TKM2 Übungsblatt 3: Lösungen

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1 | Matsubara Sums

a) Let us write

$$n_\epsilon(z) = \frac{1}{e^{\beta z} + \epsilon} = \begin{cases} n_B(z), & \epsilon = -1, \quad \text{Bosons} \\ n_F(z), & \epsilon = +1, \quad \text{Fermions} \end{cases} \tag{1}$$

The poles (singularities) of $n_\epsilon(z)$ are found for $e^{\beta z} = -\epsilon$. Writing $z = i\omega$ this yields

$$e^{i\beta\omega} = -\epsilon = \left.\begin{cases} +1, & \text{Bosons} \\ -1, & \text{Fermions} \end{cases}\right\} \Longrightarrow \omega = \omega_n = \begin{cases} \frac{2n\pi}{\beta}, & \text{Bosons} \\ \frac{(2n+1)\pi}{\beta}, & \text{Fermions} \end{cases} \tag{2}$$

The poles are thus

$$z_n = i\omega_n, \qquad \omega_n = \begin{cases} \frac{2n\pi}{\beta}, & \text{Bosons} \\ \frac{(2n+1)\pi}{\beta}, & \text{Fermions} \end{cases} \tag{3}$$

The residues are given by

$$\text{Res}_{z_n}[n_\epsilon(z)] = \lim_{z\to z_n}(z - z_n)n_\epsilon(z) = \lim_{z\to z_n}\frac{(z - z_n)}{e^{\beta z_n} + \epsilon} = \lim_{\delta\to 0}\frac{\delta}{e^{\beta\delta}e^{iz_n} + \epsilon} = (-\epsilon)\lim_{\delta\to 0}\frac{\delta}{e^{\beta\delta} - 1} \tag{4}$$

The last limit we can evaluate by expanding the denominator to first order $e^{\beta\delta} = 1 + \beta\delta$ and thus $\lim_{\delta\to 0}\frac{\delta}{e^{\beta\delta}-1} = \frac{1}{\beta}$. The residues are thus

$$\text{Res}_{z_n}[n_\epsilon(z)] = (-\epsilon)\frac{1}{\beta} = \begin{cases} +\frac{1}{\beta}, & \text{Bosons} \\ -\frac{1}{\beta}, & \text{Fermions} \end{cases} \tag{5}$$

b) According to the **Residue Theorem** we have, for a contour $\mathcal{C}$ enclosing a region Ω in the complex plane (i.e. $\partial\Omega = \mathcal{C}$), that

$$\oint_\mathcal{C} dz F(z) = 2\pi i \sum_{z_n\in\Omega} \text{Res}_{z_n}[F(z)] \tag{6}$$

For a product of functions $F(z) = n_\epsilon(z)h(z)$ where all the poles of $n_\epsilon(z)$, but none of the poles of $g(z)$ occur in Ω we have

$$\oint_\mathcal{C} dz n_\epsilon(z)h(z) = 2\pi i \sum_{z_n \text{ of } n_\epsilon} \text{Res}_{z_n}[n_\epsilon(z)]h(z_n) \tag{7}$$

given that the poles of $n_\epsilon(z)$ are found at $z_n = i\omega_n$ and the residues are given by $(-\epsilon)1/\beta$ we have

$$\oint_{\mathcal{C}} \frac{dz}{2\pi i} n_\epsilon(z) h(z) = (-\epsilon)\frac{1}{\beta}\sum_{\omega_n} h(i\omega_n) \tag{8}$$

Or written the other way around

$$\frac{1}{\beta}\sum_{\omega_n} h(i\omega_n) = (-\epsilon)\oint_{\mathcal{C}} \frac{dz}{2\pi i} n_\epsilon(z) h(z) \tag{9}$$

c) We choose the contour which covers the entire complex plane in a circle, i.e. $\mathcal{C} : z = \lim_{R\to\infty} Re^{i\theta}$. An integral over this contour gives us the poles z_n from the function $n_\epsilon(z)$ as well as the poles z_j of $g(z)$ (note that $e^{z\tau}$ does not have any poles):

$$\begin{aligned}\oint_{\mathcal{C}} \frac{dz}{2\pi i} n_\epsilon(z) g(z) e^{z\tau} &= \sum_{z_n} \mathrm{Res}_{z_n}[n_\epsilon(z)] g(z_n) e^{z_n\tau} + \sum_{z_j} \mathrm{Res}_{z_j}[g(z)] n_\epsilon(z_j) \\ &= (-\epsilon)\frac{1}{\beta}\sum_{\omega_n} g(i\omega_n) e^{i\omega_n\tau} + \sum_{z_j} \mathrm{Res}_{z_j}[g(z)] n_\epsilon(z_j)\end{aligned} \tag{10}$$

