3. Greens functions

3.1 Introduction

Greens 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

$$H = H_0 + V_t \tag{3.1}$$

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:

$$V_t = \hat{B} F_t \tag{3.2}$$

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

$$\langle \hat{A} \rangle_0 = \mathrm{Tr}(\rho_0 \hat{A}) \tag{3.3}$$

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

$$\rho_0 = \frac{e^{-\beta \mathcal{H}}}{\mathrm{Tr} e^{-\beta \mathcal{H}}} \tag{3.4}$$

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:

$$\rho_0 \to \rho_t \tag{3.5}$$

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

$$\langle \hat{A} \rangle_t = \mathrm{Tr}(\rho_t \hat{A}) \tag{3.6}$$

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

$$i\hbar \frac{\partial \rho_t}{\partial t} = \big[\mathcal{H} + V_t, \rho_t\big] \tag{3.7}$$

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 $t \to -\infty$

$$\lim_{t \to -\infty} \rho_t = \rho_0 \,. \tag{3.8}$$

We now switch to the Dirac picture where we have

$$\rho_t^D(t) = e^{\frac{i}{\hbar}\mathcal{H}_0 t} \rho_t e^{-\frac{i}{\hbar}\mathcal{H}_0 t} \tag{3.9}$$

with the equation of motion

$$\rho_t^D(t) = \frac{i}{\hbar} \big[\rho_t^D, V_t^D\big]_-(t) \,. \tag{3.10}$$

Integrating with the boundary condition

$$\lim_{t \to \infty} \rho_t^D(t) = \rho_0 \tag{3.11}$$

leads to

$$\rho_t^D(t) = \rho_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \big[V_{t'}^D(t'), \rho_{t'}^D(t')\big]_- \tag{3.12}$$

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

$$\begin{aligned} \rho_t^D(t) &= \rho_0 + \sum_{n=1}^{\infty} \rho_t^{D(n)}(t) \qquad \text{with} \\ \rho_t^{D(n)}(t) &= \Big(-\frac{i}{\hbar}\Big)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n \\ &\quad \times \big[V_{t_1}^D(t_1), \big[V_{t_2}^D(t_2), \big[\cdots \big[V_{t_n}^D(t_n), \rho_0\big] \cdots\big]_-\big]_-\big]_- \end{aligned} \tag{3.13}$$

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**:

$$\rho_t \approx \rho_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\big[V^D_{t'}(t'),\rho_0\big]_- e^{\frac{i}{\hbar}\mathcal{H}_0 t} \tag{3.14}$$

Here, we have returned to the Schrödinger representation for the density matrix. We can use this result to determine the perturbed expectation value of (3.6):

$$\begin{aligned}\langle\hat{A}\rangle_t = \mathrm{Tr}(\rho_t\hat{A}) &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\,\mathrm{Tr}\Big\{e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\big[V^D_{t'}(t'),\rho_0\big]_- e^{\frac{i}{\hbar}\mathcal{H}_0 t}\hat{A}\Big\}\\ &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\,F_{t'}\mathrm{Tr}\underbrace{\Big\{\big[\hat{B}^D(t'),\rho_0\big]_-\hat{A}^D(t)\Big\}}_{=\hat{B}\rho_0\hat{A}-\rho_0\hat{B}\hat{A}=\rho_0\hat{A}\hat{B}-\rho_0\hat{B}\hat{A}}\\ &= \langle\hat{A}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\,F_{t'}\mathrm{Tr}\Big\{\rho_0\big[\hat{A}^D(t),\hat{B}^D(t')\big]_-\Big\}\end{aligned} \tag{3.15}$$

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

$$\Delta A_t = \langle\hat{A}\rangle_t - \langle\hat{A}\rangle_0 = -\frac{i}{\hbar}\int_{-\infty}^{t} dt'\,F_{t'}\langle[\hat{A}^D(t),\hat{B}^D(t')]_-\rangle_0 \tag{3.16}$$

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

$$G^r_{AB}(t,t') = \langle\langle A(t);B(t')\rangle\rangle = -i\Theta(t,t')\big\langle\big[A(t),B(t')\big]_-\big\rangle_0 \tag{3.17}$$

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

$$\Delta A_t = -\frac{1}{\hbar}\int_{-\infty}^{\infty} dt'\,F_{t'}G^r_{AB}(t,t') \tag{3.18}$$

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

$$F_t = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, F(\omega) e^{-i(\omega+i\delta)t} \tag{3.19}$$

where $\delta > 0$ is infinitesimally small and using the later result that with a Hamiltonian that is not explicitly time dependent the Greens function depends only on time differences $t - t'$, we can rewrite (3.18) in the form of the **Kubo formula**

$$\Delta A_t = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} d\omega\, F(\omega) G^r_{AB}(\omega + i\delta) e^{-i(\omega+i\delta)t} \tag{3.20}$$

The $\delta > 0$ in the exponent enforces the boundary condition (3.8).
We will now look into two applications of response functions.

