Evaluation of Matsubara sums

$$S^F(\tau) = \frac{1}{\beta}\sum_{ik_n} g(ik_n)\, e^{ik_n\tau}, \quad ik_n = \frac{(2n+1)\pi}{\beta}$$

$\tau > 0$

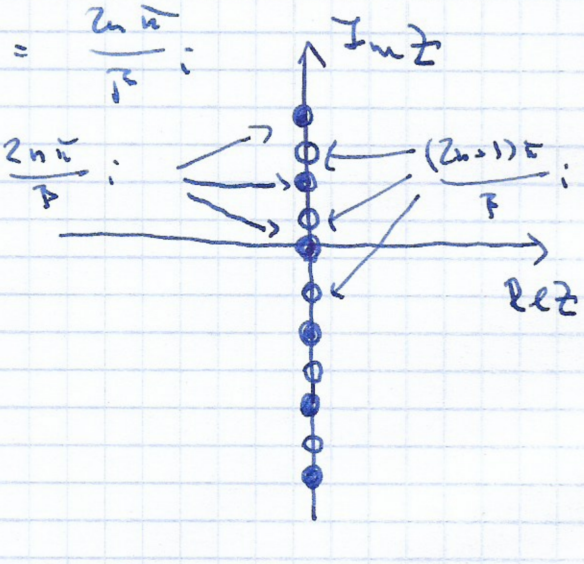
$$S^B(\tau) = \frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n)\, e^{i\omega_n\tau}, \quad i\omega_n = \frac{2n\pi}{\beta}$$

To evaluate these sums we represent them as a complex integral with using a <u>residue theory</u>

We need two functions $n(z)$ with poles at $z = ik_n$ and $z = i\omega_n$. Typical choice is

$$n_F(z) = \frac{1}{e^{\beta z}+1} \qquad \text{poles at } z = \frac{(2n+1)\pi}{\beta} i$$
odd

$$n_B(z) = \frac{1}{e^{\beta z}-1} \qquad \text{poles at } z = \frac{2n\pi}{\beta} i$$
even



Some other choice

$$n_F(z) = \frac{\beta}{2}\tanh\left(\frac{\beta z}{2}\right)$$

$$n_B(z) = \frac{\beta}{2}\coth\left(\frac{\beta z}{2}\right).$$

Indeed, $F \rightarrow e^{\beta z} = -1 = e^{(2n+1)\pi i} \rightarrow z = \frac{(2n+1)\pi}{\beta} i$

$B \Rightarrow e^{\beta z} = 1 = e^{2n\pi i} \rightarrow z = \frac{2n\pi}{\beta} i$

or

$F \rightarrow 0 = \cosh\left(\frac{\beta z}{2}\right) = \frac{1}{2}\left(e^{\beta z/2} + e^{-\beta z/2}\right) \rightarrow e^{\beta z} = (-1) \rightarrow z = \frac{(2n+1)\pi}{\beta} i$

$B \rightarrow 0 = \sinh\left(\beta z/2\right) = \frac{1}{2}\left(e^{\beta z/2} - e^{-\beta z/2}\right) \rightarrow e^{\beta z} = 1 \rightarrow z = \frac{2n\pi}{\beta} i$

Let's take the first choice.

$$\boxed{\operatorname*{Res}_{z=z_i} g(z) = \lim_{z\to z_i} \frac{d^{n-1}}{dz^{n-1}} \frac{(z-z_i)^n g(z)}{(n-1)!}}$$

The residues are

$$\operatorname*{Res}_{z=i\nu_n} n_F(z) = \lim_{z\to i\nu_n} \frac{z-i\nu_n}{e^{\beta z}+1} = \lim_{\delta\to 0} \frac{\delta}{e^{\beta i\nu_n} e^{\beta\delta}+1} =$$

$$= \lim_{\delta\to 0} \frac{\delta}{e^{(2n+1)\pi i} e^{\beta\delta}+1} = \lim_{\delta\to 0} \frac{\delta}{-e^{\beta\delta}+1} =$$

