Physics 220: Problem Set 3
due May 3, 2012.

This homework is a first exercise in Monte Carlo. Consider the one dimensional Ising model, $H = -J\sum_n \sigma_n\sigma_{n+1}$, where $\sigma_n = \pm 1$ and $J = 1$ (we take temperature units so $k_B = 1$ here as well). You can use whatever programming language you like: C, C++, fortran, python, matlab, even mathematica.

**Problem:** Write a Monte Carlo simulation for the model with $N$ 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 $N = 100$ at $\beta = 1$, $\beta = 3$, and $\beta = 6$ 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. Show (analytically) that the specific heat is given by $c_v = \left(\langle E^2 \rangle - \langle E \rangle^2\right)/(NT^2)$. Calculate this using Monte Carlo and compare it to the exact result from the transfer matrix. Try to push your simulation to get reasonable agreement with the analytic theory.
4. Make a similar comparison of the (zero field) magnetic susceptibility between Monte Carlo and theory. This is given by $\chi = \left(\langle M^2 \rangle - \langle M \rangle^2\right)/(NT)$.
5. **Extra credit:** get this to run on my iphone!