Homework 13, Statistical Mechanics: Concepts and applications 2019/20 ICFP Master (first year)

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This homework illustrates essential calculations of Lecture 13. Please study carefully.

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In lecture 13 (Bosonic quantum gases and liquid 1/2: Bose-Einstein condensation), we studied the connection of the canonical ensemble of N non-interacting Bosons with the grand canonical ensemble at fixed chemical potential. In fact, the grand-canonical partition function is simply the integrand of the canonical partition function taken at the saddle point of the integration contour. In this homework session, we will study this complex issue for the case of the three-dimensional uniform harmonic trap, although the reasoning is independent of the external potential.

I. DENSITY OF STATES

The single-particle density of states $\mathcal{N}(E)$ is the number of ways you can realize a many-body state with energy E. For the harmonic trap in three dimensions (with energy level $Ex, Ey, Ez = 0, 1, 2, \ldots$ so that $\hbar = 1$, $\omega = 1$, and the zero-point energy is subtracted), this is given by

$$\mathcal{N}(E) = \frac{(E+1)(E+2)}{2}. \tag{1}$$

For energy E, E_x could be $1, 2, ..., E$. For each E_x, E_y has $E - E_x + 1$ choices. After choosing E_x and E_y, E_z is fixed since $E = E_x + E_y + E_z$. Thus, the total number of states is

$$\mathcal{N}(E) = \sum_{E_x=0}^{E} E - E_x + 1 = \sum_{E_x=0}^{E} E_x + 1 = \frac{(E+1)(E+2)}{2}$$

Also re-derive this formula using the Kronecker δ function

$$\delta_{nm} = \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} e^{i(n-m).\lambda} \tag{2}$$

The density of state could also be written as

$$\begin{aligned}
\mathcal{N}(E) &= \sum_{E_x,E_y,E_z=0}^{E} \delta_{E,E_x+E_y+E_z} \\
&= \sum_{E_x,E_y,E_z=0}^{E} \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} \mathrm{e}^{\mathrm{i}(-E+E_x+E_y+E_z)\lambda} \\
&= \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} \mathrm{e}^{-\mathrm{i}E\lambda} \left(\sum_{E_x=0}^{E} \mathrm{e}^{\mathrm{i}E_x\lambda}\right) \left(\sum_{E_y=0}^{E} \mathrm{e}^{\mathrm{i}E_y\lambda}\right) \left(\sum_{E_z=0}^{E} \mathrm{e}^{\mathrm{i}E_z\lambda}\right) \\
&= \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} \mathrm{e}^{-\mathrm{i}E\lambda} \left(\frac{1-\mathrm{e}^{\mathrm{i}(E+1)\lambda}}{1-\mathrm{e}^{\mathrm{i}\lambda}}\right)^3 \\
&= \oint_{|z|=1} \frac{dz}{2\pi\mathrm{i}} z^{-(E+1)} \left(\frac{1-z^{E+1}}{1-z}\right)^3
\end{aligned}$$

where $z = \mathrm{e}^{\mathrm{i}\lambda}$ is a complex number. The result of the integral is thus the sum of residues of all the poles z_0 which satisfy $|z_0| < 1$. For $|z| < 1$, $1/(1-z) = 1 + z + z^2 + \ldots$. The integrand could thus be written as

$$(1 - z^{E+1})^3 \frac{1}{z^{E+1}} (1 + 3z + 6z^2 + \ldots)$$

The combinatoric factor in the last polynomial could be calculated using the identical argument as calculating $\mathcal{N}(E)$ using the naive method. Each of the three $1/(1-z)$ contributes some power of z for each term. For the ith term, the first $1/(1-z)$ contributes $z^{0\sim i}$. The second and third $1/(1-z)$ account for the rest. Thus, the Eth term, which is the only term related to determining the residue, has a factor of $\frac{(E+1)(E+2)}{2}$. Thus, $\mathcal{N}(E) = \frac{(E+1)(E+2)}{2}$.

