Linear response theory and Green's functions

The linear response theory for a conductor in presence of an external electromagnetic field is given by the Kubo formula:

$$\sigma^{\alpha\beta}(\vec{r},\vec{r}\,';\omega) = \frac{ie^2}{\omega}\,\Pi^R_{\alpha\beta}(\vec{r},\vec{r}\,';\omega) + \frac{e^2 n(\vec{r})}{i\omega m}\,\delta(\vec{r}-\vec{r}\,')\,\delta_{\alpha\beta}$$

where

$$\Pi^R_{\alpha\beta}(\vec{r},\vec{r}\,';t-t') = -i\theta(t-t')\,\left\langle\left[\hat{J}_0^{\alpha}(\vec{r},t),\,\hat{J}_0^{\beta}(\vec{r}\,',t')\right]\right\rangle_0$$

and

$\langle\bullet\rangle_0$ is the thermal average $\frac{1}{Z}\mathrm{Tr}\{e^{-\beta H_0}\,\bullet\}$ with respect of the unperturbed Hamiltonian and $\hat{J}_0^{\alpha}(\vec{r},t)$ is the current (density) operator at position $\vec{r}$ and at time t in interaction picture. The formula above is of great generality – see QTKM1 for a derivation – . We will evaluate it with the help of Green's functions. We have already introduced the concept of SINGLE PARTICLE Green's functions in the previous section. To proceed we need a generalization of the concept to a many-body system: $G^{R,A}(\vec{r},\vec{r}\,';t) = \mp i\,\theta(\pm t)\langle\vec{r}\,|\,e^{-\hat{H}t/\hbar}\,|\,\vec{r}\,'\rangle$

single particle GF
$$G^{R,A}(\vec{r}\sigma t;\vec{r}\,'\sigma' t') = \langle\vec{r}\sigma|\,e^{-i\frac{\hat{H}}{\hbar}(t-t')}\,|\vec{r}\,'\sigma'\rangle\,(\mp i)\,\theta(\pm t\mp t')$$

The single particle Green's functions of many-body systems read:

single particle GF of a many body system
$$G^{R,A}(\vec{r}\sigma t;\vec{r}\,'\sigma' t') = \left\langle\left[\,\Psi_\sigma(\vec{r}t),\,\Psi^\dagger_{\sigma'}(\vec{r}\,'t')\right]_{B,F}\right\rangle$$

where $[\ ,\ ]_{B,F}$ represents a commutator (anticommutator) of the bosonic (fermionic) field operators $\psi_\sigma(\vec{r}t)$ $\psi^\dagger_{\sigma'}(\vec{r}'t')$. The time evolution of the field operators is in Heisenberg picture. The single particle GF and the one for a many-body system coincide for the free particle case.

The expression for the Green's function is usefully transformed into the interaction picture. We obtain in this way a systematic expansion in the interacting potential.

$$H = H_0 + V$$

$$i\partial_t |\hat{\psi}(t)\rangle = \hat{V}(t) |\hat{\psi}(t)\rangle \qquad \hat{A}(t) \equiv e^{iH_0 t} A e^{-iH_0 t}$$

$$|\hat{\psi}(t)\rangle = \hat{U}(t,t_0) |\hat{\psi}(t_0)\rangle \qquad \hat{U}(t,t_0) = T_t\left(\exp\left[-i\int_{t_0}^{t} dt' \, \hat{V}(t')\right]\right)$$

The interaction picture is not enough if we work at finite temperature. There is a mathematical method that facilitates the calculation of the Green's function that requires their definition on IMAGINARY TIME. Let's introduce for clarity the correlator:

$$C_{AB}(t,t') = -\langle A(t) B(t') \rangle$$

$$C_{AB}(t,t') = -\frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} A(t) B(t')\right] =$$

$$= -\frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} \hat{U}(0,t) \hat{A}(t) \hat{U}(t,t') \hat{B}(t') \hat{U}(t',0)\right]$$

proof:

$$A(t) = e^{+i(H_0+V)t} A \, e^{-i(H_0+V)t} = e^{iHt} e^{-iH_0 t} \hat{A}(t) e^{+iH_0 t} e^{-iHt}$$

By construction $\hat{U}(t,0) \equiv e^{+iH_0 t} e^{-iHt}$

$\langle \psi(t)|A|\psi(t)\rangle = \langle A\rangle$ and it remains the same in every picture

$$\langle \psi(t)| e^{-iH_0t} e^{iH_0t} A e^{-iH_0t} |\psi(t)\rangle = \langle \psi| e^{iHt} e^{-iH_0t} \hat{A}(t) e^{iH_0t} e^{-iHt} |\psi\rangle$$

$$\Rightarrow \quad |\hat{\psi}(t)\rangle \equiv e^{iH_0t} e^{-iHt} |\psi\rangle$$