The integral over the contour cancels as the combination $n_\epsilon(z)e^{z\tau}$ goes to zero for $z = \lim_{R\to\infty} Re^{i\theta}$. Thus we have

$$\frac{1}{\beta}\sum_{\omega_n} g(i\omega_n) e^{i\omega_n\tau} = \epsilon \sum_{z_j} \mathrm{Res}_{z_j}[g(z)] n_\epsilon(z_j) \tag{11}$$

d) Let us start with the first sum which is the Fourier expansion of a Green's function $G_0(\boldsymbol{k}, -\tau)$ with $0 < \tau < \beta$. We have

$$G_0(\boldsymbol{k}, z) = \frac{1}{z - \xi_{\boldsymbol{k}}} \tag{12}$$

which has a single pole on the real axis at $z_j = \xi_{\boldsymbol{k}}$ with residue 1.

$$\frac{1}{\beta}\sum_{n} G_0(\boldsymbol{k}, i\omega_n) e^{i\omega_n\tau} = n_F(z_j) e^{\xi_{\boldsymbol{k}}\tau} = n_F(\xi_{\boldsymbol{k}}) e^{\xi_{\boldsymbol{k}}\tau} \tag{13}$$

Which is consistent with the definition of the thermal Green's function $G_0(\boldsymbol{k}, -\tau) = -\langle T_\tau c_{\boldsymbol{k}}(-\tau) c^\dagger_{\boldsymbol{k}}(0)\rangle = \langle c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}}\rangle e^{\xi_{\boldsymbol{k}}\tau}$. In the next sum we have explicitly

$$G_0(\boldsymbol{k}, z) G_0(\boldsymbol{k}+\boldsymbol{q}, z + i\omega_m) = \frac{1}{z - \xi_{\boldsymbol{k}}} \frac{1}{z + i\omega_m - \xi_{\boldsymbol{k}+\boldsymbol{q}}} \tag{14}$$

which has two poles, one at $z_1 = \xi_{\boldsymbol{k}}$ with residue $1/(i\omega_n - \xi_{\boldsymbol{k}+\boldsymbol{q}} + \xi_{\boldsymbol{k}})$, and one at $z_2 = \xi_{\boldsymbol{k}+\boldsymbol{q}} - i\omega_m$ with residue $-1/(i\omega_m - \xi_{\boldsymbol{k}+\boldsymbol{q}} + \xi_{\boldsymbol{k}})$. Thus we have

$$\frac{1}{\beta}\sum_{\omega_n} G_0(\boldsymbol{k}, i\omega_n) G_0(\boldsymbol{k}+\boldsymbol{q}, i\omega_n + i\omega_m) = \frac{n_F(\xi_{\boldsymbol{k}})}{i\omega_m - \xi_{\boldsymbol{k}+\boldsymbol{q}} + \xi_{\boldsymbol{k}}} - \frac{n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}} - i\omega_m)}{i\omega_m - \xi_{\boldsymbol{k}+\boldsymbol{q}} + \xi_{\boldsymbol{k}}} \tag{15}$$

For $\omega_m = (2m+1)\pi/\beta$, i.e. Fermionic Matsubara frequencies, we would have $n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}} - i\omega_m) = n_B(\xi_{\boldsymbol{k}+\boldsymbol{q}})$. However, since the sum consists of products of two Fermionic Green's functions, the Fourier-transform of this (i.e. the imaginary time representation) must be periodic in imaginary time, i.e. Bosonic (as opposed to anti-periodic for Fermionic). This is a general feature. Thus the $\omega_m = 2m\pi/\beta$ are Bosonic Matsubara frequencies as opposed to the $\omega_n = (2n+1)\pi/\beta$. We then have $n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}} - i\omega_m) = n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}})$. Unfortunately it was not made clear in the exercise that ω_m was Bosonic as opposed to ω_n which was Fermionic. Thus any answer is acceptable.

e) For such a problem we may choose the contour as consisting of two infinite semicircles - one in the upper complex half, $\mathcal{C}_+$ and the other in the lower complex half, $\mathcal{C}_-$. Together enclosing all the poles of $n_\epsilon(z)$ but avoiding the real line. The sum can then be written as

$$S(\tau) = (-\epsilon)\left(\oint_{\mathcal{C}_+} \frac{dz}{2\pi i} g(z) n_\epsilon(z) e^{z\tau} + \oint_{\mathcal{C}_-} \frac{dz}{2\pi i} g(z) n_\epsilon(z) e^{z\tau}\right) \tag{16}$$

The arc-pieces of the contour integral vanish due to the decay of $n_\epsilon(z)e^{z\tau}$ for $|z| \to \infty$. Thus what remains of the integral are the pieces just above (for $\mathcal{C}_+$) and just below (for $\mathcal{C}_-$) the real line going in opposite directions

$$S(\tau) = (-\epsilon)\left(\int_{\infty+i\delta}^{-\infty+i\delta} \frac{dz}{2\pi i} g(z) n_\epsilon(z) e^{z\tau} + \int_{-\infty-i\delta}^{\infty-i\delta} \frac{dz}{2\pi i} g(z) n_\epsilon(z) e^{z\tau}\right) \tag{17}$$

