vec{k}\sigma}(t-t') = \frac{1}{2\pi}\left\langle [a_{\vec{k}\sigma}(t), a^{\dagger}_{\vec{k}\sigma}(t')]_{+}\right\rangle$$

of the spectral density, due to $|\vec{k}| > k_F$ only one term can contribute; thus,

$$2\pi S_{\vec{k}\sigma}(t-t') = \langle \varphi_0(t)|\varphi_0(t')\rangle \tag{5.191}$$

This has a simple interpretation: $2\pi S_{\vec{k}\sigma}(t-t')$ is the probability that the state $|\varphi_0(t)\rangle$ that was created by addition of a $(\vec{k}, \sigma)$ electron from the state $|E_0\rangle$ at time t' will still exist at $t > t'$; $S_{\vec{k}\sigma}(t-t')$ characterizes the time evolution or **propagation** of an additional $(\vec{k}, \sigma)$ electron in the N particle system. This is why $S_{\vec{k}\sigma}$ (and $G^{\alpha}_{\vec{k}\sigma}$) are sometimes **propagators**. If we had assumed $|\vec{k}| < k_F$, $S_{\vec{k}\sigma}(t-t')$ would describe the propagation of a hole.
There are two typical states:

$$\begin{aligned}&\text{stationary state: } |\langle \varphi_0(t)|\varphi_0(t')\rangle|^2 = \text{const}\\&\text{state with finite lifetime: } |\langle \varphi_0(t)|\varphi_0(t')\rangle|^2 \xrightarrow[t-t'\to\infty]{} 0\end{aligned} \tag{5.192}$$

We now apply this consideration first to noninteracting electrons. The Hamiltonian in Bloch formulation is

$$\mathcal{H} = \sum_{\vec{k}\sigma} (\varepsilon(\vec{k}) - \mu) a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} \tag{5.193}$$

Now we can calculate

$$\left[\mathcal{H}, a^{\dagger}_{\vec{k}\sigma}\right]_{-} = \left(\varepsilon(\vec{k}) - \mu\right) a^{\dagger}_{\vec{k}\sigma} \tag{5.194}$$

and

$$\mathcal{H}_0\left(a^{\dagger}_{\vec{k}\sigma}|E_0\rangle\right) = a^{\dagger}_{\vec{k}\sigma}\mathcal{H}_0|E_0\rangle + \left[\mathcal{H}_0, a^{\dagger}_{\vec{k}\sigma}\right]_{-}|E_0\rangle = \left(E_0 + \varepsilon(\vec{k}) - \mu\right)\left(a^{\dagger}_{\vec{k}\sigma}|E_0\rangle\right) \tag{5.195}$$

In this case, $a^{\dagger}_{\vec{k}\sigma}|E_0\rangle$ turns out to be an eigenstate of $\mathcal{H}_0$ again. Further, we find

$$\begin{aligned}|\varphi_0(t)\rangle &= e^{i\mathcal{H}_0 t} a^{\dagger}_{\vec{k}\sigma} e^{-i\mathcal{H}_0 t}|E_0\rangle = e^{-iE_0 t} e^{i\mathcal{H}_0 t}\left(a^{\dagger}_{\vec{k}\sigma}|E_0\rangle\right)\\&= e^{i\left(\varepsilon(\vec{k})-\mu\right)t}\left(a^{\dagger}_{\vec{k}\sigma}|E_0\rangle\right)\end{aligned} \tag{5.196}$$

Because of $|\vec{k}| > k_F$ and $\langle E_0|E_0\rangle = 1$ we also have

$$\langle E_0|a_{\vec{k}\sigma} a^{\dagger}_{\vec{k}\sigma}|E_0\rangle = \langle E_0|E_0\rangle - \langle E_0|a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma}|E_0\rangle = 1 \tag{5.197}$$

This finally leads to

$$\langle \varphi_0(t)|\varphi_0(t')\rangle = e^{i\left(\varepsilon(\vec{k})-\mu\right)(t-t')} \tag{5.198}$$

