

Due May. 15, Thursday

Problem 1 (20 points) *Classical ideal gas from a novel approach.*

- (a) Divide the gas into many small identical volume elements such that the number of gas molecule in each volume element is $\ll 1$. Consider the statistics of counting particles this way¹ and show that $\Delta N = \sqrt{\langle N^2 \rangle_c} = \sqrt{N}$, where N is the average number of molecules. Clearly state where the ideal gas assumption is used in your reasoning.
- (b) Now, using this result, Eq. 7.13, and the discussion following that equation, set up a differential equation for N with respect to the chemical potential μ (T and V are fixed). Show that the result can be written as

$$\left. \frac{\partial N}{\partial \mu} \right|_{V,T} = \frac{N}{k_B T}$$

- (c) Show that this means that μ is a function of the form

$$\mu = k_B T \log(nA)$$

where $A = A(T)$ is a function of T only and $n = N/V$.

- (d) Consider the Gibbs free energy, $G = E - TS + PV = F + PV = \mu N$ (Eq. 2.23) and the corresponding thermodynamic identity Eq. 2.18. Show that $Nd\mu = VdP$ when T is held fixed. By plugging this result into the differential equation obtained in part (b), show that the equation of state $PV = Nk_B T$ is derived.
- (e) Combine the results of parts (c), (d) and the fact that the partition function is given by (Eq. 6.44)

$$Z = \exp(-\beta F) = (V/\lambda^3)^N / N!$$

to prove that $A(T) = \lambda(T)^3$, where $\lambda(T) = h/\sqrt{2\pi m k_B T}$ is the thermal De Broglie wavelength.

Problem 2 (20 points) For a single simple harmonic oscillator, show that the integral of the difference between the classical value of the heat capacity and the quantum heat capacity is precisely the zero point energy. That is, show that

$$\int_0^\infty dT [C(T \rightarrow \infty) - C(T)] = \frac{1}{2} \hbar \omega$$

where $C(T)$ is the heat capacity.

¹Note that this method naturally invokes a grand canonical ensemble.

Problem 3 (30 points) *Density matrix.* Consider a beam of electrons. We describe its spin polarization within the density matrix formalism.

- Show that any density matrix can be written as $\rho = \frac{1}{2}(1 + \vec{a} \cdot \vec{\sigma})$, where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, σ_i 's ($i = x, y, z$) are Pauli matrices, and $\vec{a} = (a_x, a_y, a_z)$ is a *real* three dimensional vector, to be determined by the nature of the ensemble (see later parts). [Hint: use the fact that ρ is Hermitian, and must have a unit trace.]
- Show that $\overline{\langle S_j \rangle} = \frac{\hbar}{2} a_j$ for each $j = x, y, z$.
- Bloch sphere.* Prove that $|\vec{a}| \leq 1$ for any ensemble.
- Prove that $|\vec{a}| = 1$ if and only if ρ describes a pure state. [Hint: the last sentence of point 3 of Section 9.5.]
- What is the density matrix for the completely unpolarized beam of electrons?
- Find the density matrix for the beam of electrons that are 100 % polarized along the x' direction, where $\hat{x}' \cdot \hat{x} = \frac{1}{\sqrt{2}}$, $\hat{x}' \cdot \hat{y} = \frac{1}{\sqrt{2}}$, and $\hat{x}' \cdot \hat{z} = 0$.
- The mathematics of this problem also describes the polarization of a photon beam in vacuum. What does each a_i correspond to in the photon polarization case?

Problem 4 (30 points) *Density matrix.* Consider the following Hamiltonian \mathcal{H} that corresponds to a local spin 1/2 coupled to an external field H along the z direction.

$$\mathcal{H} = -\mu_B \vec{\sigma} \cdot \vec{H}$$

where μ_B is the Bohr magneton, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, and σ_i 's ($i = x, y, z$) are Pauli matrices.

- Find the density matrix for the Gibbs² canonical ensemble defined by the above Hamiltonian, when $\vec{H} = H\hat{z}$.
- Find the ensemble average $\overline{\langle M \rangle}$, where the magnetization M is defined as $M \equiv \mu_B \vec{\sigma} \cdot \hat{H}$, and \hat{H} is the unit vector along the direction of \vec{H} , by calculating the trace of ρM .
- Repeat the calculation for parts (a) and (b) when $\vec{H} = H\hat{y}$. [Note: Clearly this calculation would be *unnecessary*, in a real world setting, since the z axis can always be defined as the direction of the \vec{H} field. Here, you are asked to carry out the calculation nonetheless. The spirit of doing so is to familiarize oneself with the representation of the density matrix.]

²With the understanding that the above Hamiltonian with a prescribed applied field H indeed defines a Gibbs canonical ensemble in the magnetic work sense, you *can* drop the word Gibbs if you are so inclined, as is done in many books. However, one must not do so carelessly. What does “carelessly” mean in this case? Here is one way to test if you are careless or not. Consider the thermodynamic identity for dE , and answer the question whether it is HdM or $-MdH$ that must appear in it. If your answer is clear, then you are all set—you are being very careful.

Problem 5 (10 points) *Maxwell-Boltzmann distribution function from Quantum Statistics.* Consider a collection of non-interacting fermions (or bosons), with the rest mass $m > 0$. Taking the semi-classical limit (fugacity $z \ll 1$), show that you can *derive* Maxwell-Boltzmann single particle distribution function, f_{MB} .

$$\begin{aligned} f_{MB}(\vec{p}, \vec{q}, t) &= \frac{\exp(-\beta[\varepsilon(\vec{p}) - \mu])}{h^3} \\ &= \frac{n}{(2\pi m k_B T)^{3/2}} \exp\left(-\frac{\vec{p}^2}{2m k_B T}\right) \end{aligned}$$

where $\varepsilon(\vec{p}) = \frac{\vec{p}^2}{2m}$ is the kinetic energy of a single particle, and n is the number density, N/V . See Section 5.8.1 for the general definition, within the semi-classical statistical mechanics, of the single particle distribution function f_1 , which becomes the above result for free particles. Note the normalization property $\int d^3\vec{p} f_1(\vec{p}) = n$.