Physics 220: Problem Set 5
due June 14, 2012.

This is a generalization of the Monte Carlo problem you did earlier to two dimensions. Consider the 2d Ising model, $H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$, where $\sigma_i = \pm 1$ and $J = 1$. You can use whatever programming language you like: C, C++, fortran, python, matlab, even mathematica. Your homework should include your program, emailed to me, and a written summary of your calculations and answers to the questions below. **Get as far as you can...**

Write a Monte Carlo simulation for the model on the square lattice of $N = L \times L$ sites with periodic boundary conditions using the Metropolis algorithm. Start from a random initial state, and choose subsequent states as follows:

- Choose the next trial configuration by randomly flipping one spin.
- Calculate the energy difference, $\Delta E$, between the trial state and the old state.
- If $\Delta E < 0$, accept the new state as the next one. If $\Delta E > 0$, generate a random number $0 \le r < 1$, and accept the trial state if and only if $e^{-\beta\Delta E} > r$.

Thermal averages can be estimated by averages over samples, $\langle\mathcal{O}\rangle = \frac{1}{M}\sum_{i=1}^{M}\mathcal{O}_i$, where the sum is over $M$ samples $i$.

1. Plot the average energy $\langle E\rangle/N$ per site for $L = 16$ at $\beta = 1$ and $\beta = 3$, as a function of the Monte Carlo step $i$. You should see an initial period in which the energy changes rapidly, before fluctuating around equilibrium. Data during this "warm up" period should not be used in the thermodynamic averages calculated below.

2. Plot the average energy per site versus temperature. Average over at least $10^5$ Monte Carlo steps per temperature. Plot the (absolute value of) the average magnetization per site $|\langle M\rangle|/N$ and the square root of the variance of the same quantity, $\langle M^2\rangle/N^2$, versus temperature. Discuss the behavior at $T \to 0$ and $T \to \infty$.

3. Calculate the specific hear $c_v = \left(\langle E^2\rangle - \langle E\rangle^2\right)/(NT^2)$ using Monte Carlo and plot it versus temperature to obtain a rough estimate of $T_c$.

4. The magnetic susceptibility is similarly given by $\chi = \left(\langle M^2\rangle - \langle M\rangle^2\right)/(NT)$. Plot $\chi$ versus $T$ for $L = 8, 12, 16$, and 20. Do the same for the quantity $\chi' = \left(\langle M^2\rangle - \langle |M|\rangle^2\right)/(NT)$. How similar are both quantities?

5. By using the exact critical temperature $T_c = 2/\ln(\sqrt{2}+1)$, collapse the data for $\chi'$ as best as possible onto one curve, plotting $\chi L^{-\gamma/\nu}$ versus $tL^{1/\nu}$, treating $\gamma$ and $\nu$ as fit parameters. What are the best fit values of these exponents? How do they compare to the exact values? What are your greatest sources of error?

6. Modify your program to simulate an antiferromagnet ($J = -1$) on the 2d **triangular** lattice. Examine the energy, specific heat, and susceptibility for a phase transition. Is there one? Calculate the entropy at very low temperature ($T < 0.1$) by integrating the specific heat:

$$\Delta S = \int_{T_{\rm low}}^{T_{\rm high}} \frac{C}{T}\,dT. \tag{1}$$

What is your numerical estimate of the "zero temperature entropy"?