

The family of Green's functions

Liqin Huang

1 Linear response theory

The time evolution of an operator \mathcal{O} is

$$\begin{aligned}\mathcal{O} &= e^{iHt} \mathcal{O}_S e^{-iHt} \\ &= e^{iHt} e^{-iH_0 t} e^{iH_0 t} \mathcal{O}_S e^{-iH_0 t} e^{iH_0 t} e^{-iHt} \\ &= e^{iHt} e^{-iH_0 t} \mathcal{O}_I e^{iH_0 t} e^{-iHt}\end{aligned}$$

We may expand $\exp(iH_0 t) \exp(-iHt)$ to first order in H_1 , and obtain

$$\mathcal{O} = \mathcal{O}_I - i \int_0^t dt' \mathcal{O}_I H_{1I} + i \int_0^t dt' H_{1I} \mathcal{O}_I$$

which means that the linear response is characterized by the commutator

$$\mathcal{O}_I H_{1I} - H_{1I} \mathcal{O}_I$$

at **different** times: \mathcal{O}_I is at time t while H_{1I} is at time t' , and we have $\int_0^t dt'$.

$$\begin{aligned}e^{iHt_2} \mathcal{O}_{2S} e^{-iHt_2} &= e^{iH_0 t_2} \mathcal{O}_{2S} e^{-iH_0 t_2} - i \int_0^{t_2} dt_1 e^{iH_0 t_2} \mathcal{O}_{2S} e^{-iH_0 t_{21}} H_{1S} e^{-iH_0 t_1} \\ &\quad + i \int_0^{t_2} dt_1 e^{iH_0 t_1} H_{1S} e^{iH_0 t_{21}} \mathcal{O}_{2S} e^{-iH_0 t_2}\end{aligned}$$

A more straightforward and perhaps more intuitive derivation is given by breaking the operator $\exp(-iHt)$ into pieces and expanding, keeping to first order in H_1 .

2 An example: The simple harmonic oscillator

The response function at zero temperature is

$$D_{\beta \rightarrow \infty} = \frac{i}{2\omega} e^{-i\omega t_{21}} \Theta_{21} - \frac{i}{2\omega} e^{-i\omega t_{12}} \Theta_{21}$$

and thus the linear response is

$$\int dt_1 \left(\frac{i}{2\omega} e^{-i\omega t_{21}} \Theta_{21} - \frac{i}{2\omega} e^{-i\omega t_{12}} \Theta_{21} \right) e^{0^+ t_1} = \frac{i}{2\omega} \left(\frac{1}{i\omega} - \frac{1}{-i\omega} \right) = \frac{1}{\omega^2}$$

which is correct, since the new equilibrium position is at $\phi = \frac{\lambda}{\omega^2}$ for $H_1 = -\lambda\phi$.

3 The Lehmann representation

1. The real-time Green's function.

$$\begin{aligned} iG_\beta &= \Theta_{21} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i e^{iE_{ij} t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} + \eta \Theta_{12} p_i e^{iE_{ij} t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \\ \tilde{G}_\beta &= p_i \frac{(\phi_{2S})_{ij} (\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij} (\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+} \end{aligned}$$

2.a. The retarded Green's function.

$$\begin{aligned} iD_{\beta+} &= \Theta_{21} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle - \eta \Theta_{21} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle - \eta \Theta_{21} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i e^{iE_{ij} t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} - \eta \Theta_{21} p_i e^{iE_{ij} t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \\ \tilde{D}_{\beta+} &= p_i \frac{(\phi_{2S})_{ij} (\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij} (\phi_{2S})_{ji}}{\omega - E_{ij} + i0^+} \end{aligned}$$

2.b. The advanced Green's function.

