Green function for Vertex solver

Ha Nul Seok

July 5, 2023

Imaginary time and tau

Answering the following question : Why is the reason that τ has its boundary condition in range : $0 < \tau < \beta$? In Statistical mechanics, quantities of interest are the partition function of the system, $Z(\beta) = Tr[e^{-\beta H}]$ and it's form is the same as the time-evolution operator $e^{iHt/\hbar}$. The Imaginary time τ is : $\tau = it$.

$$Z(\beta) = \sum_n \langle n| e^{\beta H} |n\rangle \tag{1}$$

$$= \sum_n \sum_{m_1, m_2, \ldots m_N} \langle n| e^{(1/\hbar)\delta\tau H} |m_1\rangle \langle m_1| e^{(1/\hbar)\delta\tau H} |m_2\rangle \ldots \langle m_N| e^{(1/\hbar)\delta\tau H} |n\rangle \tag{2}$$

Where,

$$e^{-\beta H} = [e^{(-1/\hbar)\delta\tau H}]^n \tag{3}$$

The time interval $\delta\tau = \hbar\Gamma$ is small on the time scales of interest. Thus, $0 < \tau < \beta$ can be deduced.

Fourier transformation of Matsubara Green function

Below, Only bosonic case considered.

$$\begin{aligned} C_{AB}(\tau) &= -\langle T(A(\tau)B(0))\rangle \\ &= -\langle T(e^{\tau H_0} a_k e^{-\tau H_0} a_k^\dagger)\rangle \end{aligned}$$

$$\leftrightarrow \quad C_{AB}(\tau) = -\theta(\tau)\langle a_k(\tau)a_k^\dagger\rangle - \theta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle$$

$$\frac{\partial}{\partial\tau} C_{AB}(\tau) = -\delta(\tau)\langle a_k(\tau)a_k^\dagger\rangle - \theta(\tau)\frac{\partial}{\partial\tau}\langle a_k(\tau)a_k^\dagger\rangle + \delta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle - \theta(-\tau)\frac{\partial}{\partial\tau}\langle a_k^\dagger a_k(\tau)\rangle$$

At given condition, $H_0 = \sum_k \omega_k a_k^\dagger a_k$.

$$\begin{aligned} \frac{\partial}{\partial\tau}\langle a_k(\tau)a_k^\dagger\rangle &= \langle \partial_\tau e^{\tau H_0} a_k e^{-\tau H_0} a_k^\dagger - e^{\tau H_0} a_k \partial_\tau e^{-\tau H_0} a_k^\dagger\rangle \\ &= \langle e^{\tau H_0} H_0 a_k e^{-\tau H_0} a_k^\dagger - e^{\tau H_0} a_k H_0 e^{-\tau H_0} a_k^\dagger\rangle \\ &= \langle e^{\tau H_0}[H_0, a]e^{-\tau H_0} a_k^\dagger\rangle \\ &\Leftrightarrow \langle e^{\tau H_0}(\sum_{k'} \omega_{k'} a_{k'} a_{k'}) a_k e^{-\tau H_0} a_k^\dagger\rangle - \langle e^{\tau H_0} a_k (\sum_{k'} \omega_{k'} a_{k'} a_{k'}) e^{-\tau H_0} a_k^\dagger\rangle \end{aligned}$$

If $k \neq k'$,

$$\langle e^{\tau H_0} \sum_{k'} a_{k'}^\dagger a_{k'} a_k e^{\tau H_0} a_k^\dagger\rangle - \langle e^{\tau H_0} a_k \sum_{k'} a_{k'}^\dagger a_{k'} e^{\tau H_0} a_k^\dagger\rangle = 0 \qquad (*) \quad [a_{k'}, a_k] = 0$$

If $k = k'$,

$$\begin{aligned} \Leftrightarrow \quad &= \omega_k\langle e^{\tau H_0} a_k^\dagger a_k a_k e^{-\tau H_0} a_k^\dagger\rangle - \omega_k\langle e^{\tau H_0} a_k a_k^\dagger a_k e^{-\tau H_0} a_k^\dagger\rangle \\ &= \omega_k\langle e^{\tau H_0}(a_k a_k^\dagger - 1) a_k e^{-\tau H_0} a_k^\dagger\rangle - \omega_k\langle e^{\tau H_0} a_k a_k^\dagger a_k e^{-\tau H_0} a_k^\dagger\rangle \\ &= -\omega_k\langle e^{\tau H_0} a_k e^{-\tau H_0} a_k^\dagger\rangle + \omega_k\langle e^{\tau H_0} a_k a_k^\dagger a_k e^{-\tau H_0} a_k^\dagger\rangle - \omega_k\langle e^{\tau H_0} a_k a_k^\dagger a_k e^{-\tau H_0} a_k^\dagger\rangle \end{aligned}$$

$$\Leftrightarrow \quad = -\omega_k\langle e^{\tau H_0} a_k e^{-\tau H_0} a_k^\dagger\rangle$$

