The family of Green's functions

Liqin Huang

1 Linear response theory

The time evolution of a Heisenberg 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 $\int_0^t dt'$.

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

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

2 An example: The simple harmonic oscillator

The response function at zero temperature is

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

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.

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

$$\widetilde{G}_\beta = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+}$$

2.a. The retarded Green's function.

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

$$\widetilde{D}_{\beta+} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} + i0^+}$$

2.b. The advanced Green's function.

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

$$\widetilde{D}_{\beta-} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} - i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+}$$

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,

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

4 The master Green's function

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

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

or equivalently,

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

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

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

which is most easily proved by working in the occupation number basis.

5 The spectral function

is defined in frequency space as

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

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

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

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

6 Kramers-Kronig relations

The master Green's function is, in fact, 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 $\operatorname{im} z > 0$,

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

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**:

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