$\hat{U}(t,0)$ is unitary.

$$A(t)B(t') = \hat{U}(0,t)\hat{A}(t)\hat{U}(t,0)\,\hat{U}(0,t')\hat{B}(t')\hat{U}(t',0)$$

$$\hat{U}(t,0)\hat{U}(0,t') = e^{iH_0t} e^{-iHt} e^{iHt'} e^{-iH_0t'} = e^{iH_0t} e^{-iH(t-t')} e^{-iH_0t'}$$

This last operator is the interaction picture evolution between t' and t

$$|\hat{\psi}(t')\rangle \equiv e^{iH_0t'} e^{-iHt'}|\psi\rangle \qquad e^{iH_0t} e^{-iH(t-t')} e^{-iH_0t'} |\hat{\psi}(t')\rangle =$$

$$|\hat{\psi}(t)\rangle \equiv e^{+iH_0t} e^{-iHt}|\psi\rangle \qquad = e^{iH_0t} e^{-iH(t-\cancel{t'})} \cancel{e^{-iH_0t'}} \cancel{e^{iH_0t'}} e^{-iHt'}|\psi\rangle = |\hat{\psi}(t)\rangle.$$

QED

As for real time one can define an imaginary time Heisenberg picture

$$A(\tau) \equiv e^{\tau H} A e^{-\tau H}$$

Similar to the interaction picture:

$$\hat{A}(\tau) \equiv e^{\tau H_0} A e^{-\tau H_0}$$

$$\hat{U}(t,t') = e^{\tau H_0} e^{-(\tau-\tau')H} e^{-\tau H_0} \qquad \partial_\tau \hat{U}(\tau,\tau') = e^{\tau H_0}(H_0 - H) e^{-(\tau-\tau')H} e^{-\tau' H_0}$$

$$= -\hat{V}(\tau)\,\hat{U}(\tau,\tau')$$

$$\Rightarrow \quad \hat{U}(\tau,\tau') = T_\tau \exp\left[-\int_{\tau'}^{\tau} d\tau''\, \hat{V}(\tau'')\right]$$

Now we are ready to see the simplification introduced by the imaginary time.

Let's consider:

$$\langle T_\tau A(\tau) B(\tau') \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H} T_\tau [A(\tau) B(\tau')] \right\}$$

$\tau > \tau'$ => the τ ordering leaves the operators in their order

$$\langle T_\tau [A(\tau) B(\tau')] \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} \hat{U}(\beta,0) \hat{U}(0,\tau) \hat{A}(\tau) \hat{U}(\tau,\tau') \hat{B}(\tau') \hat{U}(\tau',0) \right]$$

$$= \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} \hat{U}(\beta,\tau) \hat{A}(\tau) \hat{U}(\tau,\tau') \hat{B}(\tau') \hat{U}(\tau',0) \right]$$

$$= \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} T_\tau \left[\hat{U}(\beta,\tau) \hat{U}(\tau,\tau') \hat{U}(\tau',0) \hat{A}(\tau) \hat{B}(\tau') \right] \right\}$$

$$= \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} T_\tau \left[\hat{U}(\beta,0) \hat{A}(\tau) \hat{B}(\tau') \right] \right\}$$

$\tau < \tau'$ => $T_\tau [A(\tau) B(\tau')] = \pm B(\tau') A(\tau)$ ($\pm$ depends on the nature of the operators A and B)

$$\langle T_\tau [A(\tau) B(\tau')] \rangle = \pm \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} \hat{U}(\beta,0) \hat{U}(0,\tau') \hat{B}(\tau') \hat{U}(\tau',\tau) \hat{A}(\tau) \hat{U}(\tau,0) \right\}$$

$$= \pm \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} T_\tau \left[\hat{U}(\beta,0) \hat{B}(\tau') \hat{A}(\tau) \right] \right\} =$$

$$= \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} T_\tau \left[\hat{U}(\beta,0) \hat{A}(\tau) \hat{B}(\tau') \right] \right\} = \frac{\langle T_\tau [\hat{U}(\beta,0) \hat{A}(\tau) \hat{B}(\tau')] \rangle_0}{\langle \hat{U}(\beta,0) \rangle_0}$$

The imaginary time Green's function (also called <u>Matsubara</u> GF) is defined:

$$C_{AB}(\tau,\tau') \equiv - \langle T_\tau [A(\tau) B(\tau')] \rangle$$

$$T_\tau [A(\tau) B(\tau')] = \theta(\tau-\tau') A(\tau) B(\tau') \pm \theta(\tau'-\tau) B(\tau') A(\tau)$$

Which values can τ and τ' have?

