PHY 4523 Spring 2001 – Homework 2

Due at the start of class on Wednesday, February 7.

Answer both questions. To gain full credit you should explain your reasoning and show all working. Please write neatly and remember to include your name on the front page of your answers.

1. *Two-level model with level degeneracy.* Consider a system of N atoms, each of which has two low-lying sets of energy levels: g_0 ground states, each having energy 0, plus g_1 excited states, each having energy $\varepsilon > 0$.

   (a) Calculate $\Omega(E, N)$, the number of microstates having energy E.

   Hint: A microstate is completely specified by listing which of the $(g_0 + g_1)$ possible levels each atom occupies. To calculate $\Omega(E, N)$, start with the corresponding result for a nondegenerate two-level system (as discussed in class). Then figure out the extra multiplicity arising from the level degeneracy.

   (b) Use your answer to part (a) to express the temperature T as a function of E and N.

   (c) Calculate $c(T)$, the molar heat capacity. (NB: To be precise, this is the molar heat capacity at constant ε, which one would expect to correspond to constant volume.)

   (d) Derive a transcendental equation for the temperature T_S at which c attains its maximum value (the position of the Schottky peak). Simplify the equation as much as possible, but do not attempt to solve it algebraically.

   (e) Calculate the dimensionless ratios $k_B T_S/\varepsilon$ and $c(T_S)/R$ (where R is the gas constant) for the case $g_0 = 1$, $g_1 = 2$. You should find $k_B T_S/\varepsilon$ to within $\pm 2\%$.

   Hint: The transcendental equation obtained in part (d) can be solved numerically to the necessary accuracy by trial and error using a computer or a scientific calculator. Just substitute trial values of $k_B T_S/\varepsilon$ into the equation and adjust them to minimize the difference between the left and right hand sides of the equation.

   (f) A plot of the experimental molar specific heat for the material α-$NiSO_4 \cdot 6H_2O$ was distributed in class. The data appear to show a Schottky peak at 2.6 K. The peak value of c is approximately 6.3 J/K per mole-formula of α-$NiSO_4 \cdot 6H_2O$.

   It is claimed that this material corresponds to the case $g_0 = 1$, $g_1 = 2$ of the two-level model, with one two-level system per Ni ion. Use your answers to part (e) to extract ε from the data and to check whether the experimental and theoretical values of $c(T_S)$ are consistent with each other.

2. *A polymer model in two dimensions.* Consider a chain of N monomeric links, each of length a, and each constrained to point (with equal probability) along one of four directions: $+x$, $-x$, $+y$, and $-y$. Denote the number of monomers pointing along each of these directions by N_{+x}, N_{-x}, N_{+y}, and N_{-y}, respectively. In this simplified problem, all conformations of the chain are assumed to have the same energy.

(a) Write down the multiplicity function $\Omega(N; N_{+x}, N_{-x}, N_{+y}, N_{-y})$.

(b) Re-express N_{+x}, N_{-x}, N_{+y}, and N_{-y} in terms of the variables N, $l_x = N_{+x} - N_{-x}$, $l_y = N_{+y} - N_{-y}$, and $\Delta = N_{+x} + N_{-x} - N_{+y} - N_{-y}$. (Note that l_x and l_y are proportional to the x and y components of the end-to-end length, while Δ is a measure of the spatial anisotropy of the monomer distribution.)

(c) Re-express your answer to (a) as $\Omega(N; l_x, l_y, \Delta)$.

(d) Approximate $\ln \Omega(N; l_x, l_y, \Delta)$ using Stirling's formula, $\ln n! \approx n \ln n - n$.

(e) Expand $\ln \Omega(N; l_x, l_y, \Delta)$ about $l_x = l_y = \Delta = 0$, retaining all terms out to second order in the small parameters l_x/N, l_y/N, and Δ/N.

(f) Suppose that the polymer chain is maintained at a temperature T. An external agent pulls outward on each end of the chain with a force F directed along the x axis. Calculate the equilibrium values of l_x, l_y, and Δ. You may assume that the applied force is sufficiently small that you can use the result from part (e).