Sum formula including Matsubara frequencies

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This short note summarizes formulas including an infinite sum with Matsubara frequencies and their proofs. We define $\beta = 1/(k_\mathrm{B}T)$ with Boltzmann constant k_B and absolute temperature T. $\hbar$ is reduced Planck's constant. A function $g(z)$ of a complex number z is assumed to be analytic near the imaginary axis.

1 Bosonic system

First we define Bosonic Matsubara frequency $\nu_n = \frac{2\pi n}{\beta\hbar}$ where n is an integer. Following relation holds

$$\frac{1}{\beta}\sum_{n=-\infty\ (n\neq 0)}^{\infty} g(i\hbar\nu_n) = -\frac{1}{2\pi i}\int_C dz \frac{g(z)}{e^{\beta z}-1}, \tag{1}$$

where the path of the contour integration is depicted in Fig. 1. Let us examine the poles of the function $(\exp[\beta z]-1)^{-1}$ in the integral. Put $z = z_z + \epsilon$, where z_z is the zero-point and ϵ is a small number and require that $\exp[\beta(z_z+\epsilon)] - 1 = 0$ is satisfied. Then $e^{\beta z_z} = 1 \leftrightarrow z_z = \frac{2n\pi}{\beta} i = i\hbar\nu_n$ are single poles and their residues are $\epsilon = \beta^{-1}$. Noting the contour shown in the right Figure 1 is clockwise, we evaluate the contour integral as

$$\begin{aligned} -\frac{1}{2\pi i}\int_C dz \frac{g(z)}{e^{\beta z}-1} &= -\frac{1}{2\pi i}\sum_{n\neq 0}(-2\pi i)\ \frac{g(z)}{e^{\beta z}-1}(z - i\hbar\nu_n)\Big|_{z=i\hbar\nu_n} \\ &= \sum_{n\neq 0}\frac{1}{\beta}g(i\hbar\nu_n). \end{aligned} \tag{2}$$

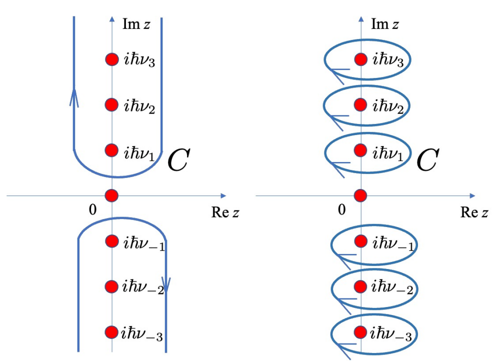

Figure 1: Integration contour in a complex plane. The two contours in the left and right figures are equivalent.

1.1 Corollary of Eq. (1)

Using the formula (1), we will show following relation[1] (we assume $\omega > 0$) :

$$\coth\left(\frac{1}{2}\beta\hbar\omega\right) = \frac{2}{\beta\hbar\omega}\left(1 + 2\sum_{n=1}^{\infty}\frac{\omega^2}{\nu_n^2 + \omega^2}\right). \tag{3}$$

Let us first define a function $g(z)$,

$$g(z) \equiv \frac{1}{(\hbar\omega)^2 - z^2}. \tag{4}$$

Putting this into the left hand side of Eq. (1), we have

$$\frac{1}{\beta}\sum_{n\neq 0} g(i\hbar\nu_n) = \frac{1}{\beta}\sum_{n\neq 0}\frac{1}{(\hbar\omega)^2 + (\hbar\nu_n)^2} = \frac{2}{\beta\hbar^2}\sum_{n=1}^{\infty}\frac{1}{\nu_n^2 + \omega^2}. \tag{5}$$

The right hand side of Eq. (1) is

$$-\frac{1}{2\pi i}\int_C dz \frac{g(z)}{e^{\beta z} - 1} = \frac{1}{2\pi i}\int_C dz \frac{1}{(e^{\beta z} - 1)(z^2 - (\hbar\omega)^2)}, \tag{6}$$

then we deform the contour as shown in Fig. 2, which contains three single poles, $z = 0, \hbar\omega, -\hbar\omega$. Hence, the integral becomes

