The Matsubara Green's function is defined as

$$G(\tau) = -\langle T c(\tau) c^\dagger \rangle = \begin{cases} -\langle c(\tau) c^\dagger \rangle, & \tau \geqslant 0 \\ \langle c^\dagger c(\tau) \rangle, & \tau < 0 \end{cases}, \tag{1}$$

where $c(\tau) = e^{\tau H} c e^{-\tau H}$. It satisify the antiperiodic condition $G(\tau) = -G(\tau+\beta), -\beta \leqslant \tau < 0$, then it can be expanded as a Fourier series in $0 \leqslant \tau < \beta$ as

$$G(\tau) = \frac{1}{\beta} \sum_{s=-\infty}^{\infty} G(i\omega_s) e^{-i\omega_s \tau}, \quad \omega_s = \frac{(2s+1)\pi}{\beta}, \tag{2}$$

where

$$G(i\omega_s) = \int_0^\beta G(\tau) e^{i\omega_s \tau} \mathrm{d}\tau. \tag{3}$$

1 Lehmann Representation

Let $|m\rangle$ be the eigenstate of the Hamiltonian, for $0 \leqslant \tau < \beta$ we can write

$$\begin{aligned} G(\tau) &= -\frac{1}{Z} \sum_m e^{-\beta E_m} \langle m | c(\tau) c^\dagger | m \rangle \\ &= -\frac{1}{Z} \sum_{mn} e^{-\beta E_m} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle e^{-\tau \omega_{nm}} \end{aligned} \tag{4}$$

where $\omega_{mn} = E_m - E_n$. The Fourier series is

$$\begin{aligned} G(i\omega_s) &= -\frac{1}{Z} \sum_{mn} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle e^{-\beta E_m - \tau \omega_{nm}} e^{i\omega_s \tau} \mathrm{d}\tau \\ &= -\frac{1}{Z} \sum_{mn} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle \frac{e^{-\beta E_m} e^{(i\omega_s - \omega_{nm})\tau}}{i\omega_s - \omega_{nm}} \Big|_0^\beta \\ &= \frac{1}{Z} \sum_{mn} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle \frac{e^{-\beta E_n} + e^{-\beta E_m}}{i\omega_s - \omega_{nm}}. \end{aligned} \tag{5}$$

Define a spectral function as

$$A(\varepsilon) = \frac{1}{Z} \sum_{mn} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle (e^{-\beta E_n} + e^{-\beta E_m}) \delta(\varepsilon - \omega_{nm}), \tag{6}$$

we can write

$$G(i\omega_s) = \int \frac{A(\varepsilon)}{i\omega_s - \varepsilon} \mathrm{d}\varepsilon. \tag{7}$$

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

$$\begin{aligned} \frac{1}{Z} \sum_{mn} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle (e^{-\beta E_n} + e^{-\beta E_m}) &= \frac{1}{Z} \sum_{mn} [e^{-\beta E_m} \langle m | c | n \rangle \langle n | c^\dagger | m \rangle + e^{-\beta E_n} \langle n | c^\dagger | m \rangle \langle m | c | n \rangle] \\ &= \frac{1}{Z} \mathrm{Tr}\, [e^{-\beta H} (c c^\dagger + c^\dagger c)] = 1, \end{aligned} \tag{8}$$

which means that

$$\int A(\varepsilon) \mathrm{d}\varepsilon = 1. \tag{9}$$

2 Asymptotic Correction for Fourier Series

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

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

Therefore if we truncated ω_s at $s_{\min}$ and $s_{\max}$ for Fourier series, we should add the asymptotic correction as

$$G(\tau) = \frac{1}{\beta} \sum_{s=s_{\min}}^{s_{\max}} \left[G(i\omega_s) - \frac{1}{i\omega_s} \right] e^{-i\omega_s\tau} + \frac{1}{\beta} \sum_{s=-\infty}^{\infty} \frac{1}{i\omega_s} e^{-i\omega_s\tau}. \tag{11}$$

