Tutorial class 2: Functional integral for a non-interacting boson gas

We consider a non-interacting boson gas with grand canonical Hamiltonian

$$\hat{H} = \sum_\alpha \xi_\alpha \hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha \qquad (\xi_\alpha = \epsilon_\alpha - \mu), \tag{1}$$

where $\{|\alpha\rangle, \epsilon_\alpha\}$ denotes a basis in which the one-body Hamiltonian is diagonal. The partition function can be written as

$$Z = \lim_{N\to\infty} \int \prod_{k=1}^N d(\psi_k^*, \psi_k) \exp\Big\{ - \sum_\alpha \sum_{k=1}^N \big[\psi^*_{k,\alpha} \left(\psi_{k,\alpha} - \psi_{k-1,\alpha}\right) + \frac{\beta}{N} \xi_\alpha \psi^*_{k,\alpha} \psi_{k-1,\alpha}) \big] \Big\}, \tag{2}$$

where $\psi^{(*)}_{k,\alpha}$ is a c-number, $\psi_{N,\alpha} = \psi_{0,\alpha}$, $\psi^*_{N,\alpha} = \psi^*_{0,\alpha}$ and

$$d(\psi_k^*, \psi_k) = \prod_\alpha \frac{d\Re[\psi_{k,\alpha}] d\Im[\psi_{k,\alpha}]}{\pi}. \tag{3}$$

1) Calculation of the partition function with discrete times

1.1) *Recall the result of the Gaussian integral*

$$\int \prod_{k=1}^N d(\psi_k^*, \psi_k) \exp\Big\{ - \sum_\alpha \sum_{k,k'=1}^N \psi^*_{k,\alpha} M^{(\alpha)}_{k,k'} \psi_{k',\alpha} \Big\}, \tag{4}$$

where $M^{(\alpha)}$ is a positive definite Hermitian $N \times N$ matrix and $\psi^{(*)}_{k,\alpha}$ a c-number.

$$\int \prod_{k=1}^N d(\psi_k^*, \psi_k) \exp\Big\{ - \sum_\alpha \sum_{k,k'=1}^N \psi^*_{k,\alpha} M^{(\alpha)}_{k,k'} \psi_{k',\alpha} \Big\} = \prod_\alpha \left[\det M^{(\alpha)} \right]^{-1} \tag{5}$$

1.2) *Deduce the expression of the partition function (2).*

The action can be written as

$$S = \sum_\alpha \sum_{k,k'=1}^N \psi^*_{k,\alpha} S^{(\alpha)}_{k,k'} \psi_{k',\alpha}, \tag{6}$$

where $S^{(\alpha)}$ is the $N \times N$ matrix

$$S^{(\alpha)} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 & -a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & -a & 1 & 0 \\ 0 & \cdots & \cdots & 0 & -a & 1 \end{pmatrix} \tag{7}$$

with $a = 1 - \frac{\beta}{N}\xi_\alpha$. Expanding with respect to the first line, one obtains

$$\lim_{N\to\infty} \det S^{(\alpha)} = \lim_{N\to\infty} \left[1 + (-a)(-1)^{N-1}(-a)^{N-1}\right] = 1 - e^{-\beta\xi_\alpha}, \tag{8}$$

so that

$$Z = \lim_{N\to\infty} \prod_\alpha \left[\det S^{(\alpha)}\right]^{-1} = \prod_\alpha \left(1 - e^{-\beta\xi_\alpha}\right)^{-1}, \tag{9}$$

which is the standard expression for non-interacting bosons.

2) Continuous-time limit

2.1) *Give the expression of the action $S[\psi^*, \psi]$ obtained from (2) in the continuous-time limit $\psi_{k,\alpha} \to \psi_\alpha(\tau)$ ($\tau \in [0, \beta]$). Express $S[\psi^*, \psi]$ as a function of the Fourier-transformed fields*

$$\psi_\alpha(i\omega_n) = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, e^{i\omega_n\tau} \psi_\alpha(\tau), \qquad \psi^*_\alpha(i\omega_n) = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, e^{-i\omega_n\tau} \psi^*_\alpha(\tau), \tag{10}$$

where $\omega_n = 2n\pi T$ ($n \in \mathbb{Z}$) is a bosonic Matsubara frequency.

$$\begin{aligned} S[\psi^*, \psi] &= \int_0^\beta d\tau \sum_\alpha \psi^*_\alpha(\tau)(\partial_\tau + \xi_\alpha)\psi_\alpha(\tau) \\ &= \sum_{\alpha,\omega_n} \psi_\alpha(i\omega_n)(-i\omega_n + \xi_\alpha)\psi_\alpha(i\omega_n) \end{aligned} \tag{11}$$