① $$C_{AB}(\tau,\tau') = C_{AB}(\tau-\tau')$$

proof: $\tau > \tau'$

$$C_{AB}(\tau,\tau') = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} e^{\tau H} A\, e^{-\tau H} e^{\tau' H} B\, e^{-\tau' H}\right]$$

cyclic property of trace plus trivial commutation

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} e^{(\tau-\tau')H} A\, e^{-(\tau-\tau')H} B\right]$$

$$= C_{AB}(\tau-\tau')$$

$\tau < \tau'$ analogous.

② Convergence is guaranteed only for $-\beta < \tau-\tau' < \beta$ as it is clearly seen using Lehmann representation. $(\tau > \tau')$

$$C_{AB}(\tau,\tau') = -\frac{1}{Z}\sum_{nm} e^{-\beta E_n} e^{(\tau-\tau')E_n} A_{nm}\, e^{-(\tau-\tau')E_m} B_{mn}$$

and likewise the second inequality for $\tau<\tau'$

③ $\tau < 0$ $$C_{AB}(\tau) = \pm\, C_{AB}(\tau+\beta)$$

$$C_{AB}(\tau+\beta) = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} e^{(\tau+\beta)H} A\, e^{-(\tau+\beta)H} B\right] =$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{\tau H} A\, e^{-\tau H} e^{-\beta H} B\right] =$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} B\, e^{\tau H} A\, e^{-\tau H}\right] =$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} B\, A(\tau)\right] =$$

$$= \pm\, C_{AB}(\tau)$$

Analogously with $\tau > 0$

Since the Matsubara GF is defined only in the "time" interval $-\beta < \tau < \beta$ => it has a discrete Fourier transform

$$C_{AB}(n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau)$$

$$C_{AB}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{+\infty} e^{-i\pi n\tau/\beta}\, C_{AB}(n)$$

Due to the symmetry property under translation of β for $C_{AB}(\tau)$

$$C_{AB}(n) = \frac{1}{2}\int_0^{\beta} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau) + \frac{1}{2}\int_{-\beta}^{0} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau)$$

$$= \frac{1}{2}\int_0^{\beta} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau) \pm \frac{1}{2}\int_{-\beta}^{0} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau+\beta)$$

$$= \frac{1}{2}\int_0^{\beta} d\tau\, e^{i\pi n\tau/\beta}\, C_{AB}(\tau) \pm \frac{1}{2}\int_0^{\beta} d\tau'\, e^{i\pi n(\tau'-\beta)/\beta}\, C_{AB}(\tau')$$

$$= \frac{1}{2}\left(1 \pm e^{-i\pi n}\right)\int_0^{\beta} e^{i\pi n\tau/\beta}\, C_{AB}(\tau)\, d\tau$$

=> bosons have only even components (n = even) and fermions only odd components (n = odd). In both cases:

$$C_{AB}(n) = \int_0^{\beta} e^{i\pi n\tau/\beta}\, C_{AB}(\tau)\, d\tau$$

Let's introduce a more suggestive notation:

$$C_{AB}(n) \rightarrow C_{AB}(i\omega_n) = \int_0^{\beta} d\tau\, e^{i\omega_n\tau}\, C_{AB}(\tau) \qquad \begin{cases} \omega_n = \dfrac{2n\pi}{\beta} & \text{for bosons} \\[2mm] \omega_n = \dfrac{(2n+1)\pi}{\beta} & \text{for fermions} \end{cases}$$

Now we shall see why at all we have introduced the Matsubara Green's functions.

The answer is that there is an analytic function $C_{AB}(z)$ that is equal to $C_{AB}(i\omega_n)$ on the imaginary axis and $C^{R,A}(\omega)$ in the vicinity of the real axis.

