

11 Lesson 11

11.1 Quantum Statistical Mechanics

11.1.1 A few additional words on Matsubara Frequencies

A flavor on how it works. We will use the contour integral method.

For example, let's inspect free Fermions,

$$f(z) = \frac{1}{e^{\beta z} + 1}. \quad (11.1)$$

This function has poles at each $z = i\omega_n$ with strength $-k_B T$. We see it immediately from

$$f(z = i\omega + \delta) = \frac{1}{e^{\beta(i\omega + \delta)} + 1} \simeq -\frac{1}{\beta\delta} = -\frac{k_B T}{\delta}. \quad (11.2)$$

Now, suppose we have a general function $F(i\omega_n)$. Then

$$k_B T \sum_n F(i\omega_n) = \int_C \frac{dz}{2\pi i} F(z) f(z), \quad (11.3)$$

and C represents some contour, and we applied Jordan's lemma.

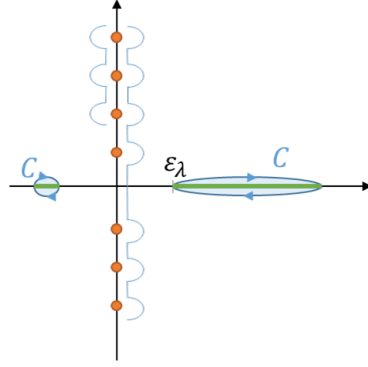


Figure 11.1: The contour on Matsubara Frequencies.

11.1.2 Free energy of a gas of free Fermions

Let's recall the Free energy of a gas of Fermions,

$$H = \sum_{\lambda} \varepsilon_{\lambda} c_{\lambda}^{\dagger} c_{\lambda}, \quad \varepsilon_{\lambda} = E = \lambda - \mu. \quad (11.4)$$

The number of particles $N(\mu)$ is given by the Green's function

$$N_{\lambda} = \langle c_{\lambda}^{\dagger} c_{\lambda} \rangle = G_{\lambda}(0^{-}), \quad (11.5)$$

where

$$G_{\lambda}(\tau) = T \sum_{i\omega_n} G_{\lambda}(\omega_n) e^{-i\omega_n \tau}. \quad (11.6)$$

Therefore,

$$N(\mu) = \sum_{\lambda} N_{\lambda} = T \sum_{\lambda, \omega_n} G_{\lambda}(i\omega_n) e^{i\omega_n 0^+}. \quad (11.7)$$

Hence,

$$N(\mu) = -\frac{\partial F}{\partial \mu} \Rightarrow F = -\int^{\mu} d\mu' N(\mu'). \quad (11.8)$$

Explicitly,

$$F = -T \sum_{\lambda, \omega_n} \int^{\mu} d\mu' \frac{e^{i\omega_n 0^+}}{i\omega_n - E_{\lambda} - \mu'} = -T \sum_{\lambda, \omega_n} e^{i\omega_n 0^+} \ln(\varepsilon_{\lambda} - i\omega_n), \quad (11.9)$$

and we have

$$F = \sum_{\lambda} \oint \frac{dz}{2\pi i} f(z) \ln(\varepsilon_{\lambda} - z) e^{z 0^+}. \quad (11.10)$$

Notice that $F(z) \equiv \ln(\varepsilon_\lambda - z)$ has a branch cut running from $\varepsilon_\lambda \rightarrow +\infty$. Hence

$$F = \sum_\lambda \int_{\varepsilon_\lambda}^{\infty} \frac{d\omega}{\pi} f(\omega) = -T \ln(1 + e^{-\beta\varepsilon_\lambda}). \quad (11.11)$$

Similarly for free Bosons we'd have the same expression, but with a $-$ sign and another set of ε_λ .

11.1.3 Another approach

Let's look on free Bosons (photon gas). Their partition function reads

$$\ln Z(T, V) = \sum_{\text{modes}} (-\ln(1 - e^{-\beta\hbar\omega})). \quad (11.12)$$

But,

$$\begin{aligned} -\ln(1 - e^{-\beta\hbar\omega}) &= \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta\hbar\omega} \\ &= \sum_{n=1}^{\infty} \frac{1}{n} \int_0^{\infty} \frac{d\tau}{\tau} \cdot \frac{e^{-\omega^2\tau}}{\sqrt{\tau}} \cdot e^{-n^2 \frac{(\hbar\beta)^2}{4\tau}} \cdot \frac{\hbar\beta n}{4\pi} \\ &= \frac{\hbar\beta}{4\pi} \int_0^{\infty} \frac{d\tau}{\tau} \frac{1}{\sqrt{\tau}} e^{-\omega^2\tau} \left(\sum_{n=1}^{\infty} e^{-n^2 \frac{(\hbar\beta)^2}{4\tau}} \right). \end{aligned} \quad (11.13)$$

