2-D Ising Model

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Ising model was invented by Wilhelm Lenz in 1920 and is named after Ernst Ising, a student of Lenz who pursued it as the subject of his doctoral dissertation in 1925. Here we have simulated 2-D Ising Model using Metropolis-Hasting algorithm and plotted net average magnetization, net average energy, magnetic susceptibility and specific heat capacity with respect to change in temperature at zero external magnetic field. The Metropolis–Hastings algorithm is the most commonly used Monte Carlo algorithm to calculate Ising model estimations. It follows single-spin-flip dynamics, which states that in each transition, we only change one of the spin sites on the lattice. Close to criticality the correlation length diverges and the magnetization goes to almost zero. In dimensions greater than four, the phase transition of the Ising model is described by mean field theory.

I. INTRODUCTION

Ferromagnetism is a phenomena that arises when a collection of spins align such that their associated magnetic moments all point in the same direction, yielding a net magnetic moment which is macroscopic in size. The simplest theoretical description of ferromagnetism is the Ising model. It's one of few exactly solvable models where we can actually compute thermodynamic quantities and interpret them. The model was not able to explain ferromagnetism in one dimension,and Ising gave arguments as to why it would not exhibit ferromagnetism in two and three dimensions. Although we now know that it does show a ferromagnetic transition in two and higher dimensions. In 1944, Lars Onsager gave a complete solution of the problem in zero magnetic field which was the first nontrivial demonstration of the existence of a phase transition from the partition function alone. Onsager solved the two dimensional Ising model exactly for the zero field case, and found a finite temperature ferromagnetic phase transition.

Considering a lattice of N sites with a spin S on each site, where each spin can take one of two possible values: +1 for spin up and -1 for spin down a total of 2N possible configurations of the system will be available. A particular configuration is specified by the orientations of the spins at each of the N sites: $\{S_i\}$ and the interaction energy is given by:

$$E_I\{S_i\} = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j - \sum_{i=1}^{N} B_i S_i \tag{1}$$

where the subscript I represents the Ising model. A factor of 2 has been absorbed into $\{J_{ij}\}$ and we set $g\mu_B = 1$ in the last term. $\langle i,j\rangle$ means nearest neighbor pairs of spins. So $\langle i,j\rangle$ is the same as $\langle j,i\rangle$. $\{J_{ij}\}$ is the exchange constant; which sets the energy scale. For simplicity, one sets $\{J_{ij}\}$ equal to a constant J independent of i and j. Different spatial separations imply different electrostatic interaction energies, and the exchange energy J measures this difference. The spins lower their energy by aligning parallel to the field. If the field $\{B_i\}$ is random, it is called the random field Ising model. Assuming a constant uniform magnetic field so that $\{B_i\}$= B, the interaction energy becomes:

$$E_I\{S_i\} = -J\sum_{\langle i,j\rangle} S_i S_j - B\sum_{i=1}^{N} S_i \tag{2}$$

where partition function is given by:

$$Z = \sum_{s_1=-1}^{+1}\sum_{s_2=-1}^{+1}\cdots\sum_{s_N=-1}^{+1} e^{-\beta E_I\{S_i\}} \tag{3}$$

In the mean field approximation:

$$H_{\text{eff}} = H + \frac{z\,J\,\bar{s}}{2\,\mu}. \tag{4}$$

where,

$$\bar{s} = \tanh\{\beta\,\mu\,H + \beta\,z\,J\,\bar{s}/2\}\,. \tag{5}$$

and critical temperature and critical field are defined by: $T_c = \frac{zJ}{2k}$ and $H_c = \frac{kT_c}{\mu} = \frac{zJ}{2\mu}$.

In the absence of any external magnetic field, it can be seen that below the critical or 'Curie' temperature, there is spontaneous magnetization: the exchange effect being sufficiently large causes neighbouring atomic spins to spontaneously align. On the other hand, thermal fluctuations completely eliminate any alignment above the critical temperature. At the critical temperature there is a discontinuity in the first derivative of the energy with respect to temperature creating a downward jump in heat capacity. The sudden loss of spontaneous magnetization as the temperature exceeds the critical temperature is a type of phase transition. According to the conventional classification of phase transitions, a transition is first-order if the energy is discontinuous with respect to the order parameter, and second-order if the energy is continuous, but its first derivative with respect to the order

parameter is discontinuous. Temperature is the order parameter here. Based on this we conclude that the loss of spontaneous magnetization in a ferromagnetic material as the temperature exceeds the critical temperature is a second-order phase transition. If we observe the behaviour of magnetization, M, as the external field, H, is varied at constant temperature, T. It can be seen that E is discontinuous, indicating the presence of a first-order phase transition. Calculations based on the mean field approximation correctly predict the existence of first and second order phase transitions when $H \neq 0$ and $H = 0$ respectively. However, mean field calculations get some of the details of the second-order phase transition wrong. Hence we shift to Monte-Carlo approach from the mean field approximation.

