Homework 5: The Ising Model

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1 Ising Model Algorithim

This program was written to numerically study the 2D Ising Model on a n x n lattice with periodic boundary condtions. The calulated lattive has a nearest neighbor interaction strength of $J = 1.5$ and no external magnetic field. The metropolis algorithim is then used to relax the system of spins to the desired temperature(s).

1.1 Equations Used

The Hamiltonian which is the energy of the system is give by the following equation:

$$H = -J \sum s_i s_j \tag{1}$$

Where J is the nearest neighboor interation between the spins in the lattice and s_i and s_j are the spin states of the neighbooring lattices which are summed and either +1 or -1.
The probability once the system is in thermal equlibrium that the configuartion of the lattice with a certain energy is given by the Boltzmann distribtuion:

$$P_\alpha \ \propto e^- E_\alpha / k_B T \tag{2}$$

Where K_B is the boltzmann constant and T is the given temperature.
The magnetization of the system is given by:

$$M = \sum M_\alpha P_\alpha \tag{3}$$

$$M_\alpha = \sum s \tag{4}$$

The average energy and average energy squared is given by:

$$\langle E \rangle = \frac{1}{N} \sum E_\alpha \tag{5}$$

$$\langle E^2 \rangle = \frac{1}{N} \sum E_\alpha^2 \tag{6}$$

The specific heat is given by:

$$C = \frac{\langle E \rangle^2 - \langle E^2 \rangle}{k_B T^2} \tag{7}$$

1.2 Monte Carlo and Metropolis Algorithim

At the equlibrium the system has a phase transition between paramagnetic and ferromagnetic states at the Curie temperature (T_C). At this temperature magnetiziation and energy are able to be measured. The steps for the Metropolis Algorithim are given below to generate lattice configurations for a given temperature (using Monte Carlo). The metropolis algorthim was run sufficently to reach equlibrium before magnetization and energy calculations were completed.

1) Initlize system: assing random spin to the system (to each lattice point). This is done using a RNG to generate a number between 0 and 1. If the number is less than or equal to 0.5 it is spin up and if its greater than 0.5 its spin down.
2) For a random given atom, calculate the change in energy of the system if the spin is flipped.
3) If $\Delta E \leq 0$, the spin is flipped. If $\Delta E \geq 0$, the spin is flipped with probability $e^{-\frac{\Delta E}{k_B T}}$. A random number is then generated to compute the probaility. If the random number is less than or equal to the probability, the spin is flipped otherwise its not flipped.
4) The new energy of the system along with its magnetization is saved.
5) Back to step 2.

1.3 Part 1 Analysis

Part one of the code calculates the magnetization, $M = N\langle s\rangle$ as a function of temperature. The number of lattice sites chosen was 50^2 and using Monte Carlo, enough iterations were allowed to reach equilibrium to determine the critical temperature T_C of the system.

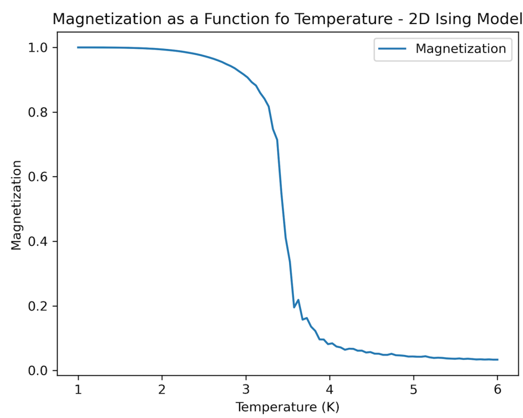

Figure 1: Magnetization, $M = N\langle s\rangle$ as a function of temperature with a lattice size of 50^2.

From the plot it was determined that the critical temperature T_C is around 3.5 K. This can also be determined analytically:

$$T_C = \frac{2J}{k_B \ln(1+\sqrt{2})} \tag{8}$$

$$T_C = \frac{2 * 1.5}{1\ln(1+\sqrt{2})} \tag{9}$$

$$T_C = 3.404 \text{ K} \tag{10}$$

1.4 Part 2 Analysis

Part two of the code calculates the specific heat per spin C/N for 10 different lattice sizes using the fluctuation-dissipation theorem, $C = \frac{\langle E\rangle^2 - \langle E^2\rangle}{k_B T^2}$. The approximate finite-size scaling relation $C_{max}/N \sim \log(n)$. When plotting specific heat vs temperature the peaks become sharper and increase as n increases. The fluctuation-dissipation theorem equation shows that fluctuations in energy increase as the temperature increases. The peak is centered around the critical temperature of the system which indicates the transition from the ferromagnetic state to the paramagnetic state.

