PHYSICS 715

Problem Set 7 **Due Friday, March 24, 2006**

Reading: Landau and Lifshitz, Secs. 33, 45–52

LD 22: Fermi, Bose, and Schrödinger statistics and the factorization properties of the canonical partition function Z_N

(a) A system containing N distinguishable particles has a set of discrete single-particle energy levels $\epsilon_1 < \epsilon_2 < \epsilon_3 \cdots$ with degeneracies $g_1, g_2, g_3, \ldots$. The total energy E_α is the sum of the energies of the occupied levels. The quantum mechanical canonical partition function Z_N is defined as the sum of $e^{-\beta E_\alpha}$ over all the energy eigenstates of the system. Label the states in terms of the occupation numbers for the different single-particle states, determine the number of ways of getting each completely labeled energy, and show that Z_N factors, with $Z_N = Z_1^N$. [The multinomial theorem will be useful. See, e.g., Abramowitz and Stegun, *Handbook of Mathematical Functions*, p. 823.]

(b) Construct the normalized wave functions $\Psi(1,2)$ allowed for two-particle Schrödinger (distinguishable particle), Bose, and Fermi systems which have just two single-particle energy levels $\epsilon_1 < \epsilon_2$ with degeneracies $g_1 = g_2 = 1$ and corresponding single-particle wave functions ψ_1 and ψ_2. Express Z_2 as the sum of the matrix elements $\langle\Psi(1,2)|e^{-\beta(H_1+H_2)}|\Psi(1,2)\rangle$ over the allowed states for each case, and show explicitly that Z_2 does not factor for Bose and Fermi statistics.

LD 23: Trace identities and derivative tricks for quantum problems: $\langle q^2\rangle$ for the quantum oscillator.

(a) Suppose that a (finite) operator $A(\lambda)$ depends on a parameter λ. Show from the properties of the trace operation that

$$\mathrm{Tr}\frac{dA(\lambda)}{d\lambda}e^{A(\lambda)} = \frac{d}{d\lambda}\mathrm{Tr}\, e^{A(\lambda)},$$

whether or not A and $dA/d\lambda$ commute.

(b) Use the result in (a) to determine the average value of q^2 for the quantum oscillator as a function of T. The oscillator Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2.$$

Determine and explain the limiting values of $\langle q^2\rangle$ for $kT \gg \hbar\omega$ and $kT \ll \hbar\omega$.

LD 24: Brillouin paramagnetism and the classical Langevin limit.

A paramagnetic solid (Brillouin paramagnet) consists of a lattice of atoms of spin J. Atoms at different lattice sites are distinguishable. There are $n = N/V$ atoms per unit volume. $H = \sum_i H_i$, where the single-particle Hamiltonian for an atom with magnetic quantum number m_i in a magnetic field $\mathcal{H}$ is

$$H_i = g\mu_B \mathcal{H} m_i.$$

m_i can take any of the values $-J, -J+1, \ldots, J$.

(a) Calculate the canonical partition function Z_N and determine the mean magnetization of the solid. [The magnetization M is the average magnetic moment per unit volume, $M = \langle \mathcal{M}/V \rangle$, where $\mathcal{M} = -\sum_i g\mu_B m_i$. The relation $\sum_0^N x^n = (1 - x^{N+1})/(1-x)$, $|x| < 1$ will be useful. Express your results in terms of the variable $x = g\mu_B \mathcal{H}/kT$.]

(b) Calculate the magnetic susceptibility $\chi = \frac{\partial M}{\partial \mathcal{H}}$. Plot the behavior of χ as a function of x, and determine how it approaches its limits for $x \to 0, \infty$. Thus, determine how $\chi(T)$ behaves for $T \to \infty, 0$ for fixed $\mathcal{H}$. Explain *physically* why χ behaves as it does in these limits.

(c) The magnetic moment of an atom is defined as $\mu = g\mu_B J$. Show that the Brillouin magnetization of part (a) reduces in the limit $J \gg 1$, μ fixed, to the classical Langevin result for the magnetization of a set of intrinsic magnetic dipoles μ. The classical problem is defined by the Hamiltonian $H = -\sum_i \boldsymbol{\mu_i} \cdot \boldsymbol{\mathcal{H}} = -\sum_i \mu \mathcal{H} \cos\theta_i$. See Probs. LD 13 (b), (c) for the analog for electric dipoles.

LD 25: The classical limit of the quantum mechanical rotator: the "freezing out" of rotational degrees of freedom.

The rotational energy of a symmetric rotator (molecule) with principal moments of inertia I_3 and $I_2 = I_1$ is given quantum mechanically by

$$E_{\ell,k,m} = \frac{h^2}{8\pi^2 I_1}\ell(\ell+1) + \frac{h^2}{8\pi^2 I_1 I_3}(I_1 - I_3)k^2,$$

where ℓ, k, m label the rotational quantum states of the molecule. Here ℓ is the total angular momentum, $\ell = 0, 1, \ldots,$ and m and k are the projections of the angular momentum ℓ on the spatial z axis and the symmetry axis of the molecule (the body axis) respectively, $k = -\ell, -\ell+1, \ldots, \ell$, and $m = -\ell, -\ell+1, \ldots, \ell$.

(a) Show that the quantum mechanical partition function may be approximated at sufficiently high temperature by the classical result,

$$Z_{cl} = \frac{8\pi^2}{h^3}(2\pi kT\, I_1)(2\pi kT\, I_3)^{1/2},$$

hence, that the energy of rotation per molecule approaches the classical result $E_{\rm rot} = \frac{3}{2}kT$. [Hint: make approximations that you can (and do) justify, and note that $\int_0^\infty e^{-at}\mathrm{erf}(\sqrt{bt}\,)dt = \frac{1}{a}\sqrt{\frac{b}{a+b}}$, where

$$\mathrm{erf}(z) = \frac{1}{\sqrt{\pi}}\int_{-z}^{z} e^{-t^2}dt$$

is the error function. It will clarify the temperature dependence of the initial expression to introduce two characteristic temperatures $\Theta_i = h^2/8\pi^2 I_i k_B$.]

(b) Suppose $I_3 \ll I_1$. Show that rotations around the body axis "freeze out" (are not excited in the quantum problem) at temperatures at which the remaining rotational modes may still be treated classically. Obtain the modified form of $Z_{\rm rot}$ appropriate to this limit, and show how the change affects the rotational specific heat of a gas of these molecules.

Estimate the temperatures at which (i), rotations around body axis, and (ii), the remaining rotational modes, freeze out for CO. [Hint: Rotations around the body axis can be described approximately as excitations of single-electron states. A typical radius for the outer electron distribution around the symmetry axis is 0.75 Å. Note that the dissociation energy of CO is 11 eV.]