First and Second Order Phase Transitions in the Ising Model of Ferromagnetism

Introduction

Write a program which simulates via Metropolis Monte Carlo algorithm the 2D Ising model on a 128×128 square lattice with *periodic* boundary conditions. The model is assumed to describe a system placed in an applied external magnetic field B. The energy of a particular state of this system is then given by:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{1}$$

where $\langle i, j\rangle$ means that the sum runs over all pairs of nearest neighbor spins, and J is the exchange coupling. The term with J models the interaction between adjacent spins and the term with B models the interaction with the magnetic field. Note that we have defined both J and B so that they have units of energy with $\sigma = \pm 1$. $J > 0$ leads to ferromagnetism, while $J < 0$ leads to antiferromagnetism in the Ising model. Normalize units so that $E_0 = J$ and $T_0 = E_0/k_B$. Show in your writeup that this is equivalent to setting $|J| = 1$ and the Boltzmann constant is $k_B = 1$ (*Hint: Examine the probability exponential* $e^{-H/k_B T}$). The free parameters of the model are then just the temperature T and the applied field B.

Part I (PHYS460 and PHYS660): First Order Phase Transition in the Ferromagnetic Ising Model

Consider the ferromagnetic Ising model with $J = 1$. Start from a case in which temperature is below the critical temperature $T_c = 2.269$, such as $T = 1.0$. In addition, the field is large and pointing down, e.g., $B = -5$. The selected initial state of the Ising model should be the one in which all spins $\sigma_i = -1$ are parallel to B, so that magnetization per spin is $m = M/N_s = -1$, where N_s is the total number of spins in the system.

Sweep the magnetic field up to a large positive value $B = 5$ and then back down to your starting value $B = -5$. When you change B, don't reset the spins in the system, but initialize the spins in this new B run with the spins at the end of the simulation with the previous B value. Choose small enough increments of δB so that you can determine with good accuracy the B at which the phase change (if any) occurs. After each change in the magnetic field B, allow sufficient Monte Carlo trials for the system to reach equilibrium and thermalize. That is, discard some number of MC sweeps before you start recording m, and be sure to report this number in your methods section and how it was chosen.

For each value of B, the mean magnetization per spin is defined as:

$$\bar{m} = \frac{1}{N_{MC}} \sum_{\alpha=1}^{N_{MC}} m_\alpha. \tag{2}$$

The sum in this expression run is over N_{MC} microstates generated by Monte Carlo simulation. Recall that this is an *estimate* for the ensemble averaged quantity $\langle m \rangle$, and therefore is subject to errors arising from finite sampling.

(a) Plot $\bar{m}$ vs. B. You should see a discontinuous change in $\bar{m}$ as B is increased, and a second discontinuous change in $\bar{m}$ as B is decreased back to its initial value. These discontinuous changes indicate a *first order phase transition.* Also note that the values of B at which discontinuities occur are not identical. This behavior is called hysteresis because $\bar{m}$ depends on the history of the system. For each value of the magnetic field, perform at least one thousand Metropolis steps, where **one step is one complete pass through the lattice (through every spin).**

(b) Repeat the calculations for a temperature $T = 4.0$ above the critical point T_c. Is there a first order phase transition? Is there hysteresis? Provide a physical explanation of any difference in behavior for the two temperatures.

(c) Compute the autocorrelation of m, $C_m(\tau)$ in order to estimate the number of independent samples in your MC runs.

$$C_m(\tau) = \frac{\langle m(t+\tau)m(t)\rangle - \langle m \rangle^2}{\langle m^2 \rangle - \langle m \rangle^2}$$

You don't need to do this for every single value of B, but do a few to get a sense for whether the number of samples depends on B, and then use a conservative estimate to add error bars to your values of $\bar{m}$. Explain your reasoning and choices in the Methods section.