Thus the propagator is an undamped harmonic oscillation with an exact excitation energy of the system $(\varepsilon(\vec{k}) - \mu)$. As

$$|\langle \varphi_0(t)|\varphi_0(t')\rangle|^2 = 1 \tag{5.199}$$

it is a stationary state.
Next we consider an interacting system. By inserting a unit operator from a complete set of eigenstates $|E_n\rangle$ we have:

$$2\pi S_{\vec{k}\sigma}(t-t') = \sum_n \left|\langle E_n|a^\dagger_{\vec{k}\sigma}|E_0\rangle\right|^2 e^{-i(E_n-E_0)(t-t')} \tag{5.200}$$

In the free system, $a^\dagger_{\vec{k}\sigma}|E_0\rangle$ is an eigenstate, and the orthogonality of the eigenstates implies that only one term in the sum is nonzero. In the interacting system, this is no longer the case; in the expansion

$$|\varphi_0(t)\rangle = a^\dagger_{\vec{k}\sigma}|E_0\rangle = \sum_m c_m|E_m\rangle \tag{5.201}$$

usually infinitely many expansion coefficients will be nonzero. The superposition of oscillations with different frequencies will lead to a sum in (5.200) that is maximal for $t = t'$ and will destructively interfere for $t - t' > 0$ so that

$$|\langle\varphi_0(t)|\varphi_0(t')\rangle|^2 \xrightarrow[t-t'\to\infty]{} 0 \tag{5.202}$$

Then, the state $|\varphi_0(t')\rangle$ created at time t' has only a finite lifetime. Under certain conditions, however, the irregular time dependence of the propagator can be represented as superposition of damped oscillations with well defined frequency:

$$2\pi S_{\vec{k}\sigma}(t-t') = \sum_i \alpha_{i\sigma}(\vec{k})e^{-i\eta_{i\sigma}(\vec{k})(t-t')} \tag{5.203}$$

This formally has the same form as the corresponding expression (5.198) for the free system, but the new single-particle energies are complex quantities:

$$\eta_{i\sigma}(\vec{k}) = \operatorname{Re}\eta_{i\sigma}(\vec{k}) + i\operatorname{Im}\eta_{i\sigma}(\vec{k}) \tag{5.204}$$

The imaginary part is responsible for the exponential damping of the oscillation. The energies $\eta_{i\sigma}(\vec{k})$ are now ascribed to a fictive particle, the so called **quasiparticle**. This is motivated by the fact that the particle number $(N+1)$ that is added to the system at time t' propagates as if it decays into several quasiparticles of energy $\operatorname{Re}\eta_{i\sigma}(\vec{k})$ and lifetime $\frac{1}{\operatorname{Im}\eta_{i\sigma}(\vec{k})}$ ($\eta_{i\sigma}$ is again measured in units of $\hbar$, i.e. it is a frequency). Every quasiparticle has a spectral weight $\alpha_{i\sigma}(\vec{k})$ for which the conservation of total particle number means

$$\sum_i \alpha_{i\sigma}(\vec{k}) = 1 \tag{5.205}$$

If we now compare

$$S^{(i)}_{\vec{k}\sigma}(t-t') = \frac{1}{2\pi}\alpha_{i\sigma}(\vec{k})e^{-i\operatorname{Re}\eta_{i\sigma}(\vec{k})(t-t')}e^{-|\operatorname{Im}\eta_{i\sigma}(\vec{k})|(t-t')} \tag{5.206}$$

to (5.189) we recognize the relationship between quasiparticle properties and electronic selfenergy:

$$\begin{aligned}&\text{quasiparticle energy: } \omega_{i\sigma}(\vec{k}) = \varepsilon(\vec{k}) - \mu + R_\sigma\big(\vec{k}, \omega = \omega_{i\sigma}(\vec{k})\big)\\ &\text{quasiparticle lifetime: } \tau_{i\sigma}(\vec{k}) = \frac{1}{|\alpha_{i\sigma}(\vec{k})I_{i\sigma}(\vec{k})|}\end{aligned} \tag{5.207}$$

The spectral weights $\alpha_{i\sigma}$ are determined by the real part of the self energy. Thus, the quasiparticle lifetime is also influenced by the real part of the self energy. Another analogy between quasiparticle and free particle is the effective mass $m^*_{i\sigma}(\vec{k})$ which is also determined by the real part of the self energy. With the same argumentation as for the Bloch density of states $\rho_0(\omega)$ we can define a quasiparticle density of states

$$\rho_\sigma(\omega) = \frac{1}{N}\sum_{\vec{k}} S_{\vec{k}\sigma}(\omega - \mu) \tag{5.208}$$

In contrast to $\rho_0(\omega)$, this density of states for the interacting system will be temperature dependent; it will also depend on the particle number.
As the spectral density represents a weighted superposition of delta functions, in the arguments of which appear the excitation energies that are required to add a $(\vec{k}\sigma)$ electron to an N particle system or remove one from it, $\rho_\sigma(\omega)$ has a direct link to the photoemission experiment.