proof Let's consider the Lehmann representation of $C^R_{AB}(\omega)$

$$C^R_{AB}(\omega) = \frac{1}{Z}\sum_{mm'} \frac{\langle m|A|m'\rangle\langle m'|B|m\rangle}{\omega + E_m - E_{m'} + i\eta}\left(e^{-\beta E_m} - (\pm)\, e^{-\beta E_{m'}}\right)$$

$$C_{AB}(\tau) = -\frac{1}{Z}\sum_{mm'} e^{-\beta E_m}\langle m|A|m'\rangle\langle m'|B|m\rangle\, e^{\tau(E_m - E_{m'})}$$

$$\Rightarrow \quad C_{AB}(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\,\frac{-1}{Z}\sum_{mm'} e^{-\beta E_m}\langle m|A|m'\rangle\langle m'|B|m\rangle e^{\tau(E_m - E_{m'})}$$

$$= \frac{-1}{Z}\sum_{mm'} e^{-\beta E_m}\frac{\langle m|A|m'\rangle\langle m'|B|m\rangle}{i\omega_n + E_m - E_{m'}}\left(e^{i\omega_n\beta}\, e^{\beta(E_m - E_{m'})} - 1\right)$$

$$= \frac{-1}{Z}\sum_{mm'} e^{-\beta E_m}\frac{\langle m|A|m'\rangle\langle m'|B|m\rangle}{i\omega_n + E_m - E_{m'}}\left(\pm\, e^{\beta(E_m - E_{m'})} - 1\right)$$

$$= \frac{1}{Z}\sum_{mm'} \frac{\langle m|A|m'\rangle\langle m'|B|m\rangle}{i\omega_n + E_m - E_{m'}}\left(e^{-\beta E_m} - (\pm)\, e^{-\beta E_{m'}}\right)$$

$$\Rightarrow \quad i\omega_n \to \omega + i\eta \qquad C_{AB}(i\omega_n) \to C^R_{AB}(\omega).$$

An important class of Matsubara GF are the single particle ones

$$\mathcal{G}(\vec r\sigma\tau; \vec r'\sigma'\tau') = -\left\langle T_\tau\left[\psi_\sigma(\vec r\tau)\,\psi^\dagger_{\sigma'}(\vec r'\tau')\right]\right\rangle$$

It is very straightforward to prove that in the $\{\nu\}$ representation the Matsubara Green's function for non interacting system described by the Hamiltonian $H_0 = \sum_\nu \xi_\nu c^\dagger_\nu c_\nu$ are

$$\mathcal{G}_0(\nu, i\omega_n) = \frac{1}{i\omega_n - \xi_\nu}$$

$i\omega_n = ik_n$ for fermions

$= iq_n$ for bosons

(EXERCISE)

Evaluation of Matsubara sums:

$$S_1(\nu, \tau) = \frac{1}{\beta} \sum_{ik_n} g(\nu, ik_n) e^{ik_n\tau} \qquad \tau > 0$$

$$S_2(\nu_1, \nu_2, i\omega_n, \tau) = \frac{1}{\beta} \sum_{ik_n} \mathcal{G}_0(\nu_1, ik_n) \mathcal{G}_0(\nu_2, ik_n + i\omega_n) e^{ik_n\tau} \qquad \tau > 0$$

These are typical sums that one can encounter in perturbation theory. More in general

$$S^F(\tau) = \frac{1}{\beta} \sum_{ik_n} g(ik_n) e^{ik_n\tau}$$

$$S^B(\tau) = \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) e^{i\omega_n\tau}$$

where g is a generic function.

The basic trick is to rewrite these sums as integrals over complex variables and to use residue theory.

$$n_F(z) = \frac{1}{e^{\beta z} + 1} \qquad \text{poles for } z = i\frac{(2n+1)\pi}{\beta}$$

$$n_B(z) = \frac{1}{e^{\beta z} - 1} \qquad \text{poles for } z = i\frac{2n\pi}{\beta}$$

The residues at these values are

$$\operatorname*{Res}_{z = ik_n} [n_F(z)] = \lim_{z \to ik_n} \frac{z - ik_n}{e^{\beta z} + 1} = \lim_{\delta \to 0} \frac{\delta}{e^{\beta ik_n} e^{\beta\delta} + 1} = -\frac{1}{\beta}$$

$$\operatorname*{Res}_{z = i\omega_n} [n_B(z)] = \lim_{z \to i\omega_n} \frac{z - i\omega_n}{e^{\beta z} - 1} = \lim_{\delta \to 0} \frac{\delta}{e^{\beta i\omega_n} e^{\beta\delta} - 1} = +\frac{1}{\beta}$$

$\Rightarrow$ If we make the integral over a contour that does not contains singularities of $g(z)$ but one of the poles for n_F or n_B

$$\oint dz\, n_F(z) g(z) = 2\pi i \operatorname*{Res}_{z=ik_n}\left[n_F(z)\, g(ik_n)\right] = -\frac{2\pi i}{\beta} g(ik_n)$$

and analogous for bosons.