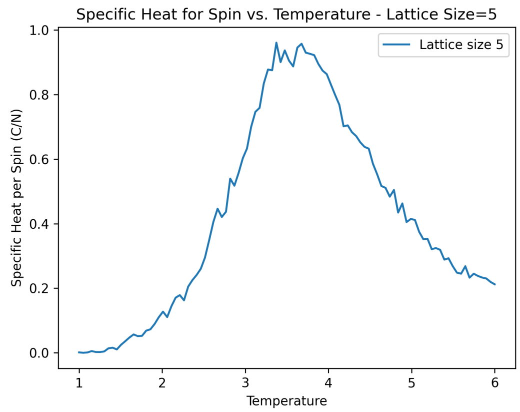

Figure 2: Specific heat per spin as a function of temperature for a lattice size of 5^2.

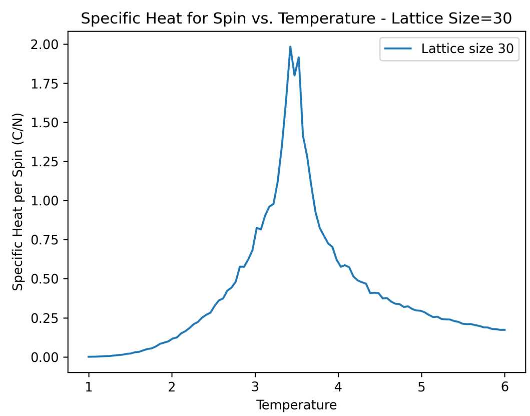

Figure 3: Specific heat per spin as a function of temperature for a lattice size of 30^2.

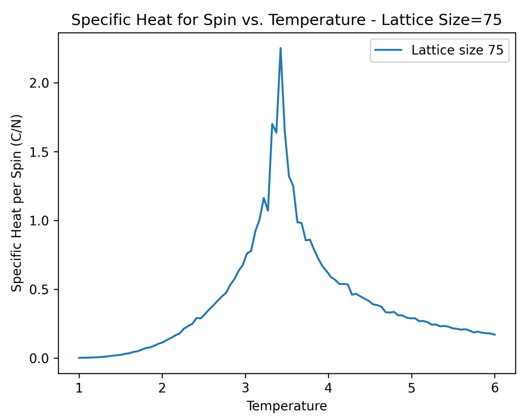

Figure 4: Specific heat per spin as a function of temperature for a lattice size of 75^2.

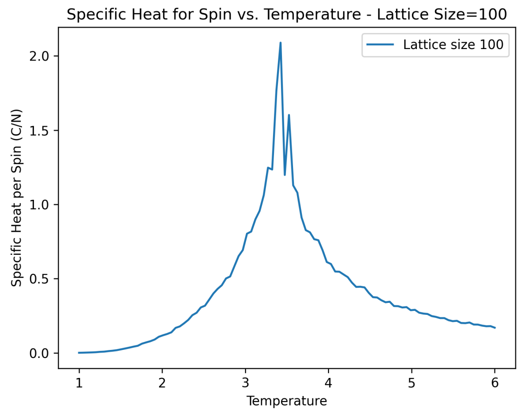

Figure 5: Specific heat per spin as a function of temperature for a lattice size of 100^2.

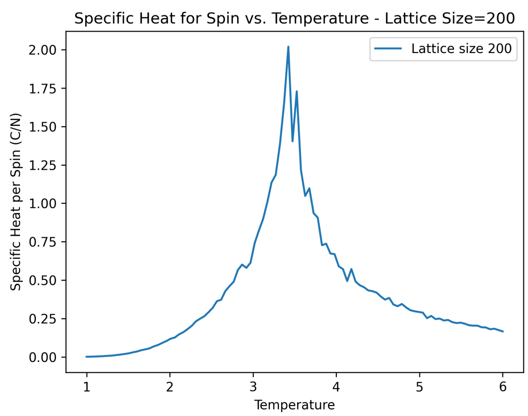

Figure 6: Specific heat per spin as a function of temperature for a lattice size of 200^2.

When plotting C_{max} vs the lattice size we see peaks at a T value that is dependent on the lattice size. It shows that the systems behavior scales with the lattice size. To verify the scaling relation, the plot shows a linear line. This is due to the finite-size effects from critical phenomena due to the specific heat forks logarithmically near the T_C. I didn't get a chance to show the remainder of the plots because I had to buy a new laptop while working on this homework and the final part of the code was taking too long.