Quantum Gas Problem 2

In the previous assignment, you wrote a function to compute the average number of bosons, $N = \langle N \rangle$, given the temperature T and the chemical potential μ. In this assignment, you will invert the function $N = N(\mu, T)$ to compute $\mu = \mu(T, N)$.

We will only consider bosons for this assignment, but write your program using the more general occupation number of a single-particle state with energy ϵ

$$\langle n_\epsilon \rangle = \left(\exp(\beta(\epsilon - \mu)) + \sigma\right)^{-1} \tag{1}$$

To invert the equation $N = N(\mu, T)$ we use the fact that N is a monotonically increasing function of μ. The basic algorithm begins with an interval (μ_-, μ_+) large enough to contain the desired value of $\mu(T, N)$. Fortunately, the choice is not very delicate. We then follow an iterative procedure until we find a value of μ that gives the correct number of particles. The suggested criterion is that $|\mu_+ - \mu_-| < \delta\mu$, where $\delta\mu \approx 10^{-4}$.

1. Calculate $\mu_{trial} = (\mu_- + \mu_+)/2$.
2. Calculate $N_{trial} = N(\mu_{trial}, T)$.
3. If $N_{trial} > N$ then set $\mu_+ = \mu_{trial}$; else if $N_{trial} < N$ then set $\mu_- = \mu_{trial}$.
4. Check to see if $\mu_+ - \mu_- < \delta\mu$. If not, return to step 1.

QUESTIONS:

1. Write a Python program to compute $\mu = \mu(T, N)$ over a set of uniformly spaced temperatures.
2. For $N = 1$ bosons in a box of edge length $L = 1$, use your program to compute and plot $\mu(T) - E_0$ (recall that the ground state energy $E_0 \neq 0$), the ground state occupation $\langle n_0(T) \rangle$, and the first excited state occupation $\Omega_1 \langle n_1 \rangle$ (Ω_1 is the degeneracy of the first excited state) for uniformly spaced values of T between $T = T_{BE}/10$ and

$T = 2T_E$, where $T_{BE} = (4\pi/k_{\mathrm{B}})(\hbar^2/2m)(N/2.612V)^{(2/3)}$ is the Bose-Einstein transition temperature.

3. Repeat for boxes of edge length $L = 2, 3, 4, 5, \ldots$ containing $N = L^3$ identical bosons. How does the behavior change with increasing L and N? Do you notice interesting behavior around T_{BE}?