Part II (PHYS460 and PHYS660): Second Order Phase Transition in the Ferromagnetic Ising Model

(a) For the case with no external magnetic field ($B = 0$), examine three different temperatures in the three physical regimes of the system: $T < T_c, T = T_c$, and $T > T_c$. Run the Monte Carlo algorithm on these three temperatures and plot the magnetization per spin and the energy per spin versus Metropolis step. These plots should reveal how many Metropolis steps are necessary to thermalize the Ising ferromagnet, i.e., bring it into the thermodynamic equilibrium with the external heat bath which is assumed to set the temperature T. Thermodynamic averages should be computed only from samples generated after the thermalization has been achieved.

(b) Generate a figure for each of the three temperatures showing the final configuration of your MC simulation, rendered as black and white pixels.

10 BONUS POINTS: Generate an mpeg showing how the lattice evolves in time for $T \simeq T_c$, which shows the growth of critical domains near T_c. For this, you may want to use a larger lattice (256×256), initialize the system in a random configuration, and then run your MC at or very near T_c, and do not discard the initial thermalization steps. Here you are modeling the effect of a quench from high T (disordered) to the critical point. You may have to try a few different temperatures, just above, at, and below T_c.

(c) In this section we examine two important thermodynamic quantities. First, the specific heat per spin is given by:

$$C_V = \frac{1}{N_s}\frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2). \tag{3}$$

Important Note: E is the total energy of a given Ising model state, not the energy per spin.

Second, we examine the magnetic susceptibility per spin given by:

$$\chi = \frac{1}{N_s}\,\frac{1}{k_B T}(\langle M^2\rangle - \langle M\rangle^2). \tag{4}$$

In the case with no external magnetic field ($B = 0$), investigate how C_V and χ change as the temperature increases. In this case we expect a second order or continuous paramagnetic-ferromagnetic phase transition at the critical temperature T_c. Around T_c, both C_V and χ diverge in the thermodynamic limit. Since your calculations are for a finite size system, repeat computation of these two quantities while increasing the lattice size (e.g., 32×32, 64×64, 256×256...) in order to observe how the peak in C_V and χ around T_c increases while its center shifts toward T_c. As shown in Equations 3 and 4 , these two quantities are divided by the lattice size to obtain their values "per spin."

A note of caution: For relatively small numbers of spin (perhaps 32×32), you have to be careful that your calculation of C_v and especially χ are not polluted by spontaneous global spin flipping. In other words, for $T < T_c$, there is a chance that the system will spontaneously flip from $m \approx +1$ to $m \approx -1$. If this occurs during the Metropolis steps where you are calculating χ, it will increase your fluctuations dramatically and give nonphysically large values of χ.

The connection between these two response functions and fluctuations

$$(\Delta X)^2 = \langle X^2\rangle - \langle X\rangle^2, \tag{5}$$

where

$$\langle X^2\rangle = \frac{1}{N_{MC}}\sum_{\alpha=1}^{N_{MC}} X_\alpha^2 \tag{6}$$

$$\langle X\rangle^2 = \left(\frac{1}{N_{MC}}\sum_{\alpha=1}^{N_{MC}} X_\alpha\right)^2 \tag{7}$$

utilizes the so-called fluctuation-dissipation theorem of statistical physics
(see http://iopscience.iop.org/article/10.1088/0034-4885/29/1/306/meta).

Part III (PHYS660 Only): Second Order Phase Transition in the Antiferromagnetic Ising Model

Compute the temperature dependence of C_V, χ, and $\bar{m}$ in the absence of magnetic field ($B = 0$) for the antiferromagnetic Ising model with $J = -1$. The initial configuration can be chosen as all spins up ($\sigma_i = +1$) on a 128×128 lattice. What configuration of spins corresponds to the thermodynamic state below the Neel temperature $T_N = 2.269$? Draw a schematic to show this state. At the so-called Neel temperature this type of materials exhibits a continuous antiferromagnetic-paramagnetic phase transition.

References

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