Matsubara Summary(3)

May 18, 2023

Trial for Inverse Fourier transformation

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.

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

$$\leftrightarrow C_{AB}(\tau) = -\theta(\tau)\langle a_k(\tau)a_k^\dagger\rangle - \theta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle \tag{4}$$

$$\begin{aligned} \partial_\tau C_{AB}(\tau) &= -\delta(\tau)\langle a_k(\tau)a_k^\dagger\rangle + \omega_k\langle a_k(\tau)a_k^\dagger\rangle + \delta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle + \omega_k\theta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle \\ &= -\delta(\tau)\langle a_k(\tau)a_k^\dagger - a_k^\dagger a_k(\tau)\rangle + \omega_k\theta(\tau)\langle a_k(\tau)a_k^\dagger\rangle + \omega_k\theta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle \\ &= -\delta(\tau)\langle a_k(\tau)a_k^\dagger - a_k^\dagger a_k(\tau)\rangle + \omega_k\{-\theta(\tau)\langle a_k(\tau)a_k^\dagger\rangle - \theta(-\tau)\langle a_k^\dagger a_k(\tau)\rangle\} \end{aligned}$$

$$\partial C_{AB}(\tau) = -\delta(\tau) - \omega_k C_{AB} \tag{5}$$

The definition of Fourier transform of Matsubara Green function in time-domain 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,

$$\partial \frac{1}{\beta}\sum_n i\omega_n e^{i\omega_n\tau} C_{AB}(i\omega_n) + \frac{1}{\beta}\sum_n i\omega_k e^{i\omega_n\tau} C_{AB}(i\omega_n) = \tag{6}$$

The result is,

$$C_{AB}(\tau) = \frac{1}{-\omega_k + i\omega_n} \quad \leftrightarrow \quad \left(\frac{1}{iq_n - \xi}\right) \tag{7}$$

Steps to derive the inverse fourier transform

$$S(\nu,\tau) = \frac{1}{\beta}\sum_{ik_n} G(\nu, ik_n)e^{ik\tau} \tag{8}$$

$$S_2(\nu_1,\nu_2,i\omega,\tau) = \frac{1}{\beta}\sum_{ik_n} G_0(\nu, ik_n)G_0\nu_2, ik_n + i\omega_n e^{ik\tau} \tag{9}$$

$$S^B(\tau) = \frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n)e^{i\omega_n\tau} \tag{10}$$

$$n_B(\tau) = \frac{1}{e^{\beta z}-1} \tag{11}$$

$$\begin{aligned}
\operatorname*{Res}_{z=i\omega_n}[n_B(z)] &= \lim_{z\to i\omega_n}\frac{(z-i\omega_n)}{e^{\beta z}-1} \\
&= \lim_{\delta\to 0}\frac{\delta}{e^{\beta i\omega_n}e^{\beta\delta}-1} \\
&= \frac{1}{\beta}
\end{aligned}$$

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

$$S^B = \int_C \frac{dz}{2\pi i} n_B(z)g(z) \tag{12}$$

Inverse fourier transform - single poles

$$S_0^F(\tau) = \frac{1}{\beta}\sum_{ik_n} g_0(ik_n)e^{ik_n\tau}, \qquad \tau > 0 \tag{13}$$

$$g_0(z) = \prod_j \frac{1}{z-z_j} \tag{14}$$

$$n_F(z)e^{\tau z} = \frac{e^{\tau z}}{e^{\beta z}+1} \propto \tag{15}$$

$$\begin{aligned}
0 &= \int_{C_\infty}\frac{dz}{2\pi i} n_B(z)g_0(z)e^{\tau z} \\
&= -\frac{1}{\beta}\sum_{ik_n} g_0(ik_n)e^{ik_n\tau} + \sum_j \operatorname*{Res}_{z=z_j}(g_0(z))n_F(z_j)e^{z_j\tau}
\end{aligned}$$

$$\frac{1}{\beta}\sum_{i\omega_n} e^{o\omega_n\tau} = S_0^B(\tau) = -\sum_j \operatorname*{Res}_{z=z_j}[g_0(z)]n_B(z_j)e^{z_j\tau} \tag{16}$$