II. NAIVE ENUMERATION

As we discussed in detail in Lecture 13, we may compute the partition function of non-interacting bosons by summing over all the N-body states $\sigma_1, \ldots, \sigma_N$, and by avoiding double counting through the condition $\sigma_1 < \sigma_2 < \cdots < \sigma_N$ (σ_k is a single-particle quantum state). Write such a program to compute the partition function and also the condensate fraction of $N = 5$ non-interacting bosons in a three-dimensional trap with energy states $0, 1, 2, 3, 4$ (as discussed). For your convenience, this program is already written (see `naive_bosons.py`, available on the website). Use this program to get benchmark results. You may also modify this program in order to explicitly count the number of $N = 5$ many-body states given a certain number of single-particle states (here 35).

`naive_bosons.py` *is designed to calculate the fraction of particles at the ground state. The output could be found in Fig. 1. Using this simple algorithm, it is already possible to calculate the condensate fraction for a small system.*

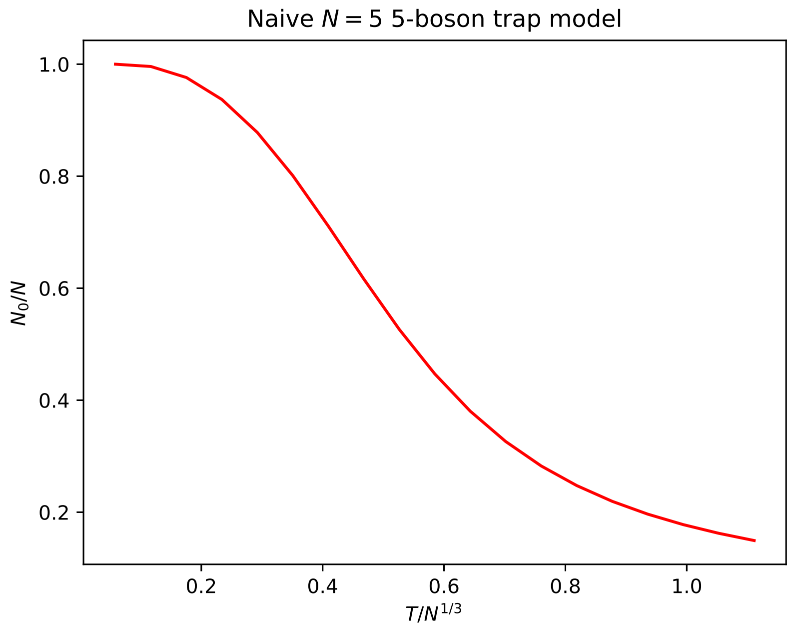

FIG. 1: The condensate fraction as a function of temperature, calculated by doing naive numeration.

III. INTEGRATION

As discussed in Lecture 13, we can also obtain the partition function, as well as thermodynamic observables, by integrating the discrete (Kronecker) δ function

$$Z_N(\beta) = \int_{-\pi+\mathrm{i}\epsilon}^{\pi+\mathrm{i}\epsilon} \frac{\mathrm{d}\lambda}{2\pi} \underbrace{\mathrm{e}^{-\mathrm{i}N\lambda} \prod_{E=0}^{E_{\max}} \left[f_E(\beta,\lambda)\right]^{\mathcal{N}(E)}}_{Z_N(\beta,\lambda)}, \tag{3}$$

with

$$f_E(\beta,\lambda) = \frac{1}{1-\exp\left(-\beta E+\mathrm{i}\lambda\right)}, \quad E > 0, \text{ (excited state)}, \tag{4}$$

a Bose-Einstein factor which comes from the sum over single-particle energy states.

In Lecture 13, we used two different formulas for $E = 0$ and for positive energies, but this is unnecessary if we move the integration contour upwards by an infinitesimal amount in the complex plane (in other words, in eq. (3) we added a little positive imaginary ϵ, to avoid the pole at $E = 0$ and $\lambda = 0$).

