Instructions manual for the Ising model code

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Introduction

The Hamiltonian for the Ising model is given as $H = -J\sum_{nn} S_i S_j$ where nn stands for interaction of nearest neighbour spins. For a 2D Ising model one has a second order phase transition from a ferromagnetic to paramagnetic state at a critical temperature that can be analytically computed. In 3D however this critical temperature can be only numerically estimated. We want to find the critical temperature from lattice computations and compare it with the analytic result in the 2D case.

To compute the thermodynamic average of a quantity A, one has to create configurations which come with the correct probability assuming a canonical ensemble, compute A on each such configuration and find a statistical average of the same quantity. A configuration consists of up or down spins sitting at each lattice site according to the Boltzmann weight. There are several algorithms which ensure that a configuration is created with the correct Boltzmann weight. These follow a Markov chain where the probability to move from one configuration to other depends only on the previous configuration. Once the probability weights follow detailed balance condition one can generate correct Boltzmann weight. One such algorithm is called a Metropolis algorithm. Here one starts from an initial spin configuration and compute the total energy. Next one spin is flipped and the new energy is measured. Now if r is a random number between 0 and 1 and $exp[-\beta J(E_{new} - E_{old})] >= r$ then the spin flip is accepted otherwise we reject the flip. We go to the next site and continue the process. After some initial iterations one obtains the configurations with the correct Boltzmann weight. This initial number of configurations which is called "cut-off" in the program has to be discarded for thermalization. The "cutoff" depends on the temperature. It should be several times the autocorrelation length of the system. One easy way to determine this "cutoff" is to begin from two different starting conditions and measure the configuration number from which observables like magnetization of the system become independent of the starting configuration. Once the configurations have thermalized then we take only statistically independent configurations to measure any observable in them. Each statistically independent configurations are separated by the autocorrelation length. Usually one has to take a large number of such independent configurations to compute the averages. If the observables are computed with these configurations then these follow a Gaussian distribution and the error bars are computed from the standard deviation.

The program needs the following parameters and we summarize the main points as follows:

- nx=no of lattice sites along the x-direction.
- ny=no of lattice sites along y-direction.
- betaJ=J/T.
- Start with cold start with all spins at each site to be up i.e 1. You can also begin with a hot start where up and down(-1) spins are distributed randomly on the lattice. In the current program I have commented out the hot start.
- Then we visit each site and flip the spin we perform a Metropolis accept-reject test.
- compile the programs using
  cc -o ising ising2d.c ran3.c -lm
- run the program using
  ./ising nx ny betaJ

Assignment 4:

- The cutoff are the initial no. of configurations that we need to throw away to thermalize the system. I have put it to be 100000. You can check later what should be the optimum value for this parameter.
- Now take every N-th configuration and compute the average magnetization given by M_{av}. I have set $N = 200$. Try to experiment with this number and check what is the optimum N.

- Now compute M_{av} for different βJ from $0.2 - 0.6$ in steps of 0.01. Plot M_{av} as a function of βJ. Find the transition temperature approximately.

- Vary $L = n_x = n_y$ and compute M_{av} and check at what values of L you have achieved the thermodynamic limit i.e. your results for intensive quantities like M_{av} are indeed independent of the volume.

- Compute susceptibility $< M^2 > -LM_{av}^2$ and determine the transition temperature T_c precisely and then compare with the theoretical prediction. Here $n_x = n_y = L$.

- **Optional:** Compute the autocorrelation time for magnetization of the system and estimate how N and cutoff are related to them.

- Near the phase transition the M_{av} follows a scaling law. Zoom in near the βJ where the phase transition occurs. Compute M_{av} for $n_x = n_y = L = 20, 30, 40, 50, 60$. Plot $M_{av} \times L^x$ as a function of temperature βJ. To find the best value of exponent x, vary x and check for what value of x there is a good intersection at one point of all the magnetization curves. Check what happens for the exact value of $x = 0.25$. Also plot $M_{av} \times L^x$ as a function of $L^{1/\nu}(T - T_c^{'})$ where $T_c^{'}$ is the value of the temperature where the curves fall on top of each other. All these curves should collapse to a single curve in the critical region. Also compare T_c with $T_c^{'}$. The ν is the scaling exponent which can be found in standard textbooks. These two temperatures should be equal in the thermodynamic limit. Here ν is the standard critical exponent for a second order phase transition whose value is given in standard textbooks. This exercise would give you an idea about the finite volume effects on the lattice.

- Find the T_c now in the 3D Ising model and compare the corresponding quantity for the $2D$ case.