$$\begin{aligned} &\frac{2\pi i}{2\pi i}\left\{ \left.\frac{z}{(e^{\beta z} - 1)(z^2 - (\hbar\omega)^2)}\right|_{z=0} + \left.\frac{z - \hbar\omega}{(e^{\beta z} - 1)(z^2 - (\hbar\omega)^2)}\right|_{z=\hbar\omega} + \left.\frac{z + \hbar\omega}{(e^{\beta z} - 1)(z^2 - (\hbar\omega)^2)}\right|_{z=-\hbar\omega}\right\} \\ &= \frac{1}{\beta}\left(-\frac{1}{(\hbar\omega)^2}\right) + \frac{1}{(e^{\beta\omega} - 1)(2\hbar\omega)} + \frac{1}{(e^{-\beta\omega} - 1)(-2\hbar\omega)} = -\frac{1}{\beta(\hbar\omega)^2} + \frac{1}{2\hbar\omega}\coth\left(\frac{1}{2}\beta\hbar\omega\right). \end{aligned} \tag{7}$$

Equating this with Eq. (5), we have the relation Eq. (3).

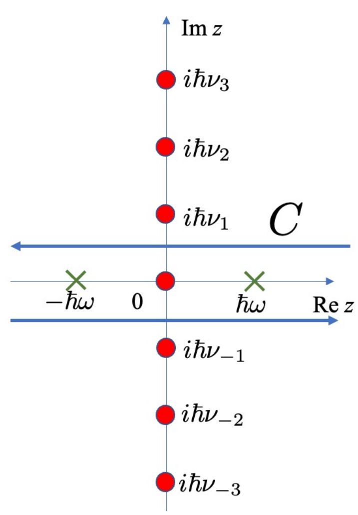

Figure 2: Deformed integration contour in a complex plane.

2 Fermionic system

We define Fermionic Matsubara frequency $\omega_n = \frac{(2n+1)\pi}{\beta\hbar}$ where n is an integer. Following relation holds[2]

$$\frac{1}{\beta}\sum_{n=-\infty}^{\infty} g(i\hbar\omega_n) = \frac{1}{2\pi i}\int_C dz \frac{g(z)}{e^{\beta z}+1}, \tag{8}$$

where the path of the contour integration is depicted in Fig. 3. Let us examine the poles of the function $(\exp[\beta z]+1)^{-1}$ in the integral. Put $z = z_z + \epsilon$, where z_z is the zero-point and ϵ is a small number and require that $\exp[\beta(z_z+\epsilon)]+1 = 0$ is satisfied. Then $e^{\beta z_z} = -1 \leftrightarrow z_z = \frac{2(n+1)\pi}{\beta} i = i\hbar\omega_n$ are single poles and their residues are $\epsilon = -\beta^{-1}$. Noting the contour shown in the right Figure 3 is clockwise, we evaluate the contour integral as

$$\begin{aligned}\frac{1}{2\pi i}\int_C dz \frac{g(z)}{e^{\beta z}+1} &= \frac{1}{2\pi i}\sum_n (-2\pi i)\left.\frac{g(z)}{e^{\beta z}+1}(z - i\hbar\omega_n)\right|_{z=i\hbar\omega_n} \\ &= -\sum_n \left(-\frac{1}{\beta}\right) g(i\hbar\nu_n).\end{aligned} \tag{9}$$

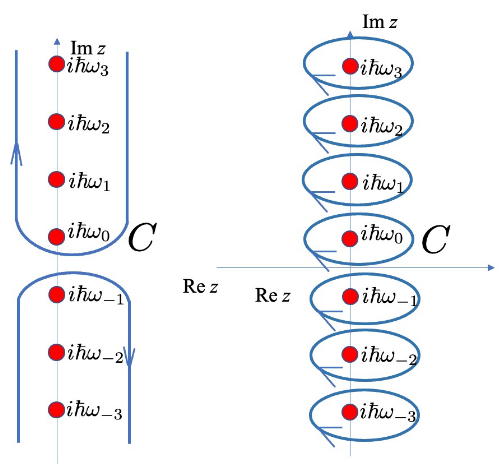

Figure 3: Integration contour in a complex plane. The two contours in the left and right figures are equivalent.

