Physics 212 – Problem Set # 6

(due Thursday, May 15)

1. Sethna, problem 8.6.

2. In Section 8.1.4, Sethna introduces the *heat bath* method for simulating an Ising model. The method is simple: keeping the neighbors of a given spin s_i fixed, reset the value of s_i according to the probabilities

$$p(+1) = \frac{e^{-\beta H(+1)}}{e^{-\beta H(+1)} + e^{-\beta H(-1)}} \qquad p(-1) = \frac{e^{-\beta H(-1)}}{e^{-\beta H(+1)} + e^{-\beta H(-1)}} \tag{1}$$

Sweep through the lattice many times, resetting each spin in turn until the system comes to equilibrium. In problem 8.6, Sethna introduces the *Metropolis* method for simulating a lattice spin system. At each site, consider the action of flipping the spin s_i, keeping the neighboring spins fixed. Carry out this action if H decreases. If H increases, carry out the action with the probability

$$p = \frac{e^{-\beta H(\text{flip})}}{e^{-\beta H(\text{no flip})}} \tag{2}$$

Implement one or the other of these algorithms on a computer for a 2-d Ising model with $J = 1$, $h = 0$, on a lattice of size at least 100×100, and answer the following questions:

   (a) Impose periodic boundary conditions. What is the value of T_c or β_c, from visual inspection of the equilibrium configurations?

   (b) Impose the boundary condition that all spins are up on the boundary. What changes? Consider temperatures both above and below T_c.

   (c) Estimate the correlation length, in lattice units, for several values of β above and below T_c.

   (d) Impose antiperiodic boundary conditions in the $\hat{x}$ direction; that is, identify the boundary values in the $\hat{x}$ direction by $s_{Lj} = -s_{0j}$. What changes, both above and below T_c?

3. Consider a d-dimensional lattice model of a magnet in which the spin variables are unit vectors in 2 dimensions.

$$s_i = (\cos\phi_i, \sin\phi_i) \tag{3}$$

and the Hamiltonian is

$$H = -J \sum_{<ij>} \vec{s}_i \cdot \vec{s}_j \tag{4}$$

This is called the 'XY model'. Write the mean field equation for $\langle \vec{s} \rangle$. You will encounter modified Bessel functions from the identity

$$I_n(z) = \int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{z\cos\theta}\, \cos n\theta \tag{5}$$

but please have no fear, since you can look up the properties of these functions. Show that mean field theory predicts a magnetized phase, compute T_c, and compute the behavior of the spontaneous magnetization in the vicinity of T_c.

4. Consider next a d-dimensional model of a magnet in which the spins are unit vectors in N dimensions. Write the mean field equation for $\langle \vec{s} \rangle$. Compute T_c, and compute the behavior of the spontaneous magnetization in the vicinity of T_c. Some integrals will appear, but (using insights from Problem 3), you should not need to evaluate these integrals explicitly. You should only need to evaluate the integrals in a power series expansion in $\langle \vec{s} \rangle$.

5. Consider a 2-dimensional Ising model at high temperature, on a square lattice of finite but large size $N \times N$, with the boundary condition that all spins on the boundary are up.

   (a) Let s_{nj} be a spin located n steps from the boundary in the horizontal direction and far from either boundary in the vertical direction. At high temperature, we might expect that this spin has a tendency to be up rather than down, but that this tendency would go to zero exponentially as n increases. Using the high-temperature expansion presented in class, find the leading nonzero term in $\langle s_{nj} \rangle$ and show that this has the form, with $A < 1$,

   $$\langle s_{nj} \rangle \sim CA^n = C\exp[-n\log(1/A)] \tag{6}$$

   The correlation length in the model would be $\xi = 1/\log(1/A)$. Find ξ in terms of the model parameters β and J.

   (b) Work out 3 more terms in the high-temperature expansion for $\langle s_{nj} \rangle$. (Remember that the high-temperature series corrections also affect the denominator $Z(\beta)$.) Show that the series can be organized as an exponential decay with n. Work out the prediction for the correlation length ξ as a function of βJ.