The retarded Green's function is defined as

$$G(t) = -i\theta(t)\langle c(t)c^\dagger + c^\dagger c(t)\rangle = \begin{cases} -i & t \geqslant 0 \\ 0 & t < 0 \end{cases} \tag{1}$$

The function vanishes when $t < 0$, then its Fourier transform is

$$G(t) = \int_{-\infty}^{\infty} G(\omega) e^{-i\omega t} \frac{\mathrm{d}\omega}{2\pi}, \tag{2}$$

where

$$G(\omega) \;=\; \int_0^\infty G(t) e^{i(\omega + i\delta)t}, \quad \delta \to 0, \tag{3}$$

where the quantity δ ensures $e^{i(\omega+i\delta)t}$ vanishes at $t \to \infty$.

1 Lehmann Representation

Let $|m\rangle$ be the eigenstate of the Hamiltonian, then for $t > 0$ we have

$$\begin{aligned} iG(t) &= \frac{1}{Z}\sum_m e^{-\beta E_m} \langle m|c\,(t)c^\dagger + c^\dagger c(t)|m\rangle \\ &= \frac{1}{Z}\sum_{mn} e^{-\beta E_m} [\langle m|c|n\rangle\langle n|c^\dagger|m\rangle e^{-i\omega_{nm}t} + \langle m|c^\dagger|n\rangle\langle n|c|m\rangle e^{-i\omega_{mn}t}], \end{aligned} \tag{4}$$

where $\omega_{mn} = E_m - E_n$. Applying Fourier transform yields

$$\begin{aligned} iG(\omega) &= \frac{1}{Z}\int \sum_{mn} e^{-\beta E_m} [A_{mn} e^{i(\omega - \omega_{nm} + i\delta)t} + A_{nm} e^{i(\omega - \omega_{mn} + i\delta)t}] \mathrm{d}t \\ &= -\frac{i}{Z}\sum_{mn} \left[\frac{e^{-\beta E_m} A_{mn}}{\omega - \omega_{nm} + i\delta} + \frac{e^{-\beta E_m} A_{nm}}{\omega - \omega_{mn} + i\delta} \right] \end{aligned} \tag{5}$$

that is

$$G(\omega) = \frac{1}{Z}\sum_{mn} A_{mn} \frac{e^{-\beta E_m} + e^{-\beta E_n}}{\omega - \omega_{nm} + i\delta}. \tag{6}$$

Define a spectral function as

$$A(\varepsilon) = \frac{1}{Z}\sum_{mn} A_{mn} (e^{-\beta E_n} + e^{-\beta E_m}) \delta(\varepsilon - \omega_{nm}), \tag{7}$$

we can write

$$G(\omega) = \int \frac{A(\varepsilon)}{\omega - \varepsilon + i\delta} \mathrm{d}\varepsilon. \tag{8}$$

The spectral function defined in this way is normalized, which can be seen from the fact that

$$\begin{aligned} \frac{1}{Z}\sum_{mn} \langle m|c|n\rangle\langle n|c^\dagger|m\rangle (e^{-\beta E_n} + e^{-\beta E_m}) &= \frac{1}{Z}\sum_{mn} [e^{-\beta E_m} \langle m|c|n\rangle\langle n|c^\dagger|m\rangle + e^{-\beta E_n} \langle n|c^\dagger|m\rangle\langle m|c|n\rangle] \\ &= \frac{1}{Z} \mathrm{Tr}\,[e^{-\beta H}(cc^\dagger + c^\dagger c)] = 1, \end{aligned} \tag{9}$$

which means that

$$\int A(\varepsilon)\mathrm{d}\varepsilon = 1. \tag{10}$$

Note that

$$\frac{1}{x+i\delta} = P\frac{1}{x} - i\pi\delta(x), \tag{11}$$

then we have

$$\mathrm{Im}\, G(\omega) = -\pi\int A(\varepsilon)\delta(\omega-\varepsilon)\mathrm{d}\varepsilon = -\pi A(\omega), \tag{12}$$

that is

$$-\frac{1}{\pi}\mathrm{Im}\, G(\omega) = A(\omega). \tag{13}$$

2 Asymptotic Correction for Fourier Transform

In asymptotic limit $\omega \to \infty$, the Green's function is approxiamtely written as

$$G(\omega) \;=\; \int \frac{A(\varepsilon)}{\omega + i\delta}\mathrm{d}\varepsilon = \frac{1}{\omega + i\delta}. \tag{14}$$