Inverse fourier transform - Branch cut

$$S(\tau) = \frac{1}{\beta}\sum_{ik_n} g(ik_n)e^{ik_n\tau} \tag{17}$$

$$\begin{aligned} S(\tau) &= -\int_{C_1+C_2}\frac{dz}{2\pi}n_F(z)g(z)e^{z\tau} &(18)\\ &= -\frac{1}{2\pi}\int_{\infty}^{\infty} d\epsilon n_F(\epsilon)[g(\epsilon+i\eta)-g(\epsilon-i\eta)]e^{\epsilon\tau} &(19)\end{aligned}$$

$$\langle a_\nu^\dagger a_\nu\rangle = G(\nu, 0^-) \tag{20}$$

$$\begin{aligned}\leftrightarrow &= \frac{1}{\beta}\sum_{ik_n} G(\nu, ik_n)e^{-ik_n0^-}\\ &= G_1(\nu, 0^+)\\ &= \int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}n_F(\epsilon)A(\nu,\epsilon)\end{aligned}$$

Matsubara Green function and retarded Green function

Following the derivation in the textbook, written by Bruus and K, Ch.11 section 2, First, retarded single particle Green's function can be written as:

$$C_{AB}^R(\omega) = \frac{1}{Z}\sum_{nn'}\frac{\langle n|A|n'\rangle\langle n'|B|n\rangle}{\omega+E_n-E_{n'}+i\eta}\left(e^{\beta E_n}-(\pm)e^{-\beta E_{n'}}\right) \tag{21}$$

And by the definition of Matsubara frequency,

$$\begin{aligned}C_{AB}(\tau) &= -\frac{1}{Z}Tr[e^{\beta H}e^{\tau H}Ae^{-\tau H}B]\\ &= -\frac{1}{Z}\int \psi_n^{0*}(x)e^{\beta H}e^{\tau H}a^\dagger e^{-\tau H}a\psi_n^0(x)dx\\ &= -\frac{1}{Z}\sum_n e^{\beta E_n}\int \psi_n^{0*}(x)e^{\tau H}a^\dagger e^{-\tau H}a\psi_n^0(x)dx\\ &= -\frac{1}{Z}\sum_n e^{\beta E_n}\int \psi_n^{0*}(x)a^\dagger|\psi_{n'}\rangle\langle\psi_n|a\psi_n^0(x)dxe^{-\tau E_n-E_{n'}}\end{aligned}$$

$$\begin{aligned}C_{AB}(\tau) &= -\frac{1}{Z}Tr[e^{\beta H}e^{\tau H}Ae^{-\tau H}B] &(22)\\ &= -\frac{1}{Z}\sum_{nn'}e^{\beta H}\langle n|A|n'\rangle\langle n'|B|n\rangle\left(e^{\beta E_n}-(\pm)e^{-\beta E_{n'}}\right) &(23)\\ & &(24)\end{aligned}$$

Using Fourier Transformation,

$$\begin{aligned}C_{AB} &= \int_0^\beta d\tau e^{i\omega_n\tau}[-\frac{1}{Z}\sum_{nn'}e^{\beta H}e\langle n|A|n'\rangle\langle n'|B|n\rangle\left(e^{\beta E_n}-(\pm)e^{-\beta E_{n'}}\right)]\\ &= \frac{1}{(E_n-E\_n'+\tau\omega_n i)}(-\frac{e^{\beta H}}{Z})e^{\tau(E_n-E_{n'}+i\omega+n)}|_0^\beta\end{aligned}$$

Therefore,

$$C_{AB} = \frac{1}{Z}\sum_{nn'}\frac{\langle n|A|n'\rangle\langle n'|B|n\rangle}{i\omega_n+E_n-En'}(e^{\beta E_n}-\pm e^{\beta E_{n'}}) \tag{25}$$

Consider the function in entire complex plane, where $z = x+iy$,

$$C_{AB} = \frac{1}{Z}\sum_{nn'}\frac{\langle n|A|n'\rangle\langle n'|B|n\rangle}{z+E_n-En'}(e^{\beta E_n}-\pm e^{\beta E_{n'}}) \tag{26}$$

According to the theory of analytic functions : if two functions coincide in an a infinite set of points then they are fully identical functions within the entire domain where at least one of them is analyitc function. That is, if $C_{AB}(i\omega)$ is known, then $C^R_{AB}(\omega)$ can be found :

$$C^R_{AB}(\omega) = C_{AB}(i\omega \rightarrow \omega + i\eta) \tag{27}$$

Where η is infinitesimal real value.