The family of Green's functions

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1 Linear response theory

The time evolution of a Heisenberg operator $\mathcal{O}$ is

$$\begin{aligned}\mathcal{O} &= e^{iHt}\mathcal{O}_S e^{-iHt}\\ &= e^{iHt}e^{-iH_0t}e^{iH_0t}\mathcal{O}_S e^{-iH_0t}e^{iH_0t}e^{-iHt}\\ &= e^{iHt}e^{-iH_0t}\mathcal{O}_I e^{iH_0t}e^{-iHt}\end{aligned}$$

We may expand $\exp(iH_0t)\exp(-iHt)$ 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 $\int_0^t dt'$.

$$\begin{aligned}e^{iHt_2}\mathcal{O}_{2S}e^{-iHt_2} = e^{iH_0t_2}\mathcal{O}_{2S}e^{-iH_0t_2} - i\int_0^{t_2} dt_1\,e^{iH_0t_2}\mathcal{O}_{2S}e^{-iH_0t_{21}}H_{1S}e^{-iH_0t_1}\\ + i\int_0^{t_2} dt_1\,e^{iH_0t_1}H_{1S}e^{iH_0t_{21}}\mathcal{O}_{2S}e^{-iH_0t_2}\end{aligned}$$

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

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

The master Green's function is, in fact, given by the spectral function

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

We also 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 The Kramers-Kronig relation

The retarded Green's function is analytic on the upper-half plane

$$0 = \int_{C+} dz \, \frac{\widetilde{D}_{\beta+}}{z-\omega+i0^+} = \int dz \, \frac{\widetilde{D}_{\beta+}}{z-\omega+i0^+} = \mathcal{P}\int dz \, \frac{\widetilde{D}_{\beta+}}{z-\omega} - i\pi\widetilde{D}_{\beta+}$$

which gives us the **Kramers-Kronig relation**:

$$\widetilde{D}_{\beta+} = \mathcal{P}\int \frac{d\omega'}{i\pi}\frac{\widetilde{D}_{\beta+}}{\omega'-\omega}$$

or equivalently,

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

or equivalently,

$$\widetilde{D}_{\beta+} = i\int \frac{d\omega'}{\pi}\frac{\mathrm{re}\,\widetilde{D}_{\beta+}}{\omega-\omega'+i0^+} = -\int \frac{d\omega'}{\pi}\frac{\mathrm{im}\,\widetilde{D}_{\beta+}}{\omega-\omega'+i0^+} = \int \frac{d\omega'}{2\pi}\frac{\widetilde{A}_{\beta}}{\omega-\omega'+i0^+}$$

7 The fluctuation-dissipation theorem

1. The correlation function.

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

$$\widetilde{S}_\beta = p_i \, (\phi_{2S})_{ij}(\phi_{1S})_{ji}\, 2\pi\delta^1(\omega+E_{ij})$$

2. The spectral function.

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

from which we read the ratio between them

$$\widetilde{S}_\beta = \frac{1}{1-\eta e^{-\beta\omega}}\,\widetilde{A}_\beta$$

8 The self-energy

We have the self-consistent equation for the pole of the propagator

$$\omega = \varepsilon_{\mathbf{k}} + \Sigma\left(\omega, \mathbf{k}\right)$$

9 The density-density response

The density operator is

$$n_{\mathbf{x}} = (a_{\mathbf{x}})^{\dagger} a_{\mathbf{x}} = V^{-1} \sum_{\mathbf{kq}} (a_{\mathbf{k}})^{\dagger} a_{\mathbf{q}} \, e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\mathbf{q}\cdot\mathbf{x}}$$