2.1 Corollary of Eq. (8)

We apply the formula (8) to the calculation of the gap equation.[3] The pair potential Δ satisfies following so-called gap equation

$$\Delta^* = -g\sum_{\boldsymbol{k}} \frac{1}{\beta}\sum_{\omega_n} \tilde{F}(\boldsymbol{k}, i\omega_n) e^{-i\omega_n\delta}, \tag{10}$$

where g and δ are the attractive potential between electron pair forming Cooper pair and small positive value, respectively. The function, $\tilde{F}(\boldsymbol{k}, \imath\omega_n)$, is called anormalous Green's function defined by

$$\tilde{F}(\boldsymbol{k}, i\omega_n) \equiv \frac{-\Delta^*}{(\hbar\omega_n)^2 + \xi_{\boldsymbol{k}}^2 + |\Delta|^2} \tag{11}$$

where $\xi_{\boldsymbol{k}}$ is the electron energy of wavenumber $\boldsymbol{k}$ measured from the Fermi energy.

We first define $\Omega \equiv \sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta|^2}$ and the factor appearing in the gap equation, $\frac{1}{\beta}\sum_n \tilde{F}(\boldsymbol{k}, i\omega_n)e^{-i\omega_n\delta}$ is just appearing in the formula (8). By identifying $g(z) \equiv -\Delta^* e^{-z\delta}/(-z^2+\Omega^2)$, we have

$$\frac{1}{\beta}\sum_n \tilde{F}(\boldsymbol{k}, i\omega_n)e^{-i\omega_n\delta} = \frac{1}{2\pi i}\int_C dz \frac{-\Delta^* e^{-z\delta}}{(e^{\beta z}+1)(-z^2+\Omega^2)}, \tag{12}$$

which can be evaluated by deforming the contour C like in Fig. (2), but now there is no pole at the origin. There are two new single poles at $z = \pm\Omega$ and the integral is evaluated as

$$\begin{aligned}\frac{1}{2\pi i}\int_C dz \frac{\Delta^* e^{-z\delta}}{(e^{\beta z}+1)(z^2-\Omega^2)} &= \frac{2\pi i\Delta^*}{2\pi i}\left\{ \left.\frac{e^{-z\delta}(z-\Omega)}{(e^{\beta z}+1)(z^2-\Omega^2)}\right|_{z=\Omega} + \left.\frac{e^{-z\delta}(z+\Omega)}{(e^{\beta z}+1)(z^2-\Omega^2)}\right|_{z=-\Omega}\right\} \\ &= \Delta^*\left\{\frac{e^{-\Omega\delta}}{(e^{\beta\Omega}+1)(2\Omega)} + \frac{e^{\Omega\delta}}{(e^{-\beta\Omega}+1)(-2\Omega)}\right\} \\ &= \frac{\Delta^*}{2\Omega}\left\{\frac{1}{e^{\beta\Omega}+1} - \frac{1}{e^{-\beta\Omega}+1}\right\} \\ &= -\frac{\Delta^*}{2\Omega}\left\{1 - 2f(\Omega)\right\},\end{aligned} \tag{13}$$

where we had introduced Fermonic distribution function $f(\epsilon) = \frac{1}{e^{\beta\epsilon}+1}$. Then putting this in the gap equation (10), we have

$$\Delta^* = g\sum_{\boldsymbol{k}} \frac{\Delta^*}{2\sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta^2|^2}}\left\{1 - 2f\left(\sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta|^2}\right)\right\}. \tag{14}$$

The obtained result can be rewritten similar to Eq. (3), expanding Fermionic distribution functions as an infinite sum,

$$f(\Omega) = \frac{1}{2}\left\{1 + \frac{2\Omega}{\beta}\sum_n \frac{1}{(\hbar\omega_n)^2 + \Omega^2}\right\}. \tag{15}$$

In addition to this, the bosonic distribution function $f_b(\Omega) = 1/(e^{\beta\Omega}-1)$ is also rewritten as an infinite sum using Eq. (3),

$$\begin{aligned} f_b(\Omega) = 2 - \coth\left(\frac{1}{2}\beta\Omega\right) &= 2 - \frac{2}{\beta\Omega} - \frac{4\Omega}{\beta}\sum_{n=1}^{\infty}\frac{1}{(\hbar\nu_n)^2+\Omega^2} \\ &= 2\left\{1 - \frac{\Omega}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(\hbar\nu_n)^2+\Omega^2}\right\}. \end{aligned} \tag{16}$$

References

[1] T. Dittrich, P. Hänggi, G. -L. Ingold, B. Kramer, G. Schön, and W. Zwerger, “Quantum Transport and Dissipation”, Wiley-VCH (1998).

[2] 阿部龍蔵、「統計力学」東京大学出版会.

[3] 田仲由喜夫、「超伝導接合の物理」名古屋大学出版会 (2021). pp.30.