II. ALGORITHM

We consider a two-dimensional square array of atoms with dimension N*N. Following is the algorithm:

- Step through each atom in the array in turn:
- For a given atom, evaluate the change in energy of the system, ΔE, when the atomic spin is flipped.
- If $\Delta E < 0$ then flip the spin.
- If $\Delta E > 0$ then flip the spin with probability $P = \exp(-\beta\,\Delta E)$.
- Repeat the process many times until thermal equilibrium is achieved.

The purpose of the algorithm is to shuffle through all possible states of the system, and to ensure that the system occupies a given state with the Boltzmann probability: i.e., with a probability proportional to $\exp(-\beta\,E)$, where E is the energy of the state. In order to demonstrate that the above algorithm is correct, let us consider flipping the spin of the ith atom. Suppose that this operation causes the system to make a transition from state a (energy, E_a) to state b (energy, E_b). Suppose, further, that $E_a < E_b$. According to the above algorithm, the probability of a transition from state a to state b is

$$P_{a\rightarrow b} = \exp[-\beta\,(E_b - E_a)],$$

whereas the probability of a transition from state b to state a is

$$P_{b\rightarrow a} = 1.$$

In thermal equilibrium, the well-known principal of detailed balance implies that

$$P_a\,P_{a\rightarrow b} = P_b\,P_{b\rightarrow a},$$

where P_a is the probability that the system occupies state a, and P_b is the probability that the system occupies state b. Equation (369) simply states that in thermal equilibrium the rate at which the system makes transitions from state a to state b is equal to the rate at which the system makes reverse transitions. The previous equation can be rearranged to give

$$\frac{P_b}{P_a} = \exp[-\beta\,(E_b - E_a)],$$

which is consistent with the Boltzmann For this system we should have N $\rightarrow \infty$, meaning very large N, but this is very expensive computation wise. One way of increasing the accuracy of the results without increasing the size of the matrix is to use periodic boundary conditions. This is easily achieved by using modulo operator: taking the neighbouring sites to be ((i + 1) mod (N), j) etc., instead of ((i + 1) , j) etc.

III. ANALYSIS

Once the system has been simulated, the aim is to investigate its properties by calculating various observables and determine whether or not it undergoes a phase transition. This can be done by calculating the several observables and investigating their properties; in particular, how they depend on the temperature of the system. The average energy per spin is determined by:

$$\langle E\rangle = \left\langle \sum_{\langle i,j\rangle} H_{ij} \right\rangle = \frac{1}{2}\left\langle \sum_{i,j} H_{ij} \right\rangle \tag{6}$$

the 1/2 accounting for the fact that every pair is counted twice in the sum. If the system is ferromagnetic, then the expected value of $\langle E\rangle$ for the 2D square lattice would be -2J when the spins are all aligned. $\langle E\rangle$should be a continuous function of temperature, with a point of inflection at , and should approach 0 after this point, signifying that a phase change has ocurred and the material has become disordered and paramagnetic. The average magnetisation per unit spin is given by:

$$\langle M\rangle = \frac{1}{N^2}\sum_{(i,j)} \sigma_{ij} \tag{7}$$

Calculating M allows determination of the time taken for the system to reach equilibrium at a given system size. The average magnetisation is seen to approach a constant value, when plotted against the number of iterations after each implementation of the Metropolis algorithm signifying an equilibrium, and the minimum number of iterations required to achieve is thus determined. The magnetisation can also be used to show that a phase transition has occurred in the material and approximate the Curie temperature, T_C. For calculating specific heat a standard equilibrium statistical thermodynamics rela-

tion is used:

$$\begin{aligned} C_V &= \frac{\partial(E)}{\partial T} \\ &= -\frac{\beta}{T}\frac{\partial\langle E\rangle}{\partial\beta} \\ &= \frac{\beta}{T}\frac{\partial^2 \ln(Z)}{\partial\delta^2} \\ &= \frac{\beta}{T}\left(\langle E^2\rangle - (E\rangle^2\right) \end{aligned} \tag{8}$$

$$C_V = \frac{\sigma_E^2}{k\,T^2}$$

Deviation in E is calculated from step to step in Monte-Carlo iteration scheme. The heat capacity peaks at the critical temperature. Similarly, the magnetic susceptibility is defined as:

$$\begin{aligned} \chi &= \frac{\partial(M)}{\partial H} \\ &= \beta\left(\langle M^2\rangle - \langle M\rangle^2\right) = \frac{\sigma_M^2}{k\,T} \end{aligned} \tag{9}$$

The mean field model yields $T_c = 2\,T_0$. The exact answer for a two-dimensional array of ferromagnetic atoms is

$$T_c = \frac{2\,T_0}{\ln(1+\sqrt{2})} = 2.27\,T_0,$$

where T_0 is defined as:

$$T_0 = \frac{J}{k}.$$

This analytic result was first obtained by Onsager in 1944. Onsager's analytic solution of the 2-D Ising model is one of the most complicated. In our case T_0 is 1 as both J and k are 1, hence T_C should be close to 2.27. In the plots we can see a critical behavior close to 2.5K.