A. Explicit integration in the complex plane

Integrate eq. (3) in the complex plane, from $-\pi$ to π and show that you obtain exactly the same result for the partition function as the one you obtained from `naive_bosons`, if you use $E_{\max} = 4$. For your convenience, this integration program is already written (see `canonic_bosons.py` on the website).

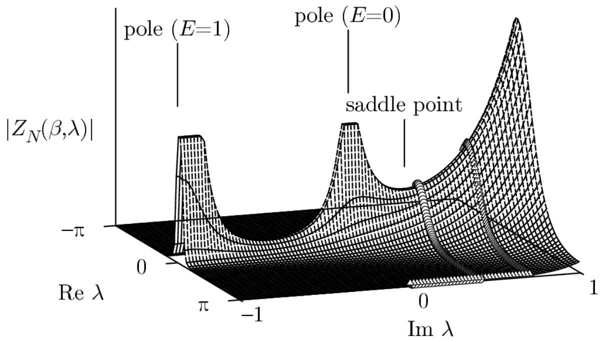

FIG. 2: Absolute value of the partition function $Z_N(\beta, \lambda)$ in the complex λ plane (for $N = 5$ and $\beta = 1$).

Using both naive numeration and explicit integration, $Z_5(\beta)$ could be evaluated. The results are shown in Table III A. As expected, the results are almost identical.

B. Experiments with the partition-function integration

In Fig. 2, you see different integration contours. Implement the integration along these contours in `canonic_bosons.py` and demonstrate that the result for the partition function Z does not change (this is simply a check of the integration theorem for analytic functions. In addition, show that the fluctuations of the integrand around the maximum changes the least if you pass through the saddle point, defined through

$$\begin{Bmatrix} \text{saddle} \\ \text{point} \end{Bmatrix} : \frac{\partial}{\mathrm{i}\partial\lambda} \left\{ -\mathrm{i}N\lambda + \sum_E \mathcal{N}(E) \log\left(1 - \mathrm{e}^{-\beta E + \mathrm{i}\lambda}\right) \right\} = 0.$$

Up to a complex i, the saddle point is equal to the chemical potential. Notice that at the saddle point $\langle N \rangle$ (for the grand-canonical formulation) equals N of the canonic model. For other extensive

T	Z(Naive numeration)	Z(Explicit integral)
0.1	1.000136224526684	1.0001366706682846-5.752221319839128e-12i
0.2	1.0207705099637532	1.0207709472344733-5.66231262437847e-12i
0.3	1.1242278972612432	1.1242282961212084-5.251378153956728e-12i
0.4	1.3548875017920095	1.3548878388740533-4.5628035926415995e-12i
0.5	1.7802348636085865	1.780235130342653-3.751763004014194e-12i
0.6	2.535546223596034	2.5355464224802655-2.926415058985978e-12i
0.7	3.8732495947558716	3.8732497353832103-2.169193002748062e-12i
0.8	6.236889859832073	6.236889954689107-1.5377737214062471e-12i
0.9	10.359307259678479	10.3593073214196-1.0747844707466746e-12i
1.0	17.373297218268803	17.373297257032995-7.664083532655879e-13i
1.1	28.915064997929925	28.915065022157002-4.608466832193404e-13i
1.2	47.199028344469035	47.1990283595266-6.141479609765191e-13i
1.3	75.04767620163041	75.04767621199802-7.21618993812497e-13i
1.4	115.86961428002716	115.86961428608755+9.439059218282899e-13i

TABLE I: $Z_5(\beta)$, calculated by naive numeration and explicit integration. Two methods give almost identical results. The infinitesimal imaginary shift is set to 0.01i.

observables, the equivalence between the two ensembles is reached only in the limit $N \to \infty$. For non-intensive quantities, there are important difference may subsist up to the thermodynamic limit.