$$\begin{aligned} -iD_{\beta-} &= \Theta_{12} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle - \eta \Theta_{12} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{12} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle - \eta \Theta_{12} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{12} p_i e^{iE_{ij} t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} - \eta \Theta_{12} p_i e^{iE_{ij} t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \\ \tilde{D}_{\beta-} &= p_i \frac{(\phi_{2S})_{ij} (\phi_{1S})_{ji}}{\omega + E_{ij} - i0^+} - \eta p_i \frac{(\phi_{1S})_{ij} (\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+} \end{aligned}$$

3. The imaginary-time Green's function.

$$\begin{aligned} -\mathcal{G}_\beta &= \Theta_{21} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i e^{E_{ij} \tau_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} + \eta \Theta_{12} p_i e^{E_{ij} \tau_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \end{aligned}$$

and we have, setting $t_1 = 0$ such that the Θ_{12} term does not contribute,

$$\tilde{\mathcal{G}}_\beta = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{i\omega_l + E_{ij}} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{i\omega_l - E_{ij}}$$

4 The master Green's function

We define the so-called master Green's function as

$$\tilde{\mathcal{M}}_\beta \equiv p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{z + E_{ij}} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{z - E_{ij}}$$

or equivalently,

$$\tilde{\mathcal{M}}_\beta \equiv \frac{(p_i - \eta p_j)(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{z + E_{ij}}$$

For a non-interacting Hamiltonian, when $\phi_{1S} = a^\dagger$ and $\phi_{2S} = a$, the master Green's function takes a very simple form:

$$\tilde{\mathcal{M}}_\beta = \frac{1}{z - \varepsilon}$$

which is most easily proved by taking $|\psi_i\rangle$ to be the occupation number basis.

5 The spectral function

is defined as

$$\tilde{A}_\beta = i\tilde{D}_{\beta+} - i\tilde{D}_{\beta-}$$

which is equal to

$$p_i (\phi_{2S})_{ij}(\phi_{1S})_{ji} 2\pi\delta^1(\omega + E_{ij}) - \eta p_i (\phi_{1S})_{ij}(\phi_{2S})_{ji} 2\pi\delta^1(\omega - E_{ij})$$

or equivalently,

$$(p_i - \eta p_j)(\phi_{2S})_{ij}(\phi_{1S})_{ji} 2\pi\delta^1(\omega + E_{ij})$$

We have the following exact identity

$$\int \frac{d\omega}{2\pi} \tilde{A}_\beta = 1$$

for a general Hamiltonian, when $\phi_{1S} = a^\dagger$ and $\phi_{2S} = a$.

6 Kramers-Kronig relations

The master Green's function is given by the spectral function

$$\widetilde{\mathcal{M}}_\beta = \int \frac{d\omega}{2\pi} \frac{\widetilde{A}_\beta}{z - \omega}$$

which is easily verified, thanks to the delta function. Now we have, if $\text{im } z > 0$,

$$\begin{aligned} \widetilde{\mathcal{M}}_\beta &= \int \frac{d\omega}{2\pi} \frac{\widetilde{A}_\beta}{z - \omega} \\ &= i \int \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta+} - \widetilde{D}_{\beta-}}{z - \omega} = i \int_{C-} \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta+} - \widetilde{D}_{\beta-}}{z - \omega} = i \int_{C-} \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta+}}{z - \omega} = i \int \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta+}}{z - \omega} \end{aligned}$$

which gives us

$$\begin{aligned} \widetilde{D}_{\beta+} &= i \int \frac{d\omega'}{2\pi} \frac{\widetilde{D}_{\beta+}}{\omega - \omega' + i0^+} \\ \Rightarrow \widetilde{D}_{\beta+} &= i\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\widetilde{D}_{\beta+}}{\omega - \omega'} \end{aligned}$$

or equivalently, the **Kramers-Kronig relations**,

$$\begin{aligned} \text{re } \widetilde{D}_{\beta+} &= -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{im } \widetilde{D}_{\beta+}}{\omega - \omega'} \\ \text{im } \widetilde{D}_{\beta+} &= \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{re } \widetilde{D}_{\beta+}}{\omega - \omega'} \end{aligned}$$