Major Project: Ising Model

PHZ 5156

This problem combines what we have learned about the technique of Monte-Carlo simulation with the physics of magnetic phase transitions. In a magnetic material (e.g. Ni, Fe, etc.) at high temperatures, each atom has a large local magnetic moment, but they tend to be unaligned. By contrast, at low temperatures, exchange interactions tend to align the spins and create a macroscopic magnetic moment. We will make a simple model of the interactions and then use statistical physics to describe the phase transition from the paramagnetic to ferromagnetic state.

The Hamiltonian H_Ω for a two-dimensional spin system is given by

$$H_\Omega = -\frac{1}{2} J \sum_{i=1}^{N} \sum_{j=1}^{N} S_{ij} \left(S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1} \right) \tag{1}$$

We can also consider adding an applied external field H which adds a term to the Hamiltonian $-H \sum_{i=1}^{N} \sum_{j=1}^{N} S_{ij}$. A more shorthand way to write this is

$$H_\Omega = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \tag{2}$$

where the summation is over nearest neighbor spins and H is an externally applied field.

Determine the "mean field" result for the Ising model. In other words, compare your computed result to the mean field result. Mean-field theory begins formally by rewriting the above Hamiltonian as,

$$H_\Omega = -J \sum_{\langle ij \rangle} S_i \langle S_j \rangle - J \sum_{\langle ij \rangle} S_i \left(S_j - \langle S_j \rangle \right) - H \sum_i S_i \tag{3}$$

and then ignore the *fluctuation term* and solve the rather simple problem

$$H_\Omega = H_\Omega = -J \sum_{\langle ij \rangle} S_i \langle S_j \rangle - H \sum_i S_i \tag{4}$$

The term $\langle S_j \rangle$ is the average spin on site j given by

$$\langle S_j \rangle = \frac{Tr S_j \exp\left(-H_\Omega / k_B T\right)}{Tr \exp\left(-H_\Omega / k_B T\right)} \tag{5}$$

where the H_Ω is given by the mean-field approximation in Eq. 4 with $H = 0$. The magnetization M is given by,

$$M = \frac{1}{N(\Omega)} \sum_{i=1}^{N(\Omega)} \langle S_i \rangle \tag{6}$$

Show that the transition temperature of the mean-field model at zero field ($H = 0$) is given by $k_B T_c = 4J$ for a two-dimensional square lattice. The transition state is where the system alternates between paramagnetic (high temperatures) and ferromagnetic (low temperatures). (Hint: Write an equation for M and determine at what temperature it has solutions other than $M = 0$). The exact result found by Onsager is $k_B T_c = \frac{2J}{log(1+\sqrt{2})} \approx 2.2692J$.

2. Write a code that uses a Metropolis Monte-Carlo algorithm to approximately compute the average properties of the system for a two-dimensional Ising model. Write your code in terms of the dimensionless parameter $J/k_B T$. Use periodic boundary conditions so that spins on the edge of your square interact with spins on the opposite edge. Write a function cluster(i,j) which computes the energy in a cluster of spins centered on spin i, j. Write another function which uses cluster(i,j) to compute the total energy of your square lattice of spins. Now here is the Monte-Carlo algorithm which samples random states with probability in accord with the partition function:

0. Begin with a random array of spins.

1. Compute the energy E_1 of the current spin state.

2. Choose a spin on the lattice at random and flip its spin state.

3. Recompute the energy E_2 of the new spin state.

4. Determine the energy difference $\Delta = E_1 - E_2$.

5. If $\Delta \leq 0$, accept the current step in the ensemble. Save the current spins and energy and return to 1.

6. If $\Delta > 0$, draw a random number between 0 and 1.

7. If the random number is less than $\exp(-\frac{\Delta}{k_B T})$, accept the current step into the ensemble and save the current spins and energy. Return to 1.

8. If the random number is greater than or equal to $\exp(-\frac{\Delta}{k_B T})$, then reject the current step. Reset the spins to what they were before the spin was flipped in step 2. Return to step 1.

Evolve a lattice of 32×32 spins. Make a plot of energy vs. iteration. You will find that the system will equilibrate after a certain amount of time. After equilibrating, average properties can be obtained. Accumulate the average magnetization. Obtain expressions for the spin susceptibility and heat capacity. Compute these quantities during your Monte-Carlo simulation. Establish (approximately) the transition point $k_B T_c/J$. For your presentation, compare to the mean-field and exact results from Onsager's solution. We will discuss and compare critical exponents in each case. You should run your code at $k_B T/J = 1$, 1.5, 1.75, 2.0, 2.25, 2.5, and 3.0. Finite-size effects are important near the transition point. Consider also an explanation for why it is much harder to equilibrate n near $k_B T/J = 2.25$.

For three-dimensional systems, no one has obtained an exact result for the Ising model, and usually either computational or theoretical techniques using the renormalization group are used. A good reference for this is "Lectures on Phase Transitions and the Renormalization Group" by Nigel Goldenfeld.