Magnetic Susceptibility

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

$$B_t = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, B(\omega) e^{-i(\omega+i\delta)t}\,, \tag{3.21}$$

which couples to the magnetic moment

$$\vec{m} = \sum_i m_i = \frac{g\mu_B}{\hbar}\sum_i \vec{S}_i\,. \tag{3.22}$$

Thus, the perturbing potential term in the Hamiltonian becomes

$$V_t = -\vec{m}\cdot\vec{B}_t = -\frac{1}{2\pi}\sum_\alpha \int_{-\infty}^{\infty} d\omega\, m^\alpha B^\alpha(\omega) e^{-i(\omega+i\delta)t} \tag{3.23}$$

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

$$\vec{M} = \frac{1}{V}\langle\vec{m}\rangle = \frac{g\mu_B}{\hbar V}\sum_i \langle\vec{S}_i\rangle\,, \tag{3.24}$$

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

$$M^\beta_t - M^\beta_0 = -\frac{1}{V}\sum_\alpha \int_{-\infty}^{\infty} dt'\, B^\alpha_{t'} \left\langle\!\!\left\langle m^\beta(t); m^\alpha(t')\right\rangle\!\!\right\rangle\,. \tag{3.25}$$

Only in a ferromagnet there is a finite magnetization M_0^β without a field. Eq. (3.25) defines the **magnetic susceptibility tensor**

$$\chi_{ij}^{\beta\alpha}(t,t') = -\frac{\mu_0}{V}\frac{g\mu_B^2}{\hbar^2}\langle\langle S_i^\beta(t); S_j^\alpha(t')\rangle\rangle \tag{3.26}$$

as a retarded Greens function. Thus

$$\Delta M_t^\beta = \frac{1}{\mu_0}\sum_{ij}\int_{-\infty}^{\infty} dt'\, B_{t'}^\alpha \chi_{ij}^{\beta\alpha}(t,t') \tag{3.27}$$

or in terms of frequency

$$\Delta M_t^\beta = \frac{1}{2\pi\mu_0}\sum_{ij}\sum_{\alpha}\int_{-\infty}^{\infty} d\omega\, e^{-i(\omega+i\delta)t}\chi_{ij}^{\beta\alpha}(\omega)B^\alpha(\omega) \tag{3.28}$$

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

$$\chi_{ij}^{zz}(\omega) = \frac{\mu_0}{V}\frac{g\mu_B^2}{\hbar^2}\langle\langle S_i^z; S_j^z\rangle\rangle_\omega \tag{3.29}$$

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

$$\chi_{\vec{q}}^{zz}(\omega) = \frac{1}{N}\sum_{ij}\chi_{ij}^{zz}(\omega)e^{i\vec{q}\cdot\left(\vec{R}_i-\vec{R}_j\right)} \tag{3.30}$$

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

$$\left\{\lim_{(\vec{q},\omega)\to\infty}\chi_{\vec{q}}^{zz}(\omega)\right\}^{-1} = 0 \tag{3.31}$$

are studied; they indicate the paramagnetic $\leftrightarrow$ ferromagnetic transition.
The other interesting case is the **transversal susceptibility**

$$\chi_{ij}^{+-}(\omega) = -\frac{\mu_0}{V}\frac{g\mu_B^2}{\hbar^2}\langle\langle S_i^+; S_j^-\rangle\rangle_\omega \quad \text{where} \quad S_i^\pm = S_i^x \pm iS_i^y \tag{3.32}$$

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

$$\left\{\chi^{+-}_{\vec{q}}(\omega)\right\}^{-1} = 0 \Longleftrightarrow \omega = \omega(\vec{q})\,. \tag{3.33}$$

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:

$$\vec{E}_t = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \vec{E}(\omega) e^{-i(\omega+i\delta)t}\,. \tag{3.34}$$

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

$$\vec{P} = \int d^3r\, \vec{r} n(\vec{r})\,. \tag{3.35}$$

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

$$n(\vec{r}) = \sum_{i=1}^{N} q_i \delta(\vec{r} - \vec{r}_i)\,. \tag{3.36}$$

This gives a dipole moment operator

$$\vec{P} = \sum_{i=1}^{N} q_i \vec{r}_i\,. \tag{3.37}$$

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

$$V_t = -\vec{P}\cdot\vec{E}_t = -\frac{1}{2\pi}\sum_{\alpha}\int_{-\infty}^{\infty} d\omega\, P^{\alpha} E^{\alpha}(\omega) e^{-i(\omega+i\delta)t}\,. \tag{3.38}$$

