Computational Methods: Homework 3: Two-dimensional Ising model

D. J. Dean
(Dated: March 9, 2005)

Homework is due on 29 March.

I. THE SCIENCE PROBLEM :ISING MODEL IN 2-DIMENSIONS

We are now going to work on the problem of the Ising model in 2-dimensions. The spins are taken as classical degrees of freedom. The Hamiltonian is given by

$$H = -J \sum_{\langle\alpha\beta\rangle} S_\alpha S_\beta - B \sum_\alpha S_\alpha \tag{1}$$

where $\langle\alpha\beta\rangle$ means that we sum over nearest neighbor pairs of spins. These spins interact with strength J. We will assume periodic boundary conditions such that $i = N_x$ is the same as $i = 1$, and $j = N_y$ is the same as $j = 1$. Note that the total number of lattice points is $L^2 = N_x \times N_y$.

Physically, for $J > 0$ we have spin alignment favored which means that the system behaves like a ferromagnet, whereas for $J < 0$ the system behaves like an antiferromagnet. We can measure various quantities on the lattice as a function of the temperature and as a function of J and B. The partition function is given by

$$Z(J, B, \beta) = \sum_{\vec{S}} \exp(-\beta H(\vec{S})) \ , \tag{2}$$

and the weight of integration is given by

$$w(\vec{S}) = \frac{\exp(-\beta H(\vec{S}))}{Z} \tag{3}$$

Because of the way we are constructing the algorithm (using importance sampling), we can make a simple measure of the magnetization for a given Monte Carlo configuration:

$$M_i = \sum_{j=1}^{L^2} s_j \tag{4}$$

and the magnetization per spin is

$$m_i = \frac{M_i}{L^2} \ , \tag{5}$$

and the average magnetization over many configurations is

$$\langle m \rangle = \frac{1}{N} \sum_i m_i \ . \tag{6}$$

The energy is given by

$$E = H \ , \tag{7}$$

while the specific heat is given by

$$C_B = -\beta^2 \frac{dE}{d\beta} \tag{8}$$

The magnetic susceptibility, ξ is

$$\xi = \sum_{j=1}^{L^2} s_j^2 - \left(\sum_{j=1}^{L^2} s_j \right)^2 \ . \tag{9}$$

You have been supplied with a basic code for this algorithm. Initially, we assume $B = 0.0$, so that you really only have the first term with the J coefficient. In what follows, we use JKT as the value of J/k_bT. Note that this quantity represents the scale of the problem, so that your plots should usually be in terms of $J\beta$.

You have several things to do:

- First, you need to find the autocorrelation function $C(k)$ as described in the notes for various values of $J\beta$. What values of k should one use to obtain statistically independent samples for various observables? ($B = 0$ here.)
- Why do I code the absolute value of the magnetism rather than the magnetism? ($B = 0$ here.)
- As you increase the lattice size, are you able to see sharper transitions from an ordered to a disordered phase? Can you find the critical tempearture? You should try lattice sizes 5x5, 10x10, 20x20, 30x30, and 50x50. Make plots of both the magnetization and magnetic susceptibility of the system. ($B = 0$ here.)
- Start the MC calculation with an initial lattice of all spins up, and then a random lattice (spins randomly distributed between up and down). How many thermalization steps do you need before you can sample when all spins are initially pointed up and when the spins are randomized? Is this affected by the lattice size? by the temperature? ($B = 0$ here.)
- Let's add the Zeeman-splitting term to the Hamiltonian: $B\sum_i s_i$. Repeat your $J\beta$ simulations for magnetic field $B = 1.0$ and for the different lattice sizes mentioned above. You will have to modify the code to do this. What can you say about the behavior of the material as a function of $J\beta$ when the field is turned on? Is there still a critical temperature? Can you extract it?