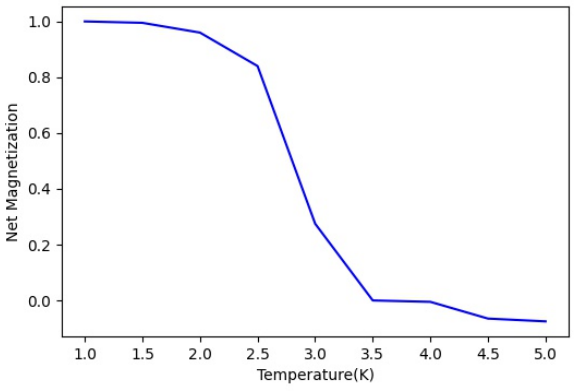

FIG. 1. Net Magnetization vs. Temperature

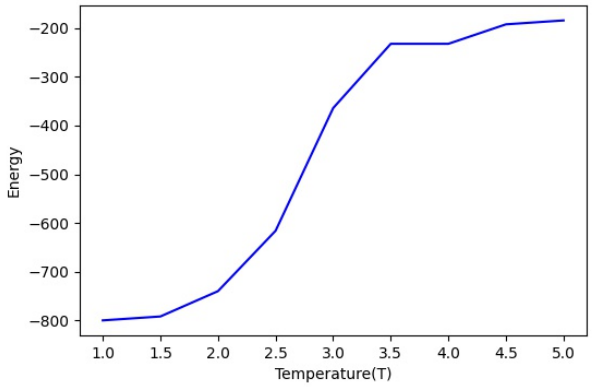

FIG. 2. Energy vs. Temperature, The Energy of a 20×20 ising lattice as a function of the temperature, T, in the absence of an external magnetic field,Monte-Carlo simulation.

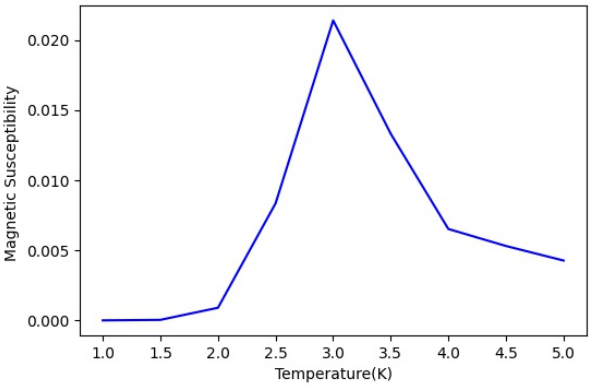

FIG. 3. Magnetic susceptibility vs. Temperature
The magnetic susceptibility , χ, of a 20×20 ising lattice as a function of the temperature, T, in the absence of an external magnetic field,Monte-Carlo simulation.

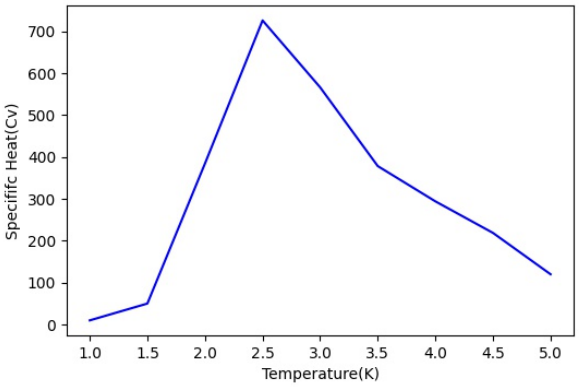

FIG. 4. Heat capacity vs. Temperature
The heat capacity, C, of a 20×20 ising lattice as a function of the temperature, T, in the absence of an external magnetic field,Monte-Carlo simulation.

IV. CONCLUSION

The analytical solution for critical temperature of 2-D Ising model is $T_C = 2.27 T_0$. Defining T_0 as 1, gives $T_C = 2.27$. The result from our simulations are close but not in exact agreement with the analytical solution and is evident in the above plots. Our plots show the approximate behavior of different observables, e.g. magnetization, energy, magnetic susceptibility and specific heat close to criticality.