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

$$\vec{j} = \frac{1}{V}\sum_{i=1}^{N} q_i \vec{r}_i = \frac{1}{V}\vec{P}\,. \tag{3.39}$$

Its expectation value without field disappears:

$$\langle \vec{j} \rangle_0 = 0\,. \tag{3.40}$$

After switching the field on, we have

$$\langle j^\beta \rangle_t = -\frac{1}{\hbar} \sum_\alpha \int_{-\infty}^{\infty} dt'\, E^\alpha_{t'} \langle\langle j^\beta(t); P^\alpha(t') \rangle\rangle\,. \tag{3.41}$$

In terms of the Fourier transforms this becomes

$$\langle j^\beta \rangle_t = \frac{1}{2\pi} \sum_\alpha \int_{-\infty}^{\infty} d\omega\, e^{-i(\omega+i\delta)t} \sigma^{\beta\alpha}(\omega) E^\alpha(\omega) \tag{3.42}$$

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

$$\sigma^{\beta\alpha}(\omega) \equiv -\langle\langle j^\beta; P^\alpha \rangle\rangle_\omega \tag{3.43}$$

that has retarded Greens functions as components. This can be rewritten as

$$\sigma^{\beta\alpha}(\omega) = i\frac{N}{V}\frac{q^2}{m(\omega+i\delta)}\delta_{\alpha\beta} + \frac{i}{\hbar}\frac{\langle\langle j^\beta; j^\alpha \rangle\rangle}{\omega+i\delta} \tag{3.44}$$

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 Greens function represents the interaction between the particles.

3.2 Matsubara method

In the solid state theory class, Greens functions were introduced as response functions; they can be used to determine the quasiparticle density of states. They also appear as correlation functions, and they give us access to excitation energies. But so far, everything was done at zero temperature. The ojective is now to extend the methods for $T = 0$ to finite temperatures.[1] As a reminder, the two-time Greens functions were defined as (with $\varepsilon = -1$ for fermionic operators, $\varepsilon = +1$ for bosonic operators)

$$\begin{aligned}
\text{retarded:} \quad & G^r_{AB}(t,t') \equiv \langle\langle A(t); B(t') \rangle\rangle^r = -i\theta(t-t')\langle [A(t), B(t')]_{-\varepsilon} \rangle \\
\text{advanced:} \quad & G^a_{AB}(t,t') \equiv \langle\langle A(t); B(t') \rangle\rangle^a = i\theta(t-t')\langle [A(t), B(t')]_{-\varepsilon} \rangle \\
\text{causal:} \quad & G^c_{AB}(t,t') \equiv \langle\langle A(t); B(t') \rangle\rangle^c = -i\langle T_\varepsilon(A(t)B(t')) \rangle
\end{aligned}$$

[1] This chapter is based on K. Elk, W. Gasser, *"Die Methode der Greenschen Funktionen in der Festkörperphysik"*, Akademie-Verlag Berlin 1979, and W. Nolting, *"Grundkurs Theoretische Physik 7, Viel-Teilchen-Theorie"*, Springer 2009.

(3.45)

with the Wick time ordering operator T_ε:

$$T_\varepsilon(A(t)B(t')) = \theta(t-t')A(t)B(t') + \varepsilon\theta(t'-t)B(t')A(t) \tag{3.46}$$

$\langle \dots \rangle$ indicates an average over the grand canonical ensemble

$$\langle X\rangle = \frac{\mathrm{Tr}(e^{-\beta\mathcal{H}}X)}{\mathrm{Tr}(e^{-\beta\mathcal{H}})} \qquad \text{where } \beta = \frac{1}{k_B T},\quad \mathcal{H} = H - \mu N \tag{3.47}$$

If the Hamiltonian has no explicit time dependence, the Greens functions are homogeneous in time:

$$\frac{\partial\mathcal{H}}{\partial t} = 0 \Rightarrow G^\alpha_{AB}(t,t') = G^\alpha_{AB}(t-t')\,, \qquad \alpha = r, a, c \tag{3.48}$$

This can be shown using the cyclic invariance of the trace.
For the correlation functions that are needed for G^r and G^a, we have

$$\begin{aligned}\langle (A(t)B(t')\rangle &= \langle A(t-t')B(0)\rangle = \langle A(0)B(t'-t)\rangle \\ \langle (B(t')A(t)\rangle &= \langle B(t'-t)A(0)\rangle = \langle B(0)A(t-t')\rangle\end{aligned} \tag{3.49}$$