Changing variables $\varepsilon = -z + i\delta$ for the former and $\varepsilon = z + i\delta$ for the latter we get

$$S(\tau) = (-\epsilon)\left(\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} g(\varepsilon + i\delta) n_\epsilon(\varepsilon + i\delta) e^{(\varepsilon+i\delta)\tau} - \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} g(\varepsilon - i\delta) n_\epsilon(\varepsilon - i\delta) e^{(\varepsilon-i\delta)\tau}\right) \tag{18}$$

Since $n_\epsilon(z)e^{z\tau}$ is continuous over the branch-cut (real axis) we can write

$$S(\tau) = (-\epsilon)\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i}\Big(g(\varepsilon + i\delta) - g(\varepsilon - i\delta)\Big) n_\epsilon(\varepsilon) e^{\varepsilon\tau} \tag{19}$$

If we define $a(\varepsilon) = i\Big(g(\varepsilon + i\delta) - g(\varepsilon - i\delta)\Big)$ then we have

$$S(\tau) = \epsilon \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} a(\varepsilon) n_\epsilon(\varepsilon) e^{\varepsilon\tau} \tag{20}$$

f) We want to evaluate the sum

$$\begin{aligned} S_{\boldsymbol{k}} &= \frac{1}{\beta}\sum_{\omega_n} \ln\left[-i\omega_n + \xi_{\boldsymbol{k}}\right] e^{i\omega_n 0^+} \\ &= \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i}\left(\ln[-(\varepsilon + i\delta) + \xi_{\boldsymbol{k}}] - \ln[-(\varepsilon - i\delta) + \xi_{\boldsymbol{k}}]\right) n_F(\varepsilon) e^{\varepsilon 0^+} \end{aligned} \tag{21}$$

We now note that

$$\partial_\varepsilon \ln(1 + e^{-\beta\varepsilon}) = -\beta n_F(\varepsilon) \tag{22}$$

we may write

$$S_{\boldsymbol{k}} = -\frac{1}{\beta}\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i}\left(\ln[-(\varepsilon + i\delta) + \xi_{\boldsymbol{k}}] - \ln[-(\varepsilon - i\delta) + \xi_{\boldsymbol{k}}]\right) \partial_\varepsilon \ln(1 + e^{-\beta\varepsilon}) e^{\varepsilon 0^+} \tag{23}$$

Integration by parts and noting that $\ln(1+e^{-\beta\varepsilon})e^{\varepsilon 0^+}$ go to zero for $\varepsilon \to \pm\infty$ we have

$$\begin{aligned}
S_{\boldsymbol{k}} &= \frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi i}\partial_\epsilon\left(\ln[-(\varepsilon+i\delta)+\xi_{\boldsymbol{k}}]-\ln[-(\varepsilon-i\delta)+\xi_{\boldsymbol{k}}]\right)\ln(1+e^{-\beta\varepsilon})e^{\varepsilon 0^+}\\
&= -\frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi i}\left(\frac{1}{\varepsilon+i\delta-\xi_{\boldsymbol{k}}}-\frac{1}{\varepsilon-i\delta-\xi_{\boldsymbol{k}}}\right)\ln(1+e^{-\beta\varepsilon})e^{\varepsilon 0^+}\\
&= -\frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi i}\left(\mathcal{P}\frac{1}{\varepsilon-\xi_{\boldsymbol{k}}}-i\pi\delta(\varepsilon-\xi_{\boldsymbol{k}})-\mathcal{P}\frac{1}{\varepsilon-\xi_{\boldsymbol{k}}}-i\pi\delta(\varepsilon-\xi_{\boldsymbol{k}})\right)\ln(1+e^{-\beta\varepsilon})e^{\varepsilon 0^+}\\
&= \frac{1}{\beta}\int_{-\infty}^{\infty}d\varepsilon\delta(\varepsilon-\xi_{\boldsymbol{k}})\ln(1+e^{-\beta\varepsilon})e^{\varepsilon 0^+}\\
&= \frac{1}{\beta}\ln(1+e^{-\beta\xi_{\boldsymbol{k}}})
\end{aligned} \tag{24}$$

Where in the last equality I dropped the (no longer necessary) convergence factor $e^{\xi_{\boldsymbol{k}}0^+}$. Inserting this into the expression for the free energy

$$F = -\sum_{\boldsymbol{k}} S_{\boldsymbol{k}} = -\frac{1}{\beta}\sum_{\boldsymbol{k}}\ln(1+e^{-\beta\xi_{\boldsymbol{k}}}) = -k_BT\ln\left(\Pi_{\boldsymbol{k}}(1+e^{-\beta\xi_{\boldsymbol{k}}})\right) = -k_BT\ln Z \tag{25}$$