We shall now use the Poisson formula

$$\sum_{n=-\infty}^{\infty} e^{-n^2 t} = \sqrt{\frac{\pi}{t}} \sum_{n=-\infty}^{\infty} e^{-\frac{\pi^2 n^2}{t}}. \quad (11.14)$$

We also have to account for the zero point energy $\frac{\hbar\omega}{2}$ (since we are dealing with harmonic oscillators). Therefore, the partition function goes to

$$\ln Z(T, V) = \sum_{\text{modes}} \left(-\frac{\beta\hbar\omega}{2} - \ln(1 - e^{-\beta\hbar\omega}) \right), \quad (11.15)$$

and after some calculation we have

$$\ln Z(T, V) = \frac{1}{2} \sum_{\text{modes}} \int_0^{\infty} \frac{d\tau}{\tau} e^{-\omega^2\tau} \sum_{n=-\infty}^{\infty} e^{-n^2 \left(\frac{2\pi}{\hbar\omega}\right)^2 \tau}. \quad (11.16)$$

Note that τ has units of [time²].

11.1.4 Matsubara modes

Let's define $\partial_0^2 \equiv \frac{\partial^2}{\partial t^2} + \text{PBCs}$ (periodic boundary conditions). Hence

$$\partial_0^2 \varphi(t) = \lambda^2 \varphi(t), \quad \varphi(t + \hbar\beta) = \varphi(t). \quad (11.17)$$

Also,

$$\text{Tr}_M \left(e^{-\tau \partial_0^2} \right) = \sum_{n=-\infty}^{\infty} e^{-n^2 \left(\frac{2\pi}{\hbar\omega}\right)^2 \tau}. \quad (11.18)$$

We now can write

$$\ln Z(T, V) = \frac{1}{2} \sum_{\text{modes}} \int_0^{\infty} \frac{d\tau}{\tau} e^{-\omega^2\tau} \text{Tr}_M \left(e^{-\tau \partial_0^2} \right). \quad (11.19)$$

Here M represents the Matsubara frequencies. Next, let $\omega = c|\mathbf{k}|$ and $\omega^2 = c^2 k^2$ so that $e^{-\omega^2\tau} = e^{-c^2 k^2 \tau}$. Therefore

$$\sum_{\text{modes}} e^{-\omega^2\tau} = \text{Tr}_{\mathbb{M}} \left(e^{-\tau c^2 \Delta} \right), \quad (11.20)$$

where Δ is the Laplacian and \mathbb{M} is some manifold, on which we integrate.

Hence we write

$$\begin{aligned} \ln Z(T, V) &= \frac{1}{2} \int_0^{\infty} \frac{d\tau}{\tau} \text{Tr}_{\mathbb{M}} \left(e^{-\tau c^2 \Delta} \right) \text{Tr}_M \left(e^{-\tau \partial_0^2} \right) \\ &= \frac{1}{2} \int_0^{\infty} \frac{d\tau}{\tau} \text{Tr}_{\mathbb{M} \times M} \left(e^{-\tau (\partial_0^2 + c^2 \Delta)} \right) \\ &= -\frac{1}{2} \text{Tr}_{\mathbb{M} \times M} \ln (\partial_0^2 + c^2 \Delta). \end{aligned} \quad (11.21)$$

Here we used $-\int_0^\infty \frac{d\tau}{\tau} \exp(-\hat{O}\tau) = \ln \hat{O}$. We now use the identity $\text{Tr} \ln \hat{A} = \ln \det \hat{A}$, and obtain

$$\boxed{\ln Z(T, V) = -\frac{1}{2} \ln \det_{\mathbb{M} \times \mathbb{M}} (\partial_0^2 + c^2 \Delta)}. \quad (11.22)$$

Note that though it looks like the wave equation, it is not. First, we used a special time derivative ∂_0^2 . Second, the wave equation has a minus sign; we have a plus because we have an imaginary time.

11.1.5 Some Calculations

We shall now see how the equation (11.22) is useful. Let the volume of the system be $V = L^d$. Therefore

$$\begin{aligned} \ln Z(T, V) &= \int_0^\infty \frac{d\tau}{\tau} \left(\sum_{n=-\infty}^\infty e^{-n^2 \left(\frac{2\pi}{\hbar\omega}\right)^2 \tau} \right) \sum_{\text{modes}} e^{-\omega^2 \tau} \\ &= \int_0^\infty \frac{du}{u} f(u) \sum_{\text{modes}} e^{-(\hbar\beta)^2 \omega^2 u} & u &\equiv \frac{\tau}{(\hbar\beta)^2} \\ &= \int_0^\infty \frac{du}{u} f(u) \sum_n e^{-(\hbar\beta c V^{-1/d})^2 u n^2}. & \omega &= c |\mathbf{k}| = c \frac{2\pi \mathbf{n}}{V^{1/d}} \text{ (in a box)} \end{aligned} \quad (11.23)$$

Hence

$$\ln Z(T, V) = g(\hbar\beta c V^{-1/d}) = g(L_\beta/L), \quad (11.24)$$

and $L_\beta = \hbar\beta c$ is the deBroglie wavelength and L is the geometrical wavelength.

