Prof. Dr. Mathias Scheurer
Institute for Theoretical Physics III, University of Stuttgart

April 24th, 2024
SS 2024

Problem 3.1: Matsubara Summations Warmup

[**Oral** | 8 pt(s)]

ID: ex_matsubara_i:qft24

Learning objective

Due to the β periodicity arising in the imaginary time formulation of the path integral we can write (imaginary) time integrals as discrete sums over Matsubara frequencies. Those can be viewed as sums of residues which allows us to solve them very elegantly using complex analysis.

In this exercise, we will learn how sums of the form

$$S = T \sum_{n\in\mathbb{Z}} h(i\omega_n) \tag{1}$$

with $\omega_n = 2n\pi T$ for bosons ($\zeta = -1$ in the following) and $\omega_n = (2n+1)\pi T$ for fermions ($\zeta = +1$) can be very efficiently evaluated at arbitrary temperature T.

a) As a first step, determine the poles of the Fermi ($\zeta = +1$) and Bose ($\zeta = -1$) function, **1**pt(s)

$$n_\zeta(z) = \frac{1}{e^{\beta z} + \zeta}, \quad \beta = T^{-1}, \tag{2}$$

and associated residues.

b) With this in mind, show that the sum in Eq. (1) can be written as **2**pt(s)

$$S = \frac{-\zeta}{2\pi i} \oint_{\mathcal{C}} \mathrm{d}z n_\zeta(z) h(z), \tag{3}$$

where the contour $\mathcal{C}$ encloses the infinite set of points $\{i\omega_n \mid n \in \mathbb{Z}\}$ in a counter-clockwise manner and $h(z)$ is analytic in the domain bound by $\mathcal{C}$.

c) As a first example, let $h(z) = f(z)e^{z\tau}$ in Eq. (1) with $0 < \tau < \beta$ and $f(z)$ being finite at $|z| \to \infty$. By appropriately choosing/deforming the contour $\mathcal{C}$ show that **2**pt(s)

$$S = \zeta \sum_{m=1}^{N_p} n_\zeta(z_m) \mathrm{Res}[f(z), z = z_m] e^{z_m \tau} \tag{4}$$

if $f(z)$ only has simple poles at $z = z_m$, $m = 1, \ldots, N_p$ with $z_m \neq i\omega_n \,\forall n, m$. In Eq. (4), $\mathrm{Res}[f(z), z = z_m]$ denotes the residue of f at z_m.

d) Use the result from (c) to calculate (both for fermions and bosons) **1**pt(s)

$$\lim_{\tau\to 0^+} T \sum_{n\in\mathbb{Z}} G_0(i\omega_n, \boldsymbol{k}) e^{i\omega_n \tau}, \tag{5}$$

where $G_0(i\omega, \boldsymbol{k}) = (i\omega - \epsilon_{\boldsymbol{k}})^{-1}$ denotes the single-particle (Matsubara) Green's function of a noninteracting system with dispersion $\epsilon_{\boldsymbol{k}}$.

e) Perform the summation in **2pt(s)**

$$T \sum_{n \in \mathbb{Z}} G_0(i\omega_n, \boldsymbol{k}) G_0(i\omega_n + i\Omega_m, \boldsymbol{k} + \boldsymbol{q}), \tag{6}$$

where ω_n and Ω_m are fermionic and bosonic Matsubara frequencies, respectively.

Problem 3.2: Matsubara Summations (continued) [**Oral** | 5 pt(s)]

ID: ex_matsubara_ii:qft24

Learning objective

As a continuation of the previous exercise, we shall see how the the free energy F for a non-interacting fermionic system can be obtained in terms of the Matsubara Green's function.

In exercise b) of the previous problem you showed that the sum

$$S(t) = T \sum_{n \in \mathbb{Z}} f(i\omega_n) e^{i\omega_n t}, \tag{7}$$

can be written as a contour integral

$$S(t) = \frac{-\zeta}{2\pi i} \oint_{\mathcal{C}} dz n_\zeta(z) f(z) e^{zt}, \tag{8}$$

where $\mathcal{C}$ consists of two vertical lines enclosing the infinite number of poles of n_ζ. Here, $\zeta = +1(-1)$ stands for Fermions (Bosons) as before.

a) Assume now that $f(z)$ is analytic everywhere except on the real axis. By deforming C show that **3pt(s)**

$$S = \frac{-\zeta}{2\pi i} \int_{-\infty}^{\infty} d\omega n_\zeta(\omega) \left[f\left(\omega + i0^+\right) - f\left(\omega - i0^+\right) \right] e^{\omega t} \tag{9}$$

holds.