Fig. 2 indicates that, when $Re(\lambda) = \pm\pi$, the integrand is almost 0. Thus, if the path of the integration is $-\pi \to -\pi + \epsilon \mathrm{i} \to \pi + \epsilon \mathrm{i} \to \pi$, only the $-\pi + \epsilon \mathrm{i} \to \pi + \epsilon \mathrm{i}$ part contribute to the integral. And the integral could be calculated using `canonic_boson.py` *by setting the imaginary shift to ϵ. The result is shown in Table III B. The result of integration remains almost unchanged when changing the value of ϵ. This is predicted by Cauchy's integral theorem.*

With `grandcan_boson.py`*, the value of μ could be calculated. For $N = 5$ and $T = 1$, the chemical potential $\mu = -0.33$. This means the saddle point is at $\lambda = 0.33\mathrm{i}$. The real part of integrand for fixed $Im(\lambda)$ is shown in Fig. 3. When $Im(\lambda) = -\beta\mu$ (saddle point), the integrand has a blunt peak and almost no oscillation. If $Im(\lambda)$ is larger, the integrand oscillates, and error will emerge from positive value and negative value cancelling each other. When $Im(\lambda)$ is smaller, there is a sharp peak. In order to get a accurate result, $\Delta Re(\lambda)$ has to be small. Besides, the height of this sharp peak is sensitive to the cut-off energy. Thus, using small $Im(\lambda)$ to do accurate calculation is computational expensive. Thus, the integrand is best integrated when going through the saddle point.*

$Im(\lambda)$	Z(Explicit integral)
0.01	17.373297257032995-7.664083532655879e-13j
0.11	17.37329730175706-1.4853496074908346e-12j
0.21	17.37329739413363-3.031735456503147e-12j
0.31	17.37329758143781-6.125760836483261e-12j
0.41	17.373297954755387-1.2197180385133349e-11j
0.51	17.373298687050337-2.352237965898094e-11j
0.61	17.373300102467958-4.503996542257634e-11j
0.71	17.37330280119636-8.557728848009089e-11j
0.81	17.37330788238893-1.6022949955251113e-10j
0.91	17.373317338957488-2.967585704947075e-10j

TABLE II: $Z_5(\beta)$, calculated with different $Im(\lambda)$.

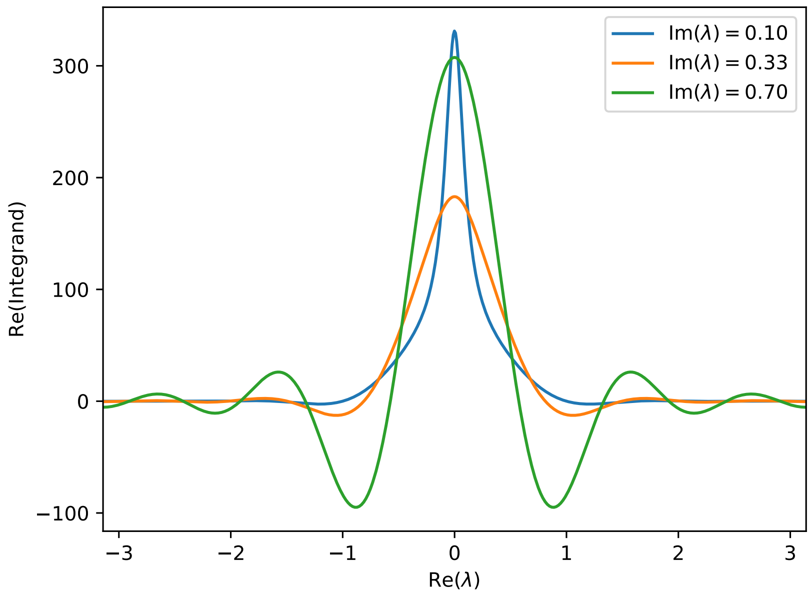

FIG. 3: The real part of integrand for fixed Im(λ).

C. Further reading

Material for this homework session is adapted from SMAC sections 4.1.2 (pp 190-191) and 4.1.3 (pp 196 - 198).

The subject of saddle point integration is best described in: C. M. Bender and S. A. Orszag

"Advanced Mathematical Methods for Scientists and Engineers" (Mc Graw Hill, 1978).