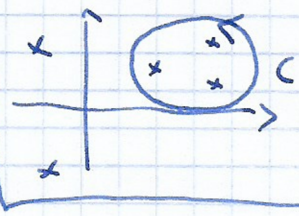
$$= \lim_{\delta\to 0} \frac{\delta}{\cancel{-1} - \beta\delta - \frac{1}{2}\beta^2\delta^2 - \dots \cancel{+1}} = \lim_{\delta\to 0} \frac{1}{-\beta - \frac{1}{2}\beta^2\delta - \dots} = \boxed{-\frac{1}{\beta}}$$

$$\operatorname*{Res}_{z=i\omega_n} n_B(z) = \lim_{z\to i\omega_n} \frac{z-i\omega_n}{e^{\beta z}-1} = \lim_{\delta\to 0} \frac{\delta}{\underbrace{e^{\beta i\omega_n}}_{=1} e^{\beta\delta}-1} =$$

$$= \lim_{\delta\to 0} \frac{\delta}{e^{\beta\delta}-1} = \lim_{\delta\to 0} \frac{\delta}{1+\beta\delta+\frac{1}{2}\beta^2\delta^2+\dots-1} = \boxed{+\frac{1}{\beta}}$$

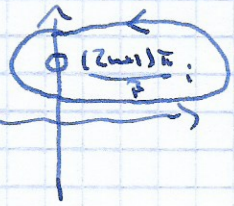
From residue theorem

$$\oint_C g(z)\,dz = 2\pi i \sum_{z_i \in C} \operatorname*{Res}_{z=z_i} g(z)$$



$$\oint_C dz\, n_F(z) g(z) = 2\pi i \operatorname*{Res}_{z=i\nu_n} [n_F(z) g(i\nu_n)] =$$

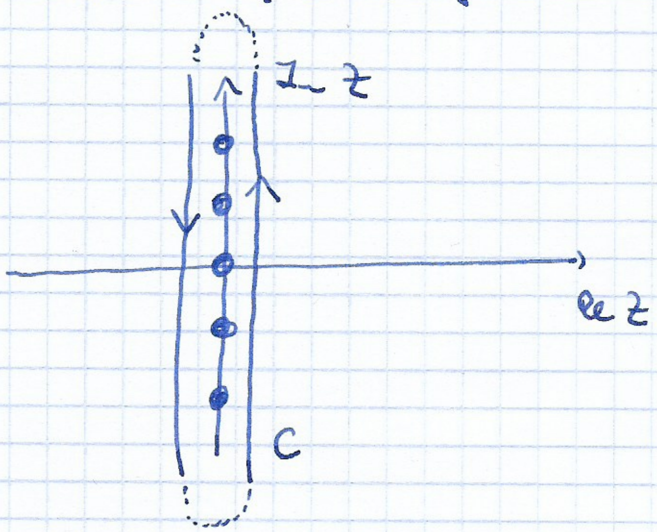
$$= -\frac{2\pi i}{\beta} g(i\nu_n)$$



in C no singularities from $g(z)$

$$\oint_C dz\, n_B(z) g(z) = 2\pi i \operatorname*{Res}_{z=i\omega_n} (n_B(z) g(i\omega_n)) = \frac{2\pi i}{\beta} g(i\omega_n)$$

The trick is to take a contour that envelopes all singular points at $z = ik_n$ or $z = i\omega_n$



and we get that

$$\varepsilon > 0 \qquad \boxed{\begin{aligned} S^F(\tau) &= \frac{1}{\beta}\sum_{ik_n} g(ik_n)e^{ik_n\tau} = -\oint_C \frac{dz}{2\pi i}\, n_F(z)\, g(z) e^{z\tau} \\ S^B(\tau) &= \frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n)e^{i\omega_n\tau} = +\oint_C \frac{dz}{2\pi i}\, n_B(z)\, g(z) e^{z\tau} \end{aligned}}$$

$\Rightarrow$ Matsubara sum is equivalent to taking a contour integral in complex plane.

Simplification comes by deforming the contour to surround singular points or cuts of $g(z)$ function only and make the integral explicit.

See the following examples.