PHYS 813: Statistical Mechanics, Assignment 6

Due 4/17/08

1. The energy levels of a quantum mechanical, one-dimensional, anharmonic oscillator are given by

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega - x\left(n + \frac{1}{2}\right)^2 \hbar\omega, \quad n = 0, 1, 2, \ldots$$

   The parameter x represents the degreee of anharmonicity and is assumed to be much smaller than 1. Find the expression for the the specific heat of a system of N such oscillators to the first order in x and the fourth order in $u = \hbar\omega/kT$. Use the canonical partition function. Note that the sum constituting this function should be truncated.

2. A system in equilibrium consists of a solid and a vapor (in contact with a thermal bath), both containing one type of atomic particles. Assume that the energy needed to transform one atom from the solid to the vapor is known and denote it by ϕ. Assume further that the solid can be approximated as a set of completely independent three-dimensional quantum harmonic oscillators (each atom being one oscillator) performing vibrations about their equilibrium position (so that the energy of each atom is $-\phi$ plus the energy due to the harmonic motion) and that the vapor is an ideal gas. Note that the zero-point vibrational energy is neglected in the definition of the sublimation energy. Evaluate the vapor pressure as a function of temperature. You may use without proof the partition functions for a set of oscillators and for the ideal gas. *Hint:* The Helmholtz free energy is at the minimum in equilibrium.

3. Consider N atoms confined on a surface of area A at temperature T. The atoms form a two-dimensional (2D) gas of classical, noninteracting particles.

   (a) Calculate the partition function for the system.

   (b) Calculate the Helmholtz free energy, F, of the gas. Compare it with the 3D case.

   (c) Calculate the internal energy of the gas. Compare it with the 3D case.

   (d) Calculate the surface tension of the gas, $\gamma = (\partial F/\partial A)_{T,N}$.

   (e) Calculate the momentum distribution $n(p)$ which determines the number of atoms $N(p)$ with momenta between p and $p + dp$: $N(p) = n(p)dp$.

4. Consider a pair of electric dipoles $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$. Assume for simplicity that one of the dipoles is placed at the center of the coordinate system and the other one at a point $\boldsymbol{R}$. The potential energy of the dipole-dipole interaction is given by

$$U = -\frac{1}{R^3}\left[3(\boldsymbol{\mu}\cdot\hat{\boldsymbol{R}})(\boldsymbol{\mu}'\cdot\hat{\boldsymbol{R}}) - \boldsymbol{\mu}\cdot\boldsymbol{\mu}'\right]$$

   and the force acting on the center of dipole $\boldsymbol{\mu}'$ is

$$\boldsymbol{F} = -\boldsymbol{\nabla}_{\boldsymbol{R}}\, U.$$

   Assume the pair to be in thermal equilibrium, their orientations governed by a canonical distribution. Find the mean force between the dipoles at high temperatures.

5. Consider three magnetic ions of spin $\frac{1}{2}$ interacting via the ("antiferromagnetic") Hamiltonian

$$H = J\left(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + \boldsymbol{S}_2 \cdot \boldsymbol{S}_3 + \boldsymbol{S}_3 \cdot \boldsymbol{S}_1\right)$$

where $\boldsymbol{S}_i$ is the spin operator for particle i and J is a positive constant.

(a) Show that the eigenvalues of H are $\frac{3}{4}J\hbar^2$ and $-\frac{3}{4}J\hbar^2$ and find the degeneracy of each level.

(b) Find the partition function for this system.

(c) Calculate the entropy and internal energy of the system as a function of temperature.

(d) What is the entropy of the system in the limit of zero temperature?

(e) Derive an expression for the specific heat.

6. Consider a large number, $N^{(0)}$, molecules contained in a volume $V^{(0)}$. Assume that there is no correlation between the locations of the molecules (ideal gas). Do not use the partition function in this problem.

(a) Calculate the probability $P(V,N)$ that an arbitrary region of volume V contains exactly N molecules.

(b) Calculate the average value $\bar{N}$ and the standard deviation of N.

(c) Show that if both V and $V^{(0)} - V$ are large, the function $P(V,N)$ assumes a Gaussian form for N close to $\bar{N}$.

(d) Show that if both $V \ll V^{(0)}$ and $N \ll N^{(0)}$, the function $P(V,N)$ assumes a Poisson form.

7. Now consider the same system using the grand canonical partition function.

(a) Find $P(V,N)$ in terms of the partition functions and fugacity.

(b) Find the particular form of $P(V,N)$ for an ideal gas. Compare with the results of the previous problem.