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Tutorial 2

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Instructions

- We encourage you to work in groups on the problems. Groups of 3 will be assigned at random at the beginning of the tutorial
- Unless otherwise specified, you can go through the tutorial in whichever order you prefer
- If you are unable to attend a tutorial, you should work on the tutorial on your own (for about 1.5 hours) and submit your written work

1 Ideal gas - canonical ensemble

This time let's consider a system of N non-interacting particles in a box of volume V with fixed temperature T. We'll work again in the continuous case.

a) Show that in the thermodynamic limit $N \to \infty$

$$F \sim -k_B T N \ln \left[\frac{V}{N\omega^3} (2m\pi kT)^{3/2} \right] - kTN. \tag{1}$$

You can use the multidimensional Gaussian integral for a $n \times n$ positive semidefinite matrix A,

$$\int_{\mathbb{R}^n} d^n x \exp\left(-\frac{1}{2} \sum_{i,j} A_{ij} x_i x_j \right) = \sqrt{\frac{(2\pi)^n}{\det A}}$$

b) Compute average energy and entropy and show that they are consistent with the results from the microcanonical ensemble.

c) Compute the pressure P and show what the ideal gas law is recovered.

d) Compute the heat capacity at constant volume.

1.1 How do we fix W_0?

Remember how the W_0 factor appearing in the definition of Gibbs entropy for a continuous system was arbitrary? In this question you'll figure out how to fix it by using information from quantum mechanics. We'll work with the canonical ensemble of N non-interacting particles in a cubic box of side L at temperature T.

a) The energy eigenvalues for each particle are

$$E_{\mathbf{n}} = \frac{h^2\|\mathbf{n}\|^2}{8mL^2}, \mathbf{n} = (n_x, n_y, n_z) \in \mathbb{N}_0^3. \tag{2}$$

Show that the canonical partition function of the discrete case is

$$Z = \frac{1}{N!}\left(\sum_{\varepsilon} e^{-\varepsilon^2/2}\right)^{3N}, \varepsilon = \frac{h}{L}\frac{n}{\sqrt{4mkT}}, n \in \mathbb{N}_0. \tag{3}$$

b) Rewrite the inner sum from the partition function as

$$\frac{1}{\Delta\varepsilon}\sum_{\varepsilon}\Delta\varepsilon e^{-\varepsilon^2/2}, \Delta\varepsilon = \frac{h}{L}\frac{1}{\sqrt{4mkT}}. \tag{4}$$

Argue that when $\Delta\varepsilon$ is small enough we can approximate the sum with an integral, and show that

$$Z \approx \frac{V^N}{N!h^{3N}}(2\pi mKT)^{3N/2}, \tag{5}$$

where $V = L^3$.

c) Discussion topic: does it make sense to assume that $\Delta\varepsilon$ is small? What is its order of magnitude for some gas at room temperature?

d) Compare the free energy obtained in the continuous case with the one you would get from eq. 5 in the discrete case to figure out what W_0 should be to get matching results.

2 Ideal gas - grand canonical ensemble

The ideal gas can also be studied using the grand canonical ensemble. Recall that in this case we have

$$Z = \sum_{N=0}^{\infty} e^{\beta\mu N} Z_N \tag{6}$$

where Z_N is the canonical partition function for N particles.

a) Use the results from the previous question to show that

$$Z = \exp\left[e^{\beta\mu}\frac{V}{h^3}(2\pi mkT)^{3/2}\right]. \tag{7}$$

b) Show that $Z = e^{\bar{N}}$ and use this to invert the expression for μ in terms of (T, V, N) as

$$\mu = -k_B T \ln\left[\frac{V}{Nh^3}(2\pi mkT)^{3/2}\right]. \tag{8}$$

c) Show that the entropy is the same as the one you get from the canonical ensemble, once you rewrite it in terms of (T, V, N). Note that there was no need to use the Stirling approximation.

d) Show that the ideal gas law $PV = Nk_BT$ still holds.

3 Occupation numbers for non-interacting quantum gas

Consider a non-interacting quantum gas, where the single particle energy levels are discrete, labeled by i, with energy ϵ_i, which can all be chosen to be non-negative, with the ground state being at energy 0. We want to derive the average number of particles in any given state, at a particular temperature.

a) Show that the grand partition function with inverse temperature β and chemical potential μ is given by,

$$Z = \prod_i \sum_{n_i} e^{-\beta n_i(\epsilon_i - \mu)}$$

See that one can rewrite this as a product of grand partition functions of each level i, Z_i.

b) Find the occupation numbers of the level i for bosons (where n_i can be $0, 1, \cdots, \infty$) and fermions (where n_i can be $0, 1$). You can use the fact that the grand potential is related to the grand partition function as $\Phi_i = -k_B T \log Z_i$. Are there any restrictions on μ for bosons or fermions?

c) For $T \to 0$, how do n_i for fermions look like, as a function of $\epsilon - \mu_0$, where μ_0 to represent the chemical potential of the system at $T = 0$. Make a plot of this mean occupation number as a function of ϵ (drawing it is fine).

4 Fermi gas

Consider the free fermi gas, which are non-interacting, non-relativistic fermions, with mean number of particles in each single-particle energy state is given by

$$\langle n_\epsilon \rangle = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}. \tag{9}$$

Assume the fermions are kept in a $L \times L \times L$ three dimensional box, and the energy is related to the wavenumber of the fermion as $E = \frac{\hbar^2 k^2}{2m}$. Assume that the fermions are electrons with two internal spin states.

a) What is the density of states for this system? You can compute this by counting the number of states at a given energy level, via the correspondence, $2\sum_n \to \int g(\epsilon) d\epsilon$.

b) The chemical potential μ_0 is generally referred to as the *Fermi energy* of the system and is denoted by ϵ_F. Using the density of states to perform an integration, the defining equation for the Fermi energy is given by

$$\int_0^{\epsilon_F} g(\epsilon) d\epsilon = N. \tag{10}$$

Show that the corresponding *Fermi momentum* is given by

$$p_F = \left(\frac{3N}{4\pi V} \right)^{1/3} h, \tag{11}$$

and the Fermi energy is given by

$$\epsilon_F = \left(\frac{3N}{4\pi V} \right)^{2/3} \frac{h^2}{2m}. \tag{12}$$

c) Show that the ground-state energy is given by

$$\frac{E_0}{N} = \frac{3}{5}\epsilon_F. \tag{13}$$

d) What is the degeneracy pressure for the free fermi gas at zero temperature?

The degeneracy pressure just completely arises from the fermionic statistics and no thermal motion ($T = 0$). The degeneracy pressure for ultrarelativistic fermions can prevent stellar collapse for old white dwarfs.