2.2) *Compute, in the continuous-time limit, the propagator $G(\alpha, i\omega_n) = -\langle \psi_\alpha(i\omega_n)\psi^*_\alpha(i\omega_n)\rangle$ and the partition function. Is the thermodynamic potential $\Omega = -\frac{1}{\beta}\ln Z$ well defined?*

$$G(\alpha, i\omega_n) = -\frac{1}{Z} \int \mathcal{D}[\psi^*, \psi]\, \psi_\alpha(i\omega_n)\psi^*_\alpha(i\omega_n) e^{-S[\psi^*,\psi]} = \frac{1}{i\omega_n - \xi_\alpha}, \tag{12}$$

and

$$\begin{aligned} Z &= \int \mathcal{D}[\psi^*, \psi]\, e^{-S[\psi^*,\psi]} = \prod_{\alpha,\omega_n} (-i\omega_n + \xi_\alpha)^{-1} \\ \Omega &= -\frac{1}{\beta}\ln Z = \frac{1}{\beta} \sum_{\alpha,\omega_n} \ln(-i\omega_n + \xi_\alpha). \end{aligned} \tag{13}$$

The partition function vanishes, $Z = 0$, and the thermodynamic potential Ω is not defined (the sum over Matsubara frequencies does not converge).

2.3) *What is the expression of the mean particle number $\langle \hat{N} \rangle$ that can be derived from Ω obtained in question (2.2)? Compare with the result obtained from (2) before taking the continuous-time limit. How should we modify the expression of Ω obtained in question 2.2 to obtain the correct result?*

From (13), one finds

$$\langle \hat{N} \rangle = -\frac{\partial\Omega}{\partial\mu} = -\frac{1}{\beta} \sum_{\alpha,\omega_n} \frac{1}{i\omega_n - \xi_\alpha} = -\sum_\alpha G(\alpha, \tau = 0). \tag{14}$$

This should be compared with the result obtained from the discrete-time expression for the partition function,

$$\langle \hat{N} \rangle = -\frac{\partial\Omega}{\partial\mu} = \frac{1}{N} \sum_{\alpha,k} \langle \psi^*_{k,\alpha}\psi_{k-a,\alpha}\rangle = \sum_\alpha \langle \psi^*_{k,\alpha}\psi_{k-a,\alpha}\rangle \quad \text{(time-translation invariance)}. \tag{15}$$

Thus, the correct expression in the continuum-time limit should be

$$\langle \hat{N} \rangle = \sum_\alpha \langle \psi^*_\alpha(\tau)\psi_\alpha(\tau^-)\rangle = -\sum_\alpha G(\alpha, \tau = 0^-) = -\frac{1}{\beta}\sum_{\alpha,\omega_n} \frac{e^{i\omega_n 0^+}}{i\omega_n - \xi_\alpha}. \tag{16}$$

This result can also be obtained by noting that, in the continuum-time limit, the chemical potential term is $\mu \sum_\alpha \psi^*_\alpha(\tau^+)\psi_\alpha(\tau)$, with ψ^*_α evaluated at a time infinitesimally larger ψ_α. In question (3), we will see that the Matsubara sum in (16) yields the expected result $\langle \hat{N} \rangle = \sum_\alpha n_B(\xi_\alpha)$, with n_B the Bose-Einstein distribution function.

To reproduce (16) from $\langle \hat{N} \rangle = -\partial\Omega/\partial\mu$, one has to consider the following expression of the grand potential,

$$\Omega = \frac{1}{\beta}\sum_{\alpha,\omega_n} \ln(-i\omega_n + \xi_\alpha) e^{i\omega_n 0^+}. \tag{17}$$

In the following, we will see that this definition yields the known expression of the grand potential of non-interacting bosons.

2.4) *Express $\langle \hat{N} \rangle$ as a time-ordered correlation function of the operators $\hat{\psi}_\alpha(\tau) = e^{\tau \hat{H}}\hat{\psi}_\alpha e^{-\tau\hat{H}}$ and $\hat{\psi}^\dagger_\alpha(\tau) = e^{\tau \hat{H}}\hat{\psi}^\dagger_\alpha e^{-\tau\hat{H}}$. Show that the corresponding expression in the functional integral formalism agrees with the discrete-time formulation.*

$$\begin{aligned}
\langle \hat{N} \rangle &= \sum_\alpha \langle \hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha \rangle \\
&= \frac{1}{Z}\sum_\alpha \mathrm{Tr}\big[e^{-\beta\hat{H}}\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha\big] \\
&= \frac{1}{Z}\sum_\alpha \mathrm{Tr}\big[e^{-\beta\hat{H}}\hat{\psi}^\dagger_\alpha(\tau) \hat{\psi}_\alpha(\tau)\big] \quad \text{(follows from cyclic invariance of the trace)} \\
&= \sum_\alpha \langle T_\tau \hat{\psi}^\dagger_\alpha(\tau^+)\hat{\psi}_\alpha(\tau)\rangle.
\end{aligned} \tag{18}$$

In the functional integral formalism, this becomes

$$\langle \hat{N} \rangle = \sum_\alpha \langle \psi^*_\alpha(\tau^+)\psi_\alpha(\tau)\rangle = -\sum_\alpha G(\alpha, \tau = 0^-). \tag{19}$$

3) Matsubara frequency sums

We now consider both bosons and fermions. The fermionic Matsubara frequencies are defined by $\omega_n = (2n+1)\pi T$ ($n \in \mathbb{Z}$).

