

Homework 13, Statistical Mechanics: Concepts and applications

2017/18 ICFP Master (first year)

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This homework illustrates essential calculations of Lecture 13. But 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 $E_x, E_y, E_z = 0, 1, 2, \dots$ so that $\hbar = 1$, $\omega = 1$, and the zero-point energy is subtracted), this is given by

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

Rederive this formula, using that $E = E_x + E_y + E_z$, and the fact that if you fix E_x , then the possible choices for E_y are easy to enumerate.

Also rederive this formula using the Kronecker δ function

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

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 $\sigma_1, \dots, \sigma_N$, and by avoiding double counting through the condition $\sigma_1 < \sigma_2 < \dots < \sigma_N$ (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).

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

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

with

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

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).

B. Experiments with the partition-function integration

In Fig. 1, 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

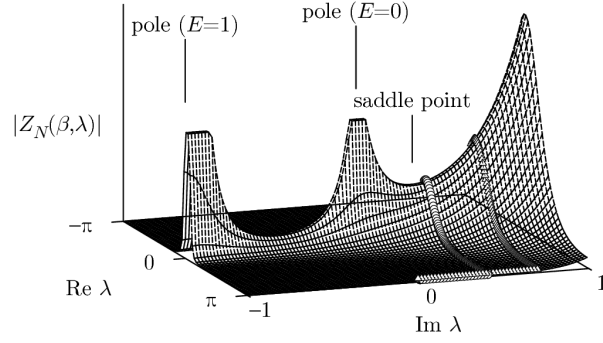


FIG. 1: Absolute value of the partition function $Z_N(\beta, \lambda)$ in the complex λ plane (for $N = 5$ and $\beta = 1$).

point, defined through

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

Up to a complex mi , 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 observables, the equivalence between the two ensembles is reached only in the limit $N \rightarrow \infty$. For non-intensive quantities, there are important differences that may persist up to the thermodynamic limit.

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).