Quantum Gas Problem 1

For this assignment, based on ideas suggested by Prof. Swendsen, you will write a program to compute the average number of particles as a function of the chemical potential μ and the temperature T by direct summation without using the integral approximation.

Consider an ideal quantum gas of N particles a cubic box with sides of length L, each with mass m. The N-particle Hamiltonian is

$$H = \sum_{j=1}^{N} \frac{|\vec{p}_j|^2}{2m} \tag{1}$$

The single-particle energy is

$$\epsilon(\mathbf{k}) = \frac{\hbar^2}{2m}|\mathbf{k}|^2 \tag{2}$$

where $\mathbf{k} = \frac{\pi}{L}(n_x, n_y, n_z)$ We will use dimensionless variables, with $\hbar^2/2m = 1$, $k_B = 1$, and $L = \pi$. Your program should still contain the constant L because we will increase L to take the thermodynamic limit in the future.

The occupation number of a single-particle state with energy ϵ

$$\langle n_\epsilon \rangle = \left(e^{\beta(\epsilon-\mu)} + \sigma\right)^{-1} \tag{3}$$

where $\sigma = -1, 0,$ and $+1$, respectively, for Bose-Einstein, Boltzmann, and Fermi-Dirac statistics. Your program should contain σ as a parameter, so that you can treat any kind of statistics. The basic equation for the average number of particles $\langle N \rangle$ (which I will write as N for simplicity) as a function of μ and T is

$$N(\mu, T) = \sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle = \sum_{\mathbf{k}} \left(e^{\beta(\epsilon(\mathbf{k})-\mu)} + \sigma\right)^{-1}. \tag{4}$$

1. Since the sum in the equation for $N(\mu, T)$ is over an infinite number of terms, it must be truncated to a finite number of terms for the program. Find a criterion for truncating

the sum such that the neglected terms are each smaller than some δ. In practice, you will find that you can choose $\delta = 10^{-8}$, or even smaller, without making the run time program too long.

2. Write a function using Python (or another programming language of your choice) to carry out the truncated sum in the equation for $N(\mu, T)$.

3. Write a loop using the function you programmed in answer to the previous question to compute $N(\mu, T)$ for uniformly spaced values of μ between arbitrary values μ_1 and μ_2.

4. On a single set of axes plot the occupation numbers of the ground state, the first excited state, and the total occupation N, as functions of μ. Plot as individual points, not connected lines. Choose $T = 1.0$, and take a total of 38 μ values from $\mu_1 = -1.0$ to $\mu_2 = 7.0$, inclusive. Repeat this calculation first for Fermi-Dirac statistics, then for Boltzmann and finally for Bose-Einstein.

5. Compare the Boltzmann and Fermi-Dirac occupations and comment on the differences.

6. Your result for the Bose-Einstein occupation numbers might look strange. Does the result make physical sense? Can you think of a change you might wish to make in your plot for Bose-Einstein occupation?