3.1) *Compute the frequency sum*

$$S = \frac{1}{\beta}\sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_n - \xi} \quad (\eta \to 0^+), \tag{20}$$

by considering the integral

$$I = \oint_{\mathcal{C}} \frac{dz}{2i\pi}\frac{e^{\eta z}}{z - \xi} n_\zeta(z), \qquad n_\zeta(z) = \frac{1}{e^{\beta z} - \zeta} \tag{21}$$

in the complex plane along the circle $\mathcal{C}$ of radius $R \to \infty$ centered at the origin $z = 0$. Deduce the expression of the expectation value $\langle \hat{N} \rangle$ as a function of the occupation number $n_\zeta(\xi_\alpha)$.

The factor $e^{\eta z} n_\zeta(z)$ ensures that the integral I over the contour $\mathcal{C}$ vanishes in the limit $R \to \infty$. We can also evaluate I by the residue theorem. Besides the poles of $n_\zeta(z)$ at the Matsubara frequencies ω_n (with residues ζ/β), there is a pole at $z = \xi$, so that

$$I = \sum_{\omega_n} \mathrm{Res}(i\omega_n) + \mathrm{Res}(\xi) = \zeta S + n_\zeta(\xi) = 0, \tag{22}$$

i.e.

$$\frac{1}{\beta}\sum_{\omega_n}\frac{e^{i\omega_n\eta}}{i\omega_n-\xi}=\begin{cases}-n_B(\xi) & \text{(bosons)},\\ n_F(\xi) & \text{(fermions)}.\end{cases} \tag{23}$$

3.2) *We want to compute the sum (with $\xi > 0$ for bosons)*

$$S=\frac{1}{\beta}\sum_{\omega_n}\ln(-i\omega_n+\xi)e^{i\omega_n\eta} \tag{24}$$

from the integral

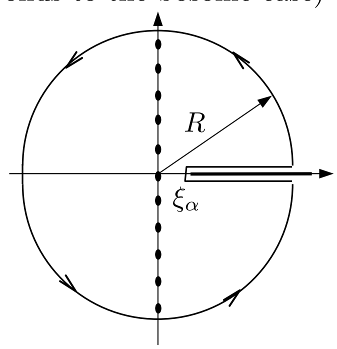
$$I=\oint_{\mathcal{C}}\frac{dz}{2i\pi}\ln(-z+\xi)n_\zeta(z)e^{\eta z}. \tag{25}$$

Why is it not possible to choose the same contour $\mathcal{C}$ as in question 3.1? By choosing an appropriate contour, show that the sum (24) can be expressed as an integral over a real variable. Compute this integral using

$$n_\zeta(\epsilon)=\frac{\zeta}{\beta}\frac{d}{d\epsilon}\ln\left|1-\zeta e^{-\beta\epsilon}\right|. \tag{26}$$

From the result obtained in question 2.3, find the usual expression of the grand potential of a non-interacting boson gas.

The function $\ln(-z+\xi)$ has a branch on the real axis for z larger than ξ. We should therefore consider the following contour (the figure corresponds to the bosonic case)



The integral vanishes on the circular part of the contour as $R\to\infty$. The contour along the branch cut gives the contribution

$$\begin{aligned} I &= \int_{\xi^-}^{\infty}\frac{d\epsilon}{2i\pi}n_\zeta(\epsilon)\ln(-\epsilon-i\eta+\xi)+\int_{\infty}^{\xi^-}\frac{d\epsilon}{2i\pi}n_\zeta(\epsilon)\ln(-\epsilon+i\eta+\xi) \\ &= \int_{\xi^-}^{\infty}\frac{d\epsilon}{2i\pi}n_\zeta(\epsilon)[\ln(-\epsilon-i\eta+\xi)-\text{c.c.}] \end{aligned} \tag{27}$$

where $\xi^-=\xi-0^+$. Using

$$n_\zeta(\epsilon)=\frac{\zeta}{\beta}\frac{d}{d\epsilon}\ln\left|1-\zeta e^{-\beta\epsilon}\right|, \tag{28}$$