Since the second term in the above expression is just the Fourier series of $-\frac{1}{2}$ for which

$$-\frac{1}{2} \int_0^\beta e^{i\omega_s\tau} \mathrm{d}\tau = -\frac{1}{2} \frac{e^{i\omega_s\tau}}{i\omega_s} |_0^\beta = \frac{1}{i\omega_s}. \tag{12}$$

Therefore we have

$$G(\tau) = \frac{1}{\beta} \sum_{s=s_{\min}}^{s_{\max}} \left[G(i\omega_s) - \frac{1}{i\omega_s} \right] e^{-i\omega_s\tau} - \frac{1}{2}. \tag{13}$$

This formula should be also used to implement the Fourier transform (3).

2.1 Higher order corrections

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

$$G(i\omega_s) \approx \sum_{n=0}^{N} \frac{a_n}{(i\omega_s)^n}. \tag{14}$$

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 $0 \leqslant \tau < \beta$ we have

$$\begin{aligned} G(\tau) &= -\frac{1}{Z} \mathrm{Tr}\,[e^{-\beta H} c c^\dagger] e^{-E_0\tau} \\ &= -(1-n) e^{-E_0\tau} \\ &= -\frac{e^{-E_0\tau}}{1+e^{-\beta E_0}} \end{aligned} \tag{15}$$

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

$$\begin{aligned} G(i\omega_s) &= -(1+e^{-\beta E_0})^{-1} \int_0^\beta e^{-E_0\tau} e^{i\omega_s\tau} \mathrm{d}\tau \\ &= -(1+e^{-\beta E_0})^{-1} \frac{e^{(i\omega_s - E_0)\tau}}{i\omega_s - E_0} |_0^\beta \quad \left[\text{Note that } \omega_s = \frac{(2s+1)\pi}{\beta} \right] \\ &= -(1+e^{-\beta E_0})^{-1} \frac{-e^{-\beta E_0} - 1}{i\omega_s - E_0} \\ &= \frac{1}{i\omega_s - E_0}. \end{aligned} \tag{16}$$

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

$$D_k(\tau) = -\langle T a_k(\tau) a_k^\dagger \rangle = -\frac{e^{-\varepsilon_k \tau}}{1 + e^{-\beta\varepsilon_k}}, \quad 0 \leqslant \tau < \beta, \tag{17}$$

and its Fourier series is

$$D_k(i\omega_s) = \frac{1}{i\omega_s - \varepsilon_k}. \tag{18}$$

The impurity Green's function becomes

$$G(i\omega_s) = \left[i\omega_s - E_0 - \sum_k \frac{V_k^2}{i\omega_s - \varepsilon_k} \right]^{-1}. \tag{19}$$

Denote

$$\Delta(i\omega_n) = \sum_k \frac{V_k^2}{i\omega_s - \varepsilon_k}, \tag{20}$$

then we have

$$G^{-1}(i\omega_s) = G_0^{-1}(i\omega_s) - \Delta(i\omega_s). \tag{21}$$

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

$$J(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k), \tag{22}$$

then we can write

$$\Delta(i\omega_s) = \int \frac{J(\varepsilon)}{i\omega_s - \varepsilon} \mathrm{d}\varepsilon. \tag{23}$$

This hybridization function is in fact the one we used in path integral formalism for which

$$\Delta(\tau) = \int J(\varepsilon) D_\varepsilon(\tau) \mathrm{d}\varepsilon, \tag{24}$$

where $D_\varepsilon(\tau) = D_k(\tau)$ for $\varepsilon_k = \varepsilon$. Its Fourier series is

$$\Delta(i\omega_s) = \int J(\varepsilon) D_\varepsilon(\tau) e^{i\omega_s \tau} \mathrm{d}\varepsilon \mathrm{d}\tau = \int J(\varepsilon) D_\varepsilon(i\omega_s) \mathrm{d}\varepsilon, \tag{25}$$

and substituting $D_\varepsilon(i\omega_s) = (i\omega_s - \varepsilon)^{-1}$ into the above expression yields (23).