Application to interacting systems

We now apply the formalism to a simple interacting problem, the Hubbard model in the limit of infinitely narrow bands. The Hamiltonian is

$$\mathcal{H} = \sum_{\varepsilon j\sigma}(t_{ij} - \mu\delta_{ij})a^\dagger_{i\sigma}a_{j\sigma} + \frac{U}{2}\sum_{i,\sigma} n_{i\sigma}n_{i\bar{\sigma}}\,, \tag{5.209}$$

where we use the notation $-\sigma \equiv \bar{\sigma}$. In order to calculate the one electron Green's function, it is convenient to proceed in the Wannier representation

$$G^\alpha_{ij\sigma}(\omega) = \langle\langle a_{i\sigma}; a^\dagger_{j\sigma}\rangle\rangle^\alpha_\omega \tag{5.210}$$

For the equation of motion, we need the commutator

$$[a_{i\sigma}, \mathcal{H}]_- = \sum_m (t_{im} - \mu\delta_{im})a_{m\sigma} + n_{ni\bar{\sigma}}a_{i\sigma} \tag{5.211}$$

The second term leads to the higher order Green's function

$$\Gamma^\alpha_{ilm;j\sigma}(\omega) = \langle\langle a^\dagger_{i\bar{\sigma}}a_{l\bar{\sigma}}a_{m\sigma}; a^\dagger_{j\sigma}\rangle\rangle^\alpha_\omega \tag{5.212}$$

This leads to the equation of motion

$$(\omega + \mu)G^\alpha_{ij\sigma}(\omega) = \delta_{ij} + \sum_m t_{im}G^\alpha_{mj\sigma}(\omega) + U\Gamma^\alpha_{iii;j\sigma}(\omega) \tag{5.213}$$

Due to the higher order Green's function Γ^α we cannot directly solve for G^α. Therefore we determine the equation of motion for Γ^α; we need

$$\begin{aligned}
[n_{i\bar{\sigma}}a_{i\sigma}, \mathcal{H}_0]_- &= \sum_m (t_{im} - \mu\delta_{im})\{n_{i\bar{\sigma}}a_{m\sigma} + a^\dagger_{i\bar{\sigma}}a_{m\bar{\sigma}}a_{i\sigma} - a^\dagger_{m\bar{\sigma}}a_{i\bar{\sigma}}a_{i\sigma}\} \\
[n_{i\bar{\sigma}}a_{i\sigma}, \mathcal{H}_1]_- &= U a_{i\sigma}n_{i\bar{\sigma}}
\end{aligned} \tag{5.214}$$

where the relation $n_{i\sigma}^2 = n_{i\sigma}$ was used. This yields

$$(\omega + \mu - U)\Gamma^{\alpha}_{iii;j\sigma}(\omega) = \delta_{ij}\langle n_{i\bar{\sigma}}\rangle + \sum_m t_{im}\{\Gamma^{\alpha}_{iim;j\sigma}(\omega) + \Gamma^{\alpha}_{imi;j\sigma}(\omega) - \Gamma^{\alpha}_{mii;j\sigma}(\omega)\} \quad (5.215)$$

Now we will specialize to the limit of infinitely narrow bands (**atomic limit**)

$$\varepsilon(\vec{k}) = t_0 \quad \Leftrightarrow \quad t_{ij} = t_0\delta_{ij} \quad (5.216)$$

Then the equation of motion hierarchy decouples and (5.215) simplifies to

$$(\omega + \mu - U - T_0)\Gamma^{\alpha}_{iii;j\sigma}(\omega) = \delta_{ij}\langle n_{\bar{\sigma}}\rangle \quad (5.217)$$