and integrating by parts,

$$\begin{aligned} I &= -\frac{\zeta}{\beta}\int_{\xi^-}^{\infty}\frac{d\epsilon}{2i\pi}\ln\left|1-\zeta e^{-\beta\epsilon}\right|\frac{d}{d\epsilon}[\ln(-\epsilon-i\eta+\xi)-\text{c.c.}] \\ &= -\frac{\zeta}{\beta}\int_{\xi^-}^{\infty}\frac{d\epsilon}{2i\pi}\ln\left|1-\zeta e^{-\beta\epsilon}\right|[-2i\pi\delta(\epsilon-\xi)] \\ &= \frac{\zeta}{\beta}\ln\left(1-\zeta e^{-\beta\xi}\right), \end{aligned} \tag{29}$$

since $\xi > 0$ for bosons ($\zeta=1$). On the other hand, the residue theorem gives

$$I=\frac{\zeta}{\beta}\sum_{\omega_n}\ln(-i\omega_n+\xi)e^{i\omega_n\eta}. \tag{30}$$

From (29) and (30), we finally deduce

$$S = \frac{1}{\beta} \sum_{\alpha} \ln\left(1 - \zeta e^{-\beta\xi}\right). \tag{31}$$

For bosons, this yields the familiar expression of the grand potential,

$$\Omega = \frac{1}{\beta} \sum_{\alpha,\omega_n} \ln(-i\omega_n + \xi_\alpha) e^{i\omega_n 0^+} = \frac{1}{\beta} \sum_{\alpha} \ln\left(1 - e^{-\beta\xi_\alpha}\right). \tag{32}$$

3.3) *Compute the sums*

$$S_1 = \frac{1}{\beta} \sum_{\omega_n} G_0(\mathbf{k}, i\omega_n) G_0(\mathbf{k}+\mathbf{q}, i\omega_n + i\omega_\nu), \tag{33}$$

$$S_2 = \frac{1}{\beta} \sum_{\omega_n} G_0(\mathbf{k}, i\omega_n) G_0(\mathbf{q}-\mathbf{k}, i\omega_\nu - i\omega_n), \tag{34}$$

where $\omega_n = (2n+1)\pi T$, $\omega_\nu = 2\nu\pi T$, and $G_0(\mathbf{k}, i\omega_n) = (i\omega_n - \xi_\mathbf{k})^{-1}$. [Hint: use the result found for the sum S in Eq. (20).]

$$\begin{aligned} S_1 &= \frac{1}{\beta} \sum_{\omega_n} G_0(k) G_0(k+q) \\ &= \frac{1}{\beta} \sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_\nu + \xi_\mathbf{k} - \xi_{\mathbf{k}+\mathbf{q}}} \left(\frac{1}{i\omega_n - \xi_\mathbf{k}} - \frac{1}{i\omega_n + i\omega_\nu - \xi_{\mathbf{k}+\mathbf{q}}} \right) \\ &= \frac{n_F(\xi_\mathbf{k}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{i\omega_\nu + \xi_\mathbf{k} - \xi_{\mathbf{k}+\mathbf{q}}}, \end{aligned} \tag{35}$$

using (23). Note that adding the factor $e^{i\omega_n\eta}$ in the second line is harmless since the sum converges.

Similarly, one finds

$$S_2 = \frac{1}{\beta} \sum_{\omega_n} G_0(\mathbf{k}, i\omega_n) G_0(\mathbf{q}-\mathbf{k}, i\omega_\nu - i\omega_n) = \frac{n_F(\xi_\mathbf{k}) + n_F(\xi_{\mathbf{q}-\mathbf{k}}) - 1}{i\omega_\nu - \xi_\mathbf{k} - \xi_{\mathbf{q}-\mathbf{k}}}. \tag{36}$$

3.4) *Show that the sum*

$$S = \frac{1}{\beta} \sum_{\omega_n} \frac{1}{|\omega_n|^3} \quad (\omega_n = (2n+1)\pi T) \tag{37}$$

can be directly expressed in terms the generalized Rieman Zeta function

$$\zeta(z, q) = \sum_{n=0}^{\infty} \frac{1}{(n+q)^z} \tag{38}$$

without performing an integral in the complex plane. The final result can be simplified using $\zeta(z, 1/2) = (2^z - 1)\zeta(z)$ where $\zeta(z) = \sum_{n=1}^{\infty} n^{-z}$ is the Riemann zeta function.

$$S = \frac{1}{\beta} \sum_{\omega_n} \frac{1}{|\omega_n|^3} = \frac{1}{4\pi^3 T^2} \sum_{n=0}^{\infty} \frac{1}{\left(n+\frac{1}{2}\right)^3} = \frac{1}{4\pi^3 T^2} \zeta\left(3, \frac{1}{2}\right) = \frac{7\zeta(3)}{4\pi^3 T^2}, \tag{39}$$