We now allow the time variables to formally take complex values:

$$\begin{aligned}\mathrm{Tr}e^{-\beta\mathcal{H}}\langle A(t-i\hbar\beta)B(t')\rangle &= \mathrm{Tr}\{e^{-\beta\mathcal{H}}e^{\frac{i}{\hbar}\mathcal{H}(t-i\hbar\beta)}A(0)e^{-\frac{i}{\hbar}\mathcal{H}(t-i\hbar\beta)}B(t')\} \\ &= \mathrm{Tr}\{B(t')e^{-\beta\mathcal{H}}e^{+\beta\mathcal{H}}e^{\frac{i}{\hbar}\mathcal{H}t}A(0)e^{-\frac{i}{\hbar}\mathcal{H}t}e^{-\beta\mathcal{H}}\} \\ &= \mathrm{Tr}\{e^{-\beta\mathcal{H}}B(t')A(t)\} \\ \Rightarrow \langle A(t-i\hbar\beta)B(t')\rangle &= \langle B(t')A(t)\rangle\end{aligned} \tag{3.50}$$

As two different correlation functions become related in this way, the extension of the Greens function to complex time seems to be advantageous. In particular, in perturbation theory in V where $\mathcal{H} = \mathcal{H}_0 + V$, V would, for finite temperatures, appear in two places, in the Heisenberg representation of time dependent operators $e^{\pm\frac{i}{\hbar}\mathcal{H}t}$ and in the density operator of the grand canonical averaging $e^{-\beta\mathcal{H}}$; two perturbation expansions would be necessary. Therefore, we join the exponential functions by introducing a complex time.
The Matsubara method introduces purely imaginary times so that the quantity $\tau = it$ is real. This leads to a modified Heisenberg representation of operators:

$$A(\tau) = e^{\frac{1}{\hbar}\mathcal{H}\tau}A(0)e^{-\frac{1}{\hbar}\mathcal{H}\tau} \tag{3.51}$$

Note that the operator $e^{\frac{i}{\hbar}\mathcal{H}\tau}$ creating imaginary time shifts is not unitary. The equation of motion (EOM) for an operator $A(\tau)$

$$-\hbar\frac{\partial}{\partial\tau}A(\tau) = -\hbar\frac{\partial}{\partial\tau}\Big[e^{\frac{1}{\hbar}\mathcal{H}\tau}A(0)e^{-\frac{1}{\hbar}\mathcal{H}\tau}\Big] = -\mathcal{H}A(\tau) + A(\tau)\mathcal{H} \quad (3.52)$$

thus becomes:

$$-\hbar\frac{\partial}{\partial\tau}A(\tau) = \big[A(\tau),\mathcal{H}\big]_- \quad (3.53)$$

Here, we use the (conventional) step function

$$\theta(\tau) = \begin{cases} 1 & \text{for } \tau > 0 \ (t = -\tau i \text{ negative imaginary}) \\ 0 & \text{for } \tau < 0 \ (t = |\tau| i \text{ positive imaginary}) \end{cases} \quad (3.54)$$

It can be used to introduce the time ordering operator.

$$T_\tau\big\{A(\tau)B(\tau')\big\} = \theta(\tau-\tau')A(\tau)B(\tau') + \varepsilon^p\theta(\tau'-\tau)B(\tau')A(\tau) \quad (3.55)$$

where p is the number of permutations of creation operators. We assume pure Fermi/Bose operators so that $p = 1$.
The definition of the Matsubara function is:

$$G^M_{AB}(\tau,\tau') = \langle\langle A(\tau); B(\tau')\rangle\rangle^M = -\langle T_\tau(A(\tau)B(\tau'))\rangle \quad (3.56)$$

Using (3.53) and (3.55) we get the EOM

$$-\hbar\frac{\partial}{\partial\tau}G^M_{AB}(\tau,\tau') = \hbar\delta(\tau-\tau')\langle[A,B]_{-\varepsilon}\rangle + \langle\langle[A(\tau),\mathcal{H}]_-; B(\tau')\rangle\rangle \quad (3.57)$$

Properties of the Matsubara Greens function introduced in this way are:
1) it depends only on time differences

$$G^M_{AB}(\tau,\tau') = G^M_{AB}(\tau-\tau',0) = G^M_{AB}(0,\tau'-\tau) \quad (3.58)$$

