PY541 Problem Set 3: Due Thursday, October 10, 2002 in class

1) Consider a simplified model of O_2 adsorption onto a hemoglobin molecule. Assume that a hemoglobin molecule consists of 2 identical strands each of which is capable of adsorbing, at most 1 O_2 molecule. Consider a single hemoglobin molecule in equilibrium with the atmosphere which acts as a reservoir which can exchange energy and also O_2 molecules. Thus we are assuming that the hemoglobin molecule, with or without O_2 molecules interacts very weakly with the molecules in the atmosphere and with the other hemoglobin molecules. Assume that the chemical potential for O_2 molecules obeys $e^{\mu/kT} = 10^{-5}$ at body temperature, $T = 37K$. Suppose that the energy, ϵ_1 of a single O_2 molecule on a hemoglobin molecule obeys $e^{-\epsilon_1/kT} = 10^4$. Suppose that 2 O_2 molecules on the same hemoglobin molecule repel each other so that the energy is $\epsilon_2 = 1.9\epsilon_1$. Calculate the fraction of hemoglobin molecules that contain zero , one or two O_2 molecules. Calculate the root mean square fluctuation in the number of O_2 molecules on a hemoglobin molecule, $\sqrt{< (n - \bar{n})^2 >}/\bar{n}$.

2) Consider the Boltzmann distribution at temperature T, for 2 non-interacting particles each of which can be in 10 different states with energies, $E_1 = i \times \Delta$ where $i = 0, 1, 2, \ldots 9$.
a) Calculate the partition function using the Maxwell-Boltzmann approximation, Z_{MB}.
b) Calculate the exact partition function if the particles obey Fermi-Dirac statistics, Z_{FD}.
c) Calculate the exact partition function if the particles obey Bose-Einstein statistics, Z_{BE}.
d) Show that $Z_{MB} = (Z_{FD} + Z_{BE})/2$.
e) Show that the 3 partition functions are fairly close to each other in the limit $kT >> \Delta$.
f) Show that they are very different in the limit $kT << \Delta$.

3) Consider an S=1/2 Heisenberg ferromagnet on a cubic lattice:

$$H = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the notation $< i, j >$ indicates that i and j are nearest neighbors. (Each nearest neighbor pair occurs *once* in the sum.)
a) Calculate the nearest neighbor spin correlation function:

$$< S_i^a S_j^b > \equiv tr \left[e^{-\beta H} S_i^a S_j^b \right] / Z, \tag{2}$$

at lowest non-vanishing order in the high-temperature expansion. Here a and b label the x, y and z components of the spin operators. That is assume that i and j are nearest neighbor sites.
b) Show that any longer range correlation is suppressed by additional powers of $1/T$ at large T. That is, show that the correlation function of Eq. (1) is smaller by at least one power of $1/T$ if i and j are further apart than nearest neighbors.
c) The zero field magnetic susceptibility can be written:

$$\chi(T) = [(2\mu_B)^2/k_B T] \sum_{i,j} < S_i^z S_j^z > . \tag{3}$$

Here the notation indicates a sum over all sites i and j. That is the two sums over i and j run independently over all sites. Calculate $\chi(T)$ up to second order in the $1/T$ expansion.
d) Suppose that $J = 1meV$. Roughly how large would T have to be for the high temperature expansion to be valid?

4) Using the Jocobian identity proved in class:

$$\frac{\partial(A,B)}{\partial(C,D)} \times \frac{\partial(C,D)}{\partial(E,F)} = \frac{\partial(A,B)}{\partial(E,F)}, \tag{4}$$

prove the identity that Joel assumed to solve the problem during the discussion session on October 2:

$$\frac{\partial(A,B)}{\partial(C,D)} \times \frac{\partial(E,F)}{\partial(G,H)} = \frac{\partial(A,B)}{\partial(G,H)} \times \frac{\partial(E,F)}{\partial(C,D)}. \tag{5}$$