Since we know the partition function, we can calculate several thermodynamic properties:

$$F(T, V) = -\frac{1}{\beta} \ln Z, \quad (11.25a)$$

$$U = -\frac{\partial}{\partial \beta} \ln Z \quad (11.25b)$$

$$P = -\left(\frac{\partial F}{\partial V}\right)_T \quad (11.25c)$$

and

$$PV = \frac{1}{d} U. \quad (11.26)$$

11.1.6 Another approach: One-loop Quantum Corrections

Now, in the previous section we cheated a bit. We obtained an equation of the form

$$\ln Z(T, V) = -\frac{1}{2} \ln \det_{\mathbb{M} \times \mathbb{M}} (\hat{A}). \quad (11.27)$$

Now, for example, the manifold as a line $\mathbb{M} = [0, L]$ and $\hat{A} = -\frac{d^2}{dx^2}$. The spectrum now is $\lambda_n = \frac{\pi^2}{L^2} n^2$, $n \in \mathbb{Z}^*$. Hence $\det \hat{A} = \prod_{n=-\infty}^\infty n^2$. In other words, we got a beautiful result (11.22), but never stopped to ask whether this $g(\hbar\beta c V^{-1/d})$ exists at all.

11.1.7 A useful representation: ζ -functions

Let's use a regularization to solve this problem. Let an operator \hat{A} with spectrum $\{\lambda_n\}$. Let us define

$$\zeta_A(s) = \sum'_n \frac{1}{\lambda_n^s}, \quad s \in \mathbb{C}. \quad (11.28)$$

Also

$$\ln \det \hat{A} = \text{Tr} \ln \hat{A} = \sum_n \ln \lambda_n. \quad (11.29)$$

Formally, we write

$$\frac{d}{ds} \zeta_A(s) = \frac{d}{ds} \sum'_n e^{-s \ln \lambda_n} = -\sum'_n \ln \lambda_n e^{-s \ln \lambda_n}, \quad (11.30)$$

hence

$$\left. \frac{d}{ds} \zeta_A(s) \right|_{s=0} = -\sum_n \ln \lambda_n = -\ln \det \hat{A}. \quad (11.31)$$

Herr RIEMANN (1859) defined the ζ -function as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \quad s \in \mathbb{C} \text{ (except for } s = 1\text{)}. \quad (11.32)$$

It has some useful relations

$$\left. \begin{aligned} \zeta(s) &= \zeta(1-s) \chi(s) \\ \chi(s) &\equiv 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s) \end{aligned} \right\} \Rightarrow \dots \Rightarrow \Gamma\left(\frac{s}{2}\right) \zeta(s) = \pi^{s-\frac{1}{2}} \Gamma\left(\frac{1-s}{2}\right) \zeta(1-s). \quad (11.33)$$

So that if it is defined somewhere, it is defined everywhere. For example, we have

$$\zeta(0) = 1 + 1 + \dots = -\frac{1}{2}. \quad (11.34)$$

Let's return to our sheep.

$$\begin{aligned} \ln Z(T, V) &= -\frac{1}{2} \text{Tr} \ln \widehat{A}^{\partial_0^2 + c^2 \Delta} \\ &= -\frac{1}{2} 2 \sum_{n=1}^{\infty} V \int \frac{d^3 k}{(2\pi)^3} \ln \left[\left(\frac{2\pi n}{\hbar\beta} \right)^2 + c^2 k^2 \right]. \end{aligned} \quad (11.35)$$

Now, use the relation

$$\int \frac{d^3 k}{(2\pi)^3} \ln(\alpha^2 + k^2) = -\frac{\Gamma(-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}} \alpha^d, \quad (11.36)$$

and have

$$\ln Z(T, V) = V \underbrace{\sum_{n=1}^{\infty} \frac{\Gamma(-\frac{3}{2})}{(4\pi)^{\frac{3}{2}}} \left(\frac{2\pi n}{\hbar\beta} \right)^3}_{\zeta(-3) \propto \zeta(4) = \frac{\pi^4}{90}} \quad (11.37)$$

hence

$$\boxed{\ln Z(T, V) = \frac{\pi^2}{90} \left(\frac{k_B T}{\hbar c} \right)^3 V.} \quad (11.38)$$

Note that all of this is for equilibrium statistical mechanics.