2) it is periodic in time: Take $\hbar\beta > \tau - \tau' + n\hbar\beta > 0$, $n \in \mathbb{Z}$; then

$$\begin{aligned}
&\mathrm{Tr} e^{-\beta\mathcal{H}} G^M_{AB}(\underbrace{\tau - \tau' + n\hbar\beta}_{>0}) \\
&= -\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} T_\tau\big(A(\tau - \tau' + n\hbar\beta)B(0)\big)\big\} \\
&= -\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} A(\tau - \tau' + n\hbar\beta)B(0)\big\} \\
&= -\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} e^{\frac{\mathcal{H}}{\hbar}(\tau-\tau'+n\hbar\beta)} A(0) e^{-\frac{\mathcal{H}}{\hbar}(\tau-\tau'+n\hbar\beta)} B(0)\big\} \\
&= -\mathrm{Tr}\big\{e^{\frac{\mathcal{H}}{\hbar}(\tau-\tau'+(n-1)\hbar\beta)} A(0) e^{-\frac{\mathcal{H}}{\hbar}(\tau-\tau'+(n-1)\hbar\beta)} e^{-\beta\mathcal{H}} B(0)\big\} \\
&= -\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} B(0) A(\underbrace{\tau - \tau' + (n-1)\hbar\beta)}_{<0}\big\} \\
&= -\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} T_\tau\big(B(0)A(\tau - \tau' + (n-1)\hbar\beta)\big)\big\} \\
&= -\varepsilon\mathrm{Tr}\big\{e^{-\beta\mathcal{H}} T_\tau\big(A(\tau - \tau' + (n-1)\hbar\beta)B(0)\big)\big\} \qquad (3.59)
\end{aligned}$$

This gives us the important result:

$$\hbar\beta > \tau - \tau' + n\hbar\beta > 0: \quad G^M_{AB}\big(\tau - \tau' + n\hbar\beta\big) = \varepsilon G^M_{AB}\big(\tau - \tau' + (n-1)\hbar\beta\big) \qquad (3.60)$$

In particular, for $n = 1$:

$$G^M_{AB}\big(\tau - \tau' + \hbar\beta\big) = \varepsilon G^M_{AB}\big(\tau - \tau'\big) \qquad \text{for } -\hbar\beta < \tau - \tau' < 0 \qquad (3.61)$$

Thus the Matsubara Greens function is periodic in an interval $2\hbar\beta$; it is enough to consider the time interval $-\hbar\beta < \tau - \tau' < 0$. This periodicity allows the Fourier expansion:

$$\begin{aligned}
G^M(\tau) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\Big[a_n \cos\frac{n\pi}{\hbar\beta}\tau + b_n \sin\frac{n\pi}{\hbar\beta}\tau\Big] \\
a_n &= \frac{1}{\hbar\beta}\int_{-\hbar\beta}^{\hbar\beta} d\tau\, G^M(\tau)\cos\Big(\frac{n\pi}{\hbar\beta}\tau\Big) \\
b_n &= \frac{1}{\hbar\beta}\int_{-\hbar\beta}^{\hbar\beta} d\tau\, G^M(\tau)\sin\Big(\frac{n\pi}{\hbar\beta}\tau\Big) \qquad (3.62)
\end{aligned}$$

Now we define discrete energies

$$E_n = \frac{n\pi}{\beta} \qquad (3.63)$$

and the Matsubara Greens function on the imaginary energy (frequency) axis

$$G(E_n) = \frac{1}{2}\hbar\beta(a_n + ib_n) \qquad (3.64)$$

Then

$$G^M(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n\tau}G^M(E_n)$$
$$G^M(E_n) = \frac{1}{2}\int_{-\hbar\beta}^{\hbar\beta} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} \tag{3.65}$$

Still, we can simplify a bit more:

$$\begin{aligned} G^M(E_n) &= \frac{1}{2}\int_0^{\hbar\beta} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} + \frac{1}{2}\int_{-\hbar\beta}^{0} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} \\ &= \frac{1}{2}\int_0^{\hbar\beta} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} + \frac{1}{2}\int_0^{\hbar\beta} d\tau\, G^M(\tau'-\hbar\beta)e^{\frac{i}{\hbar}E_n\tau'}e^{-iE_n\beta} \\ &= \left[1+\varepsilon e^{-iE_n\beta}\right]\frac{1}{2}\int_0^{\hbar\beta} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} \end{aligned} \tag{3.66}$$

where $\tau' = \tau + \hbar\beta$ was introduced. The bracket $[\ldots]$ disappears for fermions ($\varepsilon = -1$) if n is even, for bosons ($\varepsilon = 1$) if n is odd. Thus

$$G^M(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n\tau}G^M(E_n)$$
$$G^M(E_n) = \int_0^{\hbar\beta} d\tau\, G^M(\tau)e^{\frac{i}{\hbar}E_n\tau} \tag{3.67}$$

with

$$E_n = \begin{cases} 2n\frac{\pi}{\beta} & \text{for bosons} \\ (2n+1)\frac{\pi}{\beta} & \text{for fermions} \end{cases} \tag{3.68}$$