Hint: You may assume that $f(z)$ decays away in a suitable form as $z \to \infty$.

b) For a non-interacting electron gas the free energy can be written in terms of the Matsubara Green's function as **2pt(s)**

$$F = -T \sum_{\mathbf{k}} \sum_{n} \ln \left[-G_0^{-1}(\mathbf{k}, i\omega_n) \right] e^{i\omega_n 0^+}. \tag{10}$$

Using part (a), compute the sum over n and show that F is the well-known expression from non-interacting fermion theory

$$F = -k_B T \ln Z, \quad \text{with} \quad Z = \Pi_{\mathbf{k}} \left(1 + e^{-\beta \xi_{\mathbf{k}}}\right). \tag{11}$$

Hint: In order to carry out the calculation, you will have use the fact that the logarithm can only be defined with a branch-cut (if one wants to avoid multivalued functions). It is convenient to choose a definition where the logarithm $\log z$ has its branch-cut in $[-\infty, 0]$.

Problem 3.3: Kitaev Chain Model

[**Written** | 9 pt(s)]

ID: ex_kitaev_chain:qft24

> **Learning objective**
>
> As a reminder of the second quantization formalism we are going to consider the Kitaev chain model. More specifically, we shall see how this model can be naturally diagonalized with Majorana operators.

Let us consider the Kitaev chain model,

$$H = -\sum_{j=1}^{N-1} \left[t\, c_j^\dagger c_{j+1} + \Delta\, c_j c_{j+1} + \text{H.c.} \right] - \mu \sum_{j=1}^{N} \left(c_j^\dagger c_j - \frac{1}{2} \right), \tag{12}$$

$t, \Delta, \mu \in \mathbb{R}$. In this exercise, we will investigate a finite chain with edges. For this purpose, it is convenient to introduce two Hermitian operators (also known as Majorana[1] operators) $\gamma_{jA} = \gamma_{jA}^\dagger$ and $\gamma_{jB} = \gamma_{jB}^\dagger$ per site j and write

$$c_j = \frac{1}{\sqrt{2}} \left(\gamma_{jA} + i\gamma_{jB} \right), \qquad c_j^\dagger = \frac{1}{\sqrt{2}} \left(\gamma_{jA} - i\gamma_{jB} \right). \tag{13}$$

a) Determine the anticommutation relations satisfied by the Majorana operators. **2** pt(s)

b) Represent the Kitaev model (12) in terms of Majorana operators. **2** pt(s)

c) For the special case $\Delta = t$, $\mu = 0$, the Hamiltonian assumes a particularly simple form in terms of the new operators **4** pt(s)

$$b_j = \frac{1}{\sqrt{2}} \left(\gamma_{jA} + i\gamma_{j+1,B} \right), \qquad b_j^\dagger = \frac{1}{\sqrt{2}} \left(\gamma_{jA} - i\gamma_{j+1,B} \right). \tag{14}$$

Show that b_j and $b_j^\dagger$ satisfy the usual fermionic anticommutation relations. Rewrite H for $\Delta = t$, $\mu = 0$ in terms of b_j and $b_j^\dagger$ and determine the spectrum of the system.

d) Taking a closer look at the Hamiltonian expressed in terms of Majorana operators in the limit $\Delta = t$, $\mu = 0$ reveals that there are exactly two out of the $2N$ Majorana operators introduced in (13) that do not enter the Hamiltonian. Where are these operators located spatially? Show that this leads to a two-fold degeneracy of the spectrum. **1** pt(s)

Hint: Use these two Majorana operators to construct a single ordinary fermionic operator in the same way as in (13).

[1] Named after the Italian physicist E. Majorana (1906 – 1959).