Therefore if we truncated ω at ω_{min} and ω_{max} for Fourier transform, we should add the asymptotic correction as

$$G(t) = \int_{\omega_{\mathrm{min}}}^{\omega_{\mathrm{max}}} \left[G(\omega) - \frac{1}{\omega + i\delta}\right] e^{-i\omega t}\frac{\mathrm{d}\omega}{2\pi} + \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega + i\delta}\frac{\mathrm{d}\omega}{2\pi} \tag{15}$$

Since the second term in the above expression is just the Fourier series of $-i$ for which

$$-i\int_{-\infty}^{\infty} e^{i(\omega+i\delta)t}\mathrm{d}t = -\frac{e^{i(\omega+i\delta)t}}{\omega+i\delta}|_0^{\infty} = \frac{1}{\omega+i\delta}. \tag{16}$$

Therefore we have

$$G(t) \;=\; \int_{\omega_{\mathrm{min}}}^{\omega_{\mathrm{max}}} \left[G(\omega) - \frac{1}{\omega + i\delta}\right] e^{-i\omega t}\frac{\mathrm{d}\omega}{2\pi} - i. \tag{17}$$

2.1 Higher order corrections

We can assume that with high ω_s, the Green's function is

$$G(\omega) \approx \sum_{n=0}^{N} \frac{a_n}{\omega^n}. \tag{18}$$

The coefficients a_n should be determined through a least-square procedure of the data.

3 Free Impurity

The free impurity Hamiltonian is $H = E_0 c^\dagger c$, then for $t \geqslant 0$ we have

$$\begin{aligned} G(t) &= -i\frac{1}{Z}\mathrm{Tr}[cc^\dagger + c^\dagger c]e^{-iE_0 t} \\ &= -ie^{-iE_0 t}. \end{aligned} \tag{19}$$

where $n = (e^{\beta E_0} + 1)^{-1}$ is the Fermi distribution. Its Fourier transform is

$$G(\omega) = \frac{1}{\omega - E_0 + i\delta}. \tag{20}$$

4 Toulouse Model

For Toulouse model $H = E_0 c^\dagger c + \sum_k \varepsilon_k a_k^\dagger a_k + \sum_k V_k (c^\dagger a_k + a_k^\dagger c)$, the free bath Green's function is

$$D_k(t) = -i\theta(t)\langle a_k(t) a_k^\dagger + a_k^\dagger a_k(t)\rangle = -ie^{-iE_0 t} \quad t \geqslant 0 \tag{21}$$

and its Fourier series is

$$D_k(\omega) = \frac{1}{\omega - \varepsilon_k + i\delta}. \tag{22}$$

The impurity Green's function becomes

$$G(\omega) = \left[\omega - E_0 - \sum_k \frac{V_k^2}{\omega - \varepsilon_k + i\delta}\right]^{-1}. \tag{23}$$

Denote

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega - \varepsilon_k + i\delta}, \tag{24}$$

then we have

$$G^{-1}(\omega) = G_0^{-1}(\omega) - \Delta(\omega). \tag{25}$$

The function $\Delta(i\omega_n)$ is the hybridization function. If we define the spectral function

$$J(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k), \tag{26}$$

then we can write

$$\Delta(\omega) = \int \frac{J(\varepsilon)}{\omega - \varepsilon + i\delta} \mathrm{d}\varepsilon. \tag{27}$$

This hybridization function is ***not*** the hybridization function used in path integral. To obtain the hybridization function $\Delta(t, t')$ in path integral, we need to first obtain the spectral function by

$$J(\varepsilon) = -\frac{1}{\pi} \mathrm{Im}\, \Delta(\varepsilon), \tag{28}$$

and then calculate $\Delta(t, t')$ using QuaPI.