Now we need to work out a spectral representation for the Matsubara Greens function in order to relate it to the retarded Greens function. We first consider the correlation function

$$\begin{aligned} \langle A(\tau)B(0)\rangle &= \frac{1}{\mathrm{Tr}e^{-\beta\mathcal{H}}}\sum_n \langle E_n|A(\tau)B(0)|E_n\rangle e^{-\beta E_n} \\ &= \frac{1}{\mathrm{Tr}e^{-\beta\mathcal{H}}}\sum_n \langle E_n|A|E_m\rangle\langle E_m|B|E_n\rangle e^{-\beta E_n}e^{-\frac{1}{\hbar}(E_n-E_m)\tau} \end{aligned} \tag{3.69}$$

where we introduced the eigenstates of the Hamiltonian $|E_n\rangle$: $\mathcal{H}|E_n\rangle = E_n|E_n\rangle$. We recall the spectral density on the real energy axis:

$$S_{AB}(E) = \frac{\hbar}{\mathrm{Tr}e^{-\beta\mathcal{H}}} \sum_{n,m} \langle E_n|A|E_m\rangle\langle E_m|B|E_n\rangle e^{-\beta E_n}(1-\varepsilon e^{-\beta E})\delta\big(E-(E_m-E_n)\big)$$

$$\curvearrowright \langle A(\tau)B(0)\rangle = \frac{1}{\hbar}\int_{-\infty}^{\infty} dE \frac{S_{AB}(E)}{1-\varepsilon e^{-\beta E}} e^{-\frac{1}{\hbar}E\tau} \tag{3.70}$$

In the integration interval in (3.67), τ is positive; we need to evaluate

$$G^M_{AB}(E_n) = -\int_0^{\hbar\beta} d\tau\, e^{\frac{i}{\hbar}E_n\tau}\langle A(\tau)B(0)\rangle \tag{3.71}$$

Now we use the integral

$$\int_0^{\hbar\beta} d\tau\, e^{\frac{1}{\hbar}(iE_n-E)\tau} = \frac{\hbar}{iE_n-E}\big(e^{i\beta E_n}e^{-\beta E}-1\big) = \frac{\hbar}{iE_n-E}\big(\varepsilon e^{-\beta E}-1\big) \tag{3.72}$$

and put Eq. (3.70) into Eq. (3.71) to obtain

$$G^M_{AB}(E_n) = \int_{-\infty}^{\infty} dE' \frac{S_{AB}(E')}{iE_n-E'} \tag{3.73}$$

If we compare this to the spectral representation of the retarded Greens function, we only need to replace $iE_n \to E+i0^+$; thus, the retarded Greens function can be obtained from the Matsubara Greens function by analytic continuation!

3.3 Some methods for Matsubara axis functions

- The Green's function on the Matsubara axis is fairly smooth and featureless so that the determination of the sums poses no problems. But there are two points to be considered:

(1) Terms falling off as $1/(i\omega_n)$ will be badly represented by any number of frequency points; therefore, high frequency corrections are needed.

(2) In order to obtain a spectral function, we need to analytically continue the Greens function to the real axis. This is done by the Padé method.

High frequency correction

The idea is to subtract the leading terms of the high frequency expansion and calculate them analytically, *e.g.*

$$F_m(i\omega_n) = \frac{1 - n_f + \frac{n_f}{N}}{i\omega_n} + O\Big(\frac{1}{(i\omega_n)^2}\Big) \tag{3.74}$$

$$\curvearrowright n_f = T\sum_{i\omega_n'}\left(F_m(i\omega_n') - \frac{1 - n_f + \frac{n_f}{N}}{i\omega_n'}\right)e^{i\omega_n' 0^+} + \frac{1 - n_f + \frac{n_f}{N}}{2} \tag{3.75}$$

The last term of Eq. (3.75) is obtained by explicit calculation of the sum:

$$\begin{aligned} T\sum_{n=-\infty}^{\infty}\frac{1}{i\omega_n}e^{i\omega_n\tau} &= T\sum_{n=0}^{\infty}\frac{2i\sin(\omega_n\tau)}{i\omega_n} \\ &= \frac{2}{\pi}\sum_{n=0}^{\infty}\frac{\sin\big[(2n+1)\pi T\tau\big]}{2n+1} = \frac{1}{2} \end{aligned} \tag{3.76}$$

because $\tau = 0^+ \in]0; 1/T[$ and

$$\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{\sin\big[(2n+1)x\big]}{2n+1} = \begin{cases} -1 & \text{for} \quad -\pi < x < 0 \\ 0 & \text{for} \quad x = -\pi, 0, \pi \\ 1 & \text{for} \quad 0 < x < \pi \end{cases} \tag{3.77}$$

In practice, the $1/(i\omega_n)^2$ is taken into account in the same way.

