The Matsubara Green's function is defined as

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

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

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

where

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

1 Free Impurity

The free impurity Hamiltonian is $H = E_0 c^\dagger c$, then for $0 \leqslant \tau < \beta$ we have

$$\begin{aligned} G(\tau) &= -\frac{1}{Z}\mathrm{Tr}\,[e^{-\beta H} c c^\dagger] e^{-E_0\tau} \\ &= -(1-n)e^{-E_0\tau} \\ &= -\frac{e^{-E_0\tau}}{1+e^{-\beta E_0}} \end{aligned} \tag{4}$$

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

$$\begin{aligned} G(i\omega_n) &= -(1+e^{-\beta E_0})^{-1}\int_0^\beta e^{-E_0\tau}e^{i\omega_n\tau}\mathrm{d}\tau \\ &= -(1+e^{-\beta E_0})^{-1}\frac{e^{(i\omega_n - E_0)\tau}}{i\omega_n - E_0}\Big|_0^\beta \quad \left[\text{Note that } \omega_n = \frac{(2n+1)\pi}{\beta}\right] \\ &= -(1+e^{-\beta E_0})^{-1}\frac{-e^{-\beta E_0}-1}{i\omega_n - E_0} \\ &= \frac{1}{i\omega_n - E_0}. \end{aligned} \tag{5}$$

2 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

$$D_k(\tau) = -\langle T a_k(\tau) a_k^\dagger\rangle = -\frac{e^{-\varepsilon_k\tau}}{1+e^{-\beta\varepsilon_k}}, \quad 0 \leqslant \tau < \beta, \tag{6}$$

and its Fourier series is

$$D_k(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_k}. \tag{7}$$

The impurity Green's function becomes

$$G(i\omega_n) = \left[i\omega_n - E_0 - \sum_k \frac{V_k^2}{i\omega_n - \varepsilon_k}\right]^{-1}. \tag{8}$$

Denote

$$\Delta(i\omega_n) = \sum_k \frac{V_k^2}{i\omega_k - \varepsilon_k}, \tag{9}$$

then we have

$$G^{-1}(i\omega_n) = G_0^{-1}(i\omega_n) - \Delta(i\omega_n). \tag{10}$$

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

$$J(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k), \tag{11}$$

then we can write

$$\Delta(i\omega_n) = \int \frac{J(\varepsilon)}{i\omega_n - \varepsilon} \mathrm{d}\varepsilon. \tag{12}$$

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

$$\Delta(\tau) = \int J(\varepsilon) D_\varepsilon(\tau) \mathrm{d}\varepsilon, \tag{13}$$

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

$$\Delta(i\omega_n) = \int J(\varepsilon) D_\varepsilon(\tau) e^{i\omega_n \tau} \mathrm{d}\varepsilon \mathrm{d}\tau = \int J(\varepsilon) D_\varepsilon(i\omega_n) \mathrm{d}\varepsilon, \tag{14}$$

and substituting $D_\varepsilon(i\omega_n) = (i\omega_n - \varepsilon)^{-1}$ into the above expression yields (12).