So for $\tau > 0$, the green function C_{AB} become:

$$\frac{\partial}{\partial \tau} C_{AB}(\tau) = -\delta(\tau) + \omega_k C_{AB}$$

The definition of Fourier transform of Matsubara Green function in time-domain(time interval is $0 < t < \beta$) to frequency domain is : $C_{AB} = \frac{1}{\beta} \sum_n e^{i\omega_n \tau} C_{AB}(i\omega_n)$, and its bosonic frequency is : $\omega_n = \frac{2n\pi}{\beta}$. Using these definition, for $\tau > 0$,

$$\frac{1}{\beta} \sum_n i\omega_n e^{i\omega_n \tau} C_{AB}(i\omega_n) - \frac{1}{\beta} \sum_n \omega_k e^{i\omega_n \tau} C_{AB}(i\omega_n) = -\frac{1}{\beta} \sum_n e^{\omega_n \tau}$$

So the Green's function at matsubara freqency domain is,

$$C_{AB}(\tau) = \frac{1}{-\omega_k + i\omega_n} \quad \leftrightarrow \quad \left(\frac{1}{iq_n - \xi} \right)$$

Where $\omega_n(q_n)$ is bosonic matsubara frequency.

Steps to derive Matsubara Green's function at frequency domain

The Basic form of Matsubara green's function at τ domain is given as :

$$S^B(\tau) = \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) e^{i\omega_n \tau}$$

If we derive the inverse fourier transform of given function, then we can get the matsubara frequency green's function. Begin with the $\frac{1}{\beta}$,

$$n_B(\tau) = \frac{1}{e^{\beta z} - 1}$$

$$\begin{aligned}
\operatorname*{Res}_{z=i\omega_n} [n_B(z)] &= \lim_{z \to i\omega_n} \frac{(z - i\omega_n)}{e^{\beta z} - 1} \\
&= \lim_{z \to i\omega_n} \frac{1}{\beta e^{\beta z}} \\
&= \frac{1}{\beta}
\end{aligned}$$

$$\begin{aligned}
\oint dz n_B(z) g(z) &= 2\pi i \sum \operatorname*{Res}_{z=i\omega_n} (n_B(z) g_B(i\omega_n)) \\
&= \frac{2\pi i}{\beta} \sum g(i\omega_n)
\end{aligned}$$

Thus the time-domain green's function can be written in contour integral form,

$$S^B(\tau) = \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) e^{i\omega_n \tau} = \int_C \frac{dz}{2\pi i} n_B(z) g(z) e^{z\tau}$$

Where $z = i\omega_n$. Now calculate the contour term, while $z \to \infty$,

$$\int_C \frac{dz}{2\pi i} n_B(z) g(z) e^{z\tau} = 2\pi i \sum \text{Res}$$

Residue for $g(z)$,

$$\begin{aligned}
\lim_{z \to \omega_k} g(z) \frac{n_B(z) g(z) e^{z\tau}}{2\pi i} &= \lim_{z \to \omega_k} (z - \omega_k) \frac{n_B(z) e^{z\tau}}{2\pi i (z - \omega_k)} \\
&= \lim_{z \to \omega_k} \frac{n_B(z) e^{z\tau}}{2\pi i} \\
&= \frac{n_B(\omega_k) e^{\omega_k \tau}}{2\pi i}
\end{aligned}$$

and to get Residue for n_B,

$$n_B \to 0, \quad \text{if} \quad z \to \infty, \quad \frac{e^{z\tau}}{e^{\beta z}-1} \sim \frac{e^{\infty\tau}}{e^{\infty\beta}}$$
$$z \to -\infty, \quad \frac{0}{-1} \sim 0$$

Thus, Matsubara green's function at imaginary time domain is:

$$\sum_{iq_n} \frac{1}{\beta} g(iq_n) e^{iq_n\tau} = n_B(\omega_k) e^{\omega_k \tau}$$