(2) Pade approximation

This method for analytic continuation can be used

1. when the function to be continued is not given analytically (in that case, use $i\omega_n \to \omega + i\delta$)
2. when the function is given without statistical errors (for Quantum Monte Carlo Green's functions, use Maximum Entropy Method)

One has to keep in mind one drawback of the Padé approximation: it is a polynomial representation that has limited precision for functions which are hard to approximate by a polynomial. It can show the wiggles that are typical for polynomial interpolations.
The algorithm for calculating the Padé approximant was written down nicely by Vidberg and Serene (H. J. Vidberg and J. W. Serene, Solving the

Eliashberg Equations by Means of N-Point Padé Approximants, J. Low Temp. Phys. **29**, 179 (1977)).
Given the values u_i of a function at N complex points $z_i (i = 1, \ldots, N)$, we define the continued fraction

$$C_N(z) = \cfrac{a_1}{1 + \cfrac{a_2(z - z_1)}{1 + \ldots a_N(z - z_{N-1})}} \tag{3.78}$$

Here, the coefficients a_i are to be determined so that

$$C_N(z_i) = u_i\,, \quad i = 1, \ldots, N \tag{3.79}$$

The coefficients are then given by the recursion

$$\begin{aligned} a_i &= g_i(z_i)\,, \quad g_1(z_i) = u_i\,, \quad i = 1, \ldots, N \\ g_p(z) &= \frac{g_{p-1}(z_{p-1}) - g_{p-1}(z)}{(z - z_{p-1}) g_{p-1}(z)}\,, \quad p \geqslant 2 \end{aligned} \tag{3.80}$$

This requires the following calculation:

$$\begin{aligned} & g_1(z_1) = a_1 = u_1 \quad g_1(z_2) = u_2 \quad g_1(z_3) = u_3 \quad g_1(z_4) = u_4 \ \ldots \\ & g_2(z) = \frac{g_1(z_1) - g_1(z)}{(z - z_1) g_1(z)} \quad g_2(z_2) = a_2 = \frac{a_1 - g_1(z_2)}{(z_2 - z_1) g_1(z_2)} = \frac{a_1 - u_2}{(z_2 - z_1) u_2} \\ & g_2(z_3) = \frac{a_1 - g_1(z_3)}{(z_3 - z_1) g_1(z_3)} = \frac{a_1 - u_3}{(z_3 - z_1) u_3} \quad g_2(z_4) = \frac{a_1 - u_4}{(z_4 - z_1) u_4} \ \ldots \\ & g_3(z) = \frac{g_2(z_2) - g_2(z)}{(z - z_2) g_2(z)} \quad g_3(z_3) = a_3 = \frac{a_2 - g_2(z_3)}{(z_3 - z_2) g_2(z_3)} \\ & g_3(z_4) = \frac{a_2 - g_2(z_4)}{(z_4 - z_2) g_2(z_4)} \ \ldots \\ & g_4(z) = \frac{g_3(z_3) - g_3(z)}{(z - z_3) g_3(z)} \quad g_4(z_4) = a_4 = \frac{a_3 - g_3(z_4)}{(z_4 - z_3) g_3(z_4)} \ \ldots \end{aligned} \tag{3.81}$$

Thus, the following triangular matrix $p_{i,j}$ has to be calculated:

	$j = 1$	$j = 2$	$j = 3$	$j = 4$	$\ldots$
$i = 1$	$a_1 = u_1$	u_2	u_3	u_4	$\ldots$
$i = 2$		a_2	$g_2(z_3)$	$g_2(z_4)$	$\ldots$
$i = 3$			a_3	$g_3(z_4)$	$\ldots$
$i = 4$				a_4	$\ldots$
$\ldots$					$\ldots$

This can be done as follows:

$$\begin{aligned} p_{1,j} &= u_j\,, \quad j = 1,\ldots,N \\ p_{i,j} &= \frac{p_{i-1,i-1} - p_{i-1,j}}{(z_j - z_{i-1})p_{i-1,j}}\,, \quad j = 2,\ldots,N \text{ and } i = 2,\ldots,j \end{aligned} \tag{3.82}$$

The diagonal of this matrix then contains the coefficients a_i which are needed for the recursion formula for $C_N(z)$:

$$\begin{aligned} C_N(z) &= \frac{A_N(z)}{B_N(z)} \\ \text{with} \quad A_{n+1}(z) &= A_n(z) + (z - z_n)\, a_{n+1} A_{n-1}(z) \\ B_{n+1}(z) &= B_n(z) + (z - z_n)\, a_{n+1} B_{n-1}(z) \\ \text{and} \quad A_0 = 0\,, &\quad A_1 = a_1\,, \quad B_0 = B_1 = 1 \end{aligned} \tag{3.83}$$

An important fact to keep in mind: the bigger you chose N, *i.e.* the more coefficients a_i you calculate, the bigger the numbers $A_N(z)$ and $B_N(z)$ are going to be for a given z. $N = 128$ will already lead to values of order 10^{115}.

