Due May. 21, Tuesday

Problem 1 (15 point) 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

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

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

Problem 2 (10 points) *Maxwell-Boltzmann distribution function.* Consider a collection of one type of non-interacting particles, with the rest mass $m > 0$. Assuming that the fugacity $z \ll 1$, show that the single particle density function, f_1, defined in Eq. 5.23, discussed in Eqs. 5.24,5.25, becomes the following function in equilibrium.

$$\begin{aligned} f_1(\vec{p},\vec{q},t) &= \frac{\exp\left(-\beta\left[\varepsilon(\vec{p}) - \mu\right]\right)}{h^3} \\ &= \frac{n}{(2\pi m k_B T)^{3/2}}\exp\left(-\frac{\vec{p}^2}{2mk_BT}\right) \end{aligned}$$

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. The above result is, of course, the familiar Maxwell-Boltzmann distribution function, whose normalization property is such that $\int d^3\vec{p} f_1(\vec{p}) = n$.

Problem 3 (10 points) P & B 6.7 (Doppler broadening, Maxwellian gas.)

Problem 4 (20 points) P & B 6.14 (Effusion of Maxwellian gas.)

Problem 5 (15 points) P & B 6.23 (Hydrogen atom within a simple Morse potential approximation.)

Problem 6 (20 points) *Density matrix.* Consider a beam of electrons. We describe its spin polarization within the density matrix formalism.

(a) 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 next). [Hint: use the fact that ρ is Hermitian, and must have a unit trace.]

(b) Show that $\overline{\langle S_i \rangle} = \frac{\hbar}{2} a_i$ for each $i = x, y, z$.

(c) *Bloch sphere.* Prove that $|\vec{a}| \le 1$ for any ensemble.

(d) Prove that $|\vec{a}| = 1$ if and only if ρ describes a pure state. [Hint: the last sentence of point 3 of Section 10.4.]

(e) What is the density matrix for the completely unpolarized beam of electrons?

(f) 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 $\hat{x}' \cdot \hat{z} = 0$.

(g) 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 7 (20 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.

(a) Find the density matrix for the Gibbs[1] canonical ensemble defined by the above Hamiltonian, when $\vec{H} = H\hat{z}$.

(b) 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.

(c) 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.]

Problem 8 (30 points) P & B 8.3, 8.4. (C_p and C_v for Fermi gas.)

Problem 9 (20 point) A cylinder is separated into two compartments by a freely sliding piston. Two ideal Fermi gases are placed into the two compartments, numbered 1 and 2. The particles in compartment 1 has spin 1/2 and those in compartment 2 has spin 3/2, while all particles have the same mass. Find the equilibrium density ratios of the two gases at $T = 0$ and $T \to \infty$.

[1] *With* 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.