Translation symmetry implies lattice site independence of the particle number operator: $\langle n_{i\sigma}\rangle = \langle n_{\sigma}\rangle \forall i$. Eq. (5.217) can now be inserted in Eq. (5.213):

$$(\omega + \mu - t_0)G^{\alpha}_{ii\sigma} = 1 + \frac{U\langle n_{\bar{\sigma}}\rangle}{\omega - t_0 + \mu - U} \quad (5.218)$$

Then we have for the retarded Green's function

$$G^r_{ii\sigma}(\omega) = \frac{1 - \langle n_{\bar{\sigma}}\rangle}{\omega - t_0 + \mu + i0^+} + \frac{\langle n_{\bar{\sigma}}\rangle}{\omega - t_0 - U + \mu + i0^+} \quad (5.219)$$

Thus, $G^r_{ii\sigma}(\omega)$ has two poles corresponding to the excitation energies:

$$\begin{aligned} \omega_{1\sigma} &= t_0 - \mu = \omega_{1\bar{\sigma}} \\ \omega_{2\sigma} &= t_0 + U - \mu = \omega_{2\bar{\sigma}} \end{aligned} \quad (5.220)$$

The original level at t_0 splits, due to the Coulomb repulsion, into two spin independent quasiparticle levels $\omega_{1\sigma}$, $\omega_{2\sigma}$. The spectral density can be easily calculated as $S_{ii\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^r_{ii\sigma}(\omega)$ to be

$$S_{ii\sigma}(\omega) = \sum_{j=1}^{2} \alpha_{j\sigma}\delta(\omega - \omega_{j\sigma}) \quad (5.221)$$

The spectral weights

$$\alpha_{1\sigma} = 1 - \langle n_{\bar{\sigma}}\rangle\,; \quad \alpha_{2\sigma} = \langle n_{\bar{\sigma}}\rangle \quad (5.222)$$

measure the probability that a σ electron meets a $\bar{\sigma}$ electron at a site ($\alpha_{2\sigma}$) or that it finds an unoccupied site ($\alpha_{1\sigma}$). In the first case it has to pay the Coulomb interaction U. The quasiparticle density of states consists in this limit of two infinitely narrow bands at the energies t_0 and $t_0 + U$:

$$\begin{aligned} \rho_{\sigma}(\omega) &= \frac{1}{N}\sum_i S_{ii\sigma}(\omega - \mu) = S_{ii\sigma}(\omega - \mu) \\ &= (1 - \langle n_{\bar{\sigma}}\rangle)\delta(\omega - t_0) + \langle n_{\bar{\sigma}}\rangle\delta(\omega - t_0 - U) \end{aligned} \quad (5.223)$$

The lower band contains $(1 - \langle n_{\bar{\sigma}} \rangle)$, the upper $\langle n_{\bar{\sigma}} \rangle$ states per atom. Thus the number of states in the quasiparticle subbands is temperature dependent. Now we have to determine the expectation value $\langle n_{\bar{\sigma}} \rangle$ using the spectral theorem (2.100):

$$\langle n_{\bar{\sigma}} \rangle = \int_{-\infty}^{\infty} d\omega \frac{S_{ii\bar{\sigma}}(\omega)}{e^{\beta\omega} + 1} = \big(1 - \langle n_{\sigma} \rangle\big) f_{-}(t_0) + \langle n_{\sigma} \rangle f_{-}(t_0 + U) \tag{5.224}$$

with Fermi function $f_{-}(\omega)$. Using the corresponding equation for $\langle n_{\bar{\sigma}} \rangle$, we find

$$\langle n_{\bar{\sigma}} \rangle = \frac{f_{-}(t_0)}{1 + f_{-}(t_0) - f_{-}(t_0 + U)} \tag{5.225}$$

Then the complete solution for $\rho_{\sigma}(\omega)$ is

$$\rho_{\sigma}(\omega) = \frac{1}{1 + f_{-}(t_0) - f_{-}(t_0 + U)} \big\{ \big(1 - f_{-}(t_0 + U)\big) \delta(\omega - t_0) + f_{-}(t_0) \delta(\omega - t_0 - U) \big\} \tag{5.226}$$