Comparing functions on real and imaginary axes

For a first check if an analytic continuation makes sense, there are exact relations at zero frequency.
If a complex function is given around $z = 0$ as

$$f(z) = \alpha + \beta z + \gamma z^2 + \ldots \tag{3.84}$$

with complex coefficients $\alpha = \alpha' + i\alpha''$ etc., we can write it in terms of imaginary frequencies $i\omega_n$ as

$$f(i\omega_n) = \alpha' + i\alpha'' - \beta''\omega_n + i\beta'\omega_n - \gamma'\omega_n^2 - i\gamma''\omega_n^2 + \ldots \tag{3.85}$$

or of real frequencies as

$$f(\omega) = \alpha' + i\alpha'' + \beta'\omega + i\beta''\omega + \gamma'\omega^2 + i\gamma''\omega^2 + \ldots \tag{3.86}$$

and thus by comparing coefficients we find for the function value at zero

$$f(i\omega_n)|_{\omega_n=0} = f(\omega)|_{\omega=0} \tag{3.87}$$

For the derivatives of f we find

$$\frac{d}{d\omega_n} \operatorname{Re} f(i\omega_n)\Big|_{\omega_n=0} = -\frac{d}{d\omega} \operatorname{Im} f(\omega)\Big|_{\omega=0} \tag{3.88}$$

$$\frac{d}{d\omega_n}\,\mathrm{Im}\,f(i\omega_n)\Big|_{\omega_n=0} = \frac{d}{d\omega}\,\mathrm{Re}\,f(\omega)\Big|_{\omega=0} \tag{3.89}$$

$$\frac{d^2}{d\omega_n^2}\,\mathrm{Re}\,f(i\omega_n)\Big|_{\omega_n=0} = -\frac{d^2}{d\omega^2}\,\mathrm{Im}\,f(\omega)\Big|_{\omega=0} \tag{3.90}$$

$$\frac{d^2}{d\omega_n^2}\,\mathrm{Im}\,f(i\omega_n)\Big|_{\omega_n=0} = -\frac{d^2}{d\omega^2}\,\mathrm{Re}\,f(\omega)\Big|_{\omega=0} \tag{3.91}$$

Kramers Kronig relations

If the function we try to calculate is analytic in the upper complex plane as well as in the lower complex plane (this is the case for all response functions of physical systems) it must obey the Kramers-Kronig relation

$$g'(y) = -\,\mathrm{P}\int_{-\infty}^{\infty} \frac{dx}{\pi}\frac{g''(x)}{y-x} \tag{3.92}$$

where the notation $g(z) = g'(z) + ig''(z)$ is used. x, y are used for real, z and u for complex variables. This is the real-axis analog of the more general Cauchy integral formula

$$g(z) = \frac{1}{2\pi i}\oint du \frac{g(u)}{u-z} \tag{3.93}$$

which says that a holomorphic function defined on a disk is completely determined by its values on the boundary of the disk. Response functions are not analytic on the real axis, but otherwise we can deform the contour arbitrarily on the complex plane.
If g(z) falls off in infinity, we can write

$$g(z) = \int_{-\infty}^{\infty} \frac{dx}{2\pi i}\frac{[g(x+i\delta) - g(x-i\delta)]}{x-z} \tag{3.94}$$

which yields

$$g(z) = -\int_{-\infty}^{\infty} \frac{dx}{\pi}\frac{g''(x)}{z-x} \tag{3.95}$$

The real part of this equation is equal to Eq. (3.92).

The practical calculation of a Kramers Kronig transformation is straightforward but requires the subtraction of the divergent part. It will usually be implemented on a mesh from a to b large enough so that $g''(a)$ and $g''(b)$ are negligibly small.

Then

$$g'(y) = \int_a^b \frac{dx}{\pi} \frac{g''(x) - g''(y)}{x - y} + \frac{g''(y)}{\pi} \operatorname{Re}\left[\log(b - y) - \log(a - y)\right]$$

(3.96)

$$= \int_a^b \frac{dx}{\pi} \frac{g''(x) - g''(y)}{x - y} + \frac{g''(y)}{\pi} \log\left(\frac{b - y}{y - a}\right) \tag{3.97}$$

Now the integrand is smooth everywhere. At $x = y$ it should be estimated using the derivative $dg''(y)/dy$.

Kramers Kronig relations can become very useful if real or imaginary part of a Greens function are easier than the full function. Typically, the imaginary part falls off abruptly at the band edges and is exactly zero beyond. Then the imaginary part is perfectly suited for calculation on a mesh, but the corresponding real part only falls off as $1/\omega$.