$$S^F = -\int_C \frac{dz}{2\pi i} n_F(z) g(z) e^{z\tau}$$

$$S^B = +\int_C \frac{dz}{2\pi i} n_B(z) g(z) e^{z\tau}$$

We still have to overcome 2 complications:

$\boxed{A}$ Summation over functions with simple poles

$\boxed{B}$ Summation over functions with known branch cuts

$\boxed{A}$ $$S_0^F(\tau) = \frac{1}{\beta}\sum_{ik_n} g_0(ik_n)\, e^{ik_n\tau}$$

and $g_0(z)$ has a number of known simple poles. e.g.

$$g_0(z) = \prod_j \frac{1}{z - z_j}$$

We choose C as $Re^{i\theta}$ with $R \to \infty$ $\theta \in [0, 2\pi)$. The contour integral itself gives 0 since $n_F(z) e^{\tau z} \to 0$ $R \to \infty$.

$$0 = \int_{C_\infty} \frac{dz}{2\pi i} n_F(z) g_0(z) e^{z\tau} = -\frac{1}{\beta}\sum_{ik_n} g_0(ik_n) e^{ik_n\tau} +$$

$$+ \sum_j \operatorname*{Res}_{z=z_j}[g_0(z)]\, n_F(z_j) e^{z_j\tau}$$

$$\Rightarrow \quad S_0^F(\tau) = \sum_j \operatorname*{Res}_{z=z_j}[g_0(z)]\, n_F(z_j) e^{z_j\tau}$$

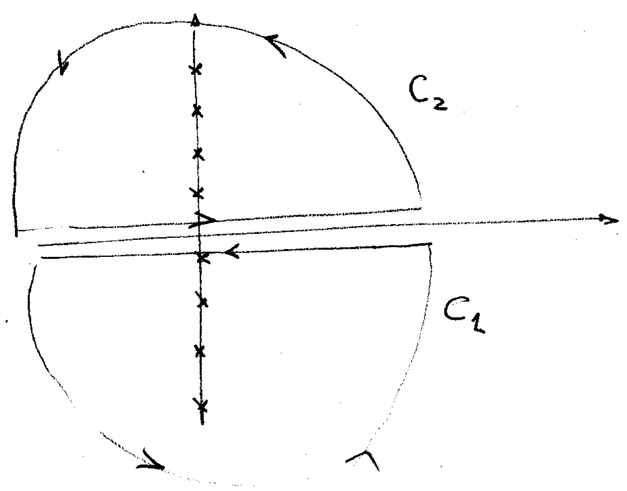
for bosons:

$$S_0^B(\tau) = -\sum_j \operatorname*{Res}_{z=z_j} [g_0(z)]\, n_B(z_j)\, e^{z_j \tau}$$

$\boxed{B}$ Consider now the sum:

$$S(\tau) = \frac{1}{\beta} \sum_{ik_n} g(ik_n)\, e^{ik_n \tau}$$

where $g(z) = \dfrac{1}{z - \xi_\nu - \Sigma(z)}$ we know it is not analytical on the real axis.



$$S(\tau) = -\int_{C_1 + C_2} \frac{dz}{2\pi i}\, n_F(z)\, g(z)\, e^{z\tau}$$

$$= -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\varepsilon\, n_F(\varepsilon) \left[g(\varepsilon + i\eta) - g(\varepsilon - i\eta) \right] e^{\varepsilon \tau}$$

For example

$$S_1(\nu, \tau) = \frac{1}{\beta} \sum_{ik_n} \mathcal{G}(\nu, ik_n)\, e^{ik_n \tau} = -\frac{1}{2\pi i} \int_{-\infty} d\varepsilon\, n_F(\varepsilon) \left[\mathcal{G}(\nu, \varepsilon + i\eta) - \mathcal{G}(\nu, \varepsilon - i\eta) \right] e^{\varepsilon\tau}$$

$$= -\int_{-\infty}^{+\infty} \frac{d\varepsilon}{\cancel{2}\pi \cancel{i}}\, n_F(\varepsilon)\, \cancel{2i}\, \operatorname{Im} G^R(\nu, \varepsilon)\, e^{\varepsilon\tau} = \int_{-\infty}^{+\infty} d\varepsilon\, n_F(\varepsilon)\, A(\nu, \varepsilon)\, e^{\varepsilon \tau}$$

$$\Rightarrow \quad \langle c_\nu^+ c_\nu \rangle = \mathcal{G}(\nu, 0^-) = \int_{-\infty}^{+\infty} d\varepsilon\, n_F(\varepsilon)\, A(\nu, \varepsilon)$$