PHYS639, Spring16, Problem 7

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In this problem set we will simulate properties of *ferromagnets* using the *Ising model*. For simplicity we will work in 2D. A 2D piece of ferromagnet consists of many atoms, each one having a spin in either a positive $s = 1$ or a negative $s = -1$ direction with respect to the z axis. We will assume that these atoms are on a regular grid. The energy of spin-interaction between neighbouring atoms (each atom in our model has four neighbours) is

$$E = -J s_i s_j \tag{1}$$

where J is a positive *exchange constant* and s_i and s_j the spins of two neighbouring atoms. The atoms prefer to have their spins aligned as this results in a lower energy. The interaction between non-neighbouring atoms is negligible. Unless the temperature is zero the atoms do not have to be in the lowest energy state. The probability of being in any particular state is proportional to the *Boltzmann factor*

$$P \sim e^{-E/k_B T}, \tag{2}$$

where k_B is the Boltzmann constant.

External magnetic field interacts with atoms of the ferromagnet and the interaction energy is

$$E = -\mu H s_i, \tag{3}$$

where μ is the *magnetic moment* and H is the strength of the magnetic field. The total energy of the ferromagnet is

$$E = -J \sum_{ij} s_i s_j - \mu H \sum_i s_i, \tag{4}$$

where i index sums over all atoms and j index sums over neighbours of each atom.

The total *magnetization* is

$$M = \sum_i s_i. \tag{5}$$

Both energy and magnetization will fluctuate in time.

The *specific heat* describes by how much the average energy of the system increases for a unit increase in temperature and is defined as

$$C = \frac{d\langle E \rangle}{dT}. \tag{6}$$

Similarly, the magnetic *susceptibility* is defined as

$$\chi = \frac{d\langle M \rangle}{dH}. \tag{7}$$

where both averages are over time.

You will simulate a 2D ferromagnet using *Monte Carlo* approach. Start by initializing a 2D regular grid of spins with all $s = 1$ initially. At each time-step go through every spin and flip it if the new (flipped) state results in a lower energy than the original state. If the new state has a higher energy then flip it with a probability of $P = \exp[-(E_{new} - E_{old})/k_B T]$ (Hint: generate a random number between 0 and 1, and if it is larger than P than do not flip). Repeat this for many time steps. Assume the units are such that $J = k_B = \mu = 1$. Produce deliverables for the scenario with no external magnetic field ($H = 0$) and a strong external magnetic field ($H = 5$). Use *periodic boundary conditions* where the spins on opposite boundaries are considered to be neighbours.

Deliverables

1. We expect the magnetization to decrease with temperature. Plot M per spin as a function of time for very low (when $\langle M \rangle \sim 1$) and very high (when $\langle M \rangle \sim 0$) temperatures.

2. Find *critical temperature* for which the system jumps sporadically from a positive magnetization state and back to a negative magnetization state and plot H as a function of time in that case.

3. Plot M per spin as a function of temperature. Identify critical temperature on the plot.

4. Plot E per spin as a function of temperature. Identify critical temperature on the plot.

5. Plot C per spin as a function of temperature. Identify critical temperature on the plot. (Hint: you can take a derivative of $\langle E \rangle$ by computing $[\langle E(T + \epsilon) \rangle - \langle E(T) \rangle]/\epsilon$, where ϵ is a small number).

6. Plot χ per spin as a function of temperature. Identify critical temperature on the plot. (Hint: compute the numerical derivative as above).