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 \( \mu \). 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 \( \epsilon \)

\[
\langle n_\epsilon \rangle = \frac{(\exp(\beta(\epsilon - \mu)) + \sigma)^{-1}}{1}
\]  

To invert the equation \( N = N(\mu, T) \) we use the fact that \( N \) is a monotonically increasing function of \( \mu \). The basic algorithm begins with an interval \((\mu_-, \mu_+)\) 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 \( \mu \) that gives the correct number of particles. The suggested criterion is that \(|\mu_+ - \mu_-| < \delta \mu\), where \( \delta \mu \approx 10^{-4} \).

1. Calculate \( \mu_{\text{trial}} = (\mu_- + \mu_+) / 2 \).
2. Calculate \( N_{\text{trial}} = N(\mu_{\text{trial}}, T) \).
3. If \( N_{\text{trial}} > N \) then set \( \mu_+ = \mu_{\text{trial}} \); else if \( N_{\text{trial}} < N \) then set \( \mu_- = \mu_{\text{trial}} \).
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 \( \Omega_1 \langle n_1 \rangle \) (\( \Omega_1 \) is the degeneracy of the first excited state) for uniformly spaced values of \( T \) between \( T = T_{BE}/10 \) and...
$T = 2T_E$, where $T_{BE} = (4\pi/k_B)(\hbar^2/2m)(N/2.612V)^{(2/3)}$ 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 $T_{BE}$?