UCSB, Physics 129AL, Computational Physics: Section Worksheet, Week 5B

Zihang Wang (UCSB), zihangwang@ucsb.edu

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Section Participation and Submission Guidelines

Section attendance is required, but you do not need to complete all the work during the section. At each section, the TA will answer any questions that you might have, and you are encouraged to work with others and look for online resources during the section and outside of sections. Unless otherwise stated, the work will be due one week from the time of assignment. The TA will give you 1 point for each task completed. You can see your grades on Canvas.

We will use GitHub for section worksheet submissions. By the due date, you should have a single public repository on GitHub containing all the work you have done for the section work. Finally, upload a screenshot or a .txt file to Canvas with your GitHub username and repository name so the TA knows who you are and which repository you are using for the section.

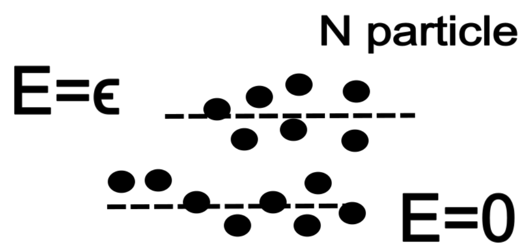
Remember: talk to your fellow students, work together, and use GPTs. You will find it much easier than working alone. Good luck! All work should be done in the Docker container, and don't forget to commit it to Git!

Task 1: Fermi-Dirac Statistics

Fermions are particles with half-integer spin (e.g., electrons, protons, neutrons), and they obey the Pauli exclusion principle, which states that no two identical fermions can occupy the same quantum state simultaneously. Let's use the same 2-level system discussed for bosons. In Fermi-Dirac statistics, The state with N particles must be considered collectively as a fraction of the states with $M \geq N$ energy levels $\epsilon, 2\epsilon, 3\epsilon, \cdots M\epsilon$, and the energy is filled one by one until there are N atoms. Derive the the partition function under grand canonical ensemble.

Task 2: Bose Einstein Condensate (BEC)

In this task, use the idea I discussed today, you are asked to create a BEC-like and a non-BEC-like system. Let's first look at the system's partition function of a N indistinguishable bosons in a 2-level system with ground state and first excited state energies $0, \epsilon$, respectively (see figure below).



a) Microstates

What are the microstates for the system in this case? This will be the microscopic view of the system.

b) (Classical) partition function under the canonical ensemble

Write down the classical partition function Z_C under the canonical ensemble. Hint: use the binomial factors. Explain why the factor must exist. What is the probability of finding a particular microstate with a given energy $\mathcal{E}$?

c) (Classical) Average particle number under the canonical ensemble

What will be the average number of particles in the ground state $\langle n_0 \rangle_C$ and the excited state $\langle n_\epsilon \rangle_C$? Plot both $\langle n_0 \rangle_C$ and $\langle n_\epsilon \rangle_C$ on the same figure. Hint: they sum to N.

d) (Quantum) partition function under the canonical ensemble

Similarly, write down the quantum partition function Z under the canonical ensemble. What is the probability of finding a particular microstate with a given energy $\mathcal{E}$?

e) (Quantum) Average particle number under the canonical ensemble

What will be the average number of particles in the ground state $\langle n_0 \rangle$ and the excited state $\langle n_\epsilon \rangle$ in the quantum case? Plot both $\langle n_0 \rangle$ and $\langle n_\epsilon \rangle$ on the same figure.

f) (Quantum) Quantum partition function under the Grand canonical ensemble

For the quantum case, modify the above partition function into the grand partition function $Z \to \Omega_G$ by introducing the chemical potential μ. What will be the condition for $\mu - \epsilon$ to ensure a normalizable system? Hint: think about the convergence. Hint: in this case, the particle number is not fixed anymore.

g) (Quantum) Particle number under the Grand canonical ensemble

Use the grand potential to calculate the average ground state particle number,

$$\langle n \rangle = k_B T \frac{\partial}{\partial \mu} \ln(\Omega_G). \tag{1}$$

h) (Quantum) Particle number under the Grand canonical ensemble

Use the grand potential to calculate the average ground state particle number, $N = 10^5$

$$\langle n \rangle = k_B T \frac{\partial}{\partial \mu} \ln(\Omega_G). \tag{2}$$

i) (Near)-degenerate Bose systems

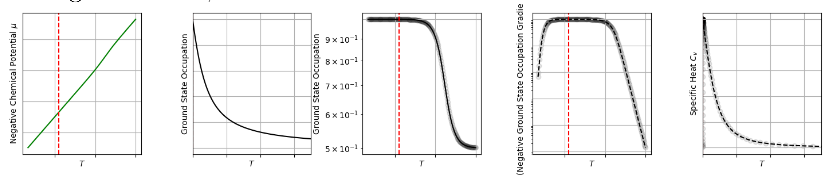
Similar to what we discussed in the class, write a Python program that introduces near-degenerate levels to the system, and numerically obtain the ground state number (in your numerical simulations, you should have a system with $N \sim 10^5$ bosons.

Your program should be able to calculate the **temperature dependence** of the listed quantities,

- negative chemical potential μ,
- Ground state occupation, $\langle n_0 \rangle$
- Ground state occupation with log-y scale , $\log(\langle n_0 \rangle)$,
- Negative ground state occupation gradient with respect to the temperature, $\frac{\partial \langle n_0 \rangle}{\partial T}$,
- Specific heat C_v.

j) (Near)-degenerate Bose system, without BEC

Design a Bose system does not experience BEC. You **should not** observe singular behaviors in thermodynamic quantities listed above. What are the degeneracy conditions and explain physically what is happening. You should see something like below,



k) (Near)-degenerate Bose systems, with BEC

Design a Bose system that experiences BEC. You **should** observe singular behaviors in thermodynamic quantities listed above. What are the degeneracy conditions and explain physically what is happening. Write a Python program that identifies the critical temperature T_c, the scaling laws of the heat capacity C_v. You should see something below.