Monte Carlo Simulation of the Ising Model

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Abstract

This paper explores the order-disorder transition at a critical temperature in the Ising model by exploring the magnetization per site and specific heat at various temperatures. A 2-D 100×100 Ising model with periodic boundary conditions was used. Each site was assigned a +1 or -1 spin. No external magnetic field effects were considered. J was set to -4 eV. A Metropolis algorithm was used to solve for the 2-D model. The algorithm was run long enough to let the system equilibrate. It was observed that the transition in mean magnetization becomes really sharp at the critical temperature. The average magnetization was zero above the critical temperature (paramagnetic phase) and one below this temperature (ferromagnetic phase).

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I. INTRODUCTION

Ising Model is a well studied model in statistical mechanics. Even though the Ising model is very simple it is extremely successful in predicting the behavior of a real system. The most important property of this model is its order-disorder phase transition. Above a critical temperature the magnetization per site m is quite small, whereas below it the magnetization is definitely non-zero and for most part close to its maximum value of 1. This seems like a sensible way for the model to behave as we know that at high temperatures all the spins are randomly aligned and at lower temperatures either all spins are aligned up or down. However, as we approach the critical temperature,T_c, the transition from small m to large m becomes really sharp. Below T_c the system randomly chooses to either have all spins aligned up or down. We are interested in studying this phase transition behavior of the Ising model. Infact, the magnetization per site and specific heat plots presented in the results section depict this behavior very clearly. This paper will use the ideas from statistical mechanics (as described above) to solve for a 2-D Ising model. We will calculate the magnetization per site and specific heat to observe the order-disorder transition in the Ising model at a critical temperature. The first section introduces some concepts necessary to understand the model. The second section describes the Ising model and its properties in detail. The third section will go over the Metropolis algorithm used to simulate the Ising model. The fourth section will present and discuss some results and finally the fifth section will provide a summary.

II. CONCEPTS FROM STATISTICAL MECHANICS

It is almost impossible to exactly solve the mathematics for systems with many atoms or molecules. In principle, it is possible to write simple equations of motion for such a system. However, the sheer number of these equations makes the task of solving them daunting. For example, one liter of oxygen at standard temperature and pressure has 3×10^{22} oxygen molecules, all moving around and interacting with each other and the walls of the container. For systems like this it is not feasible to solve the Hamiltonian's equation. However, the macroscopic properties of such systems are well-behaved and predictable. Statistical mechanics side steps the problem of solving the equations of motions for such large systems and instead calculates these gross properties by treating them in a probabilistic fashion.

Instead of looking for exact solutions we look for the probability of the system being in one state or another. Suppose our system is in a state A, we need only wait a small time before our system would be in any one of a very large number of other possible states. This is where the probabilistic treatment is relevant. A set of weights ($w(t)$) can be defined that will represent the probability of the system being in state A at time t. Given enough time our system will evolve to an equilibrium state where these weights can be represented by the Boltzmann's probability distribution,

$$p_A = \frac{e^{-E_A/kT}}{Z}, \tag{1}$$

where E_A is the energy of state A, k is the Boltzmann's constant and $Z = \sum e^{-E_A/kT}$ is the normalization constant. By using above we can obtain the expectation value of a quantity Q by,

$$\langle Q \rangle = \sum_A Q_A \times p_A, \tag{2}$$

where Q_A is the value of the quantity in state A and p_A is the probability for the system to be in state A. The above holds for systems in equilibrium state. Non-equilibrium systems are treated in a complex way that will not be discussed in this paper.

III. ISING MODEL

The Ising model is a model of a magnet. The essential concept behind it, or any magnetic model, is that the magnetism of a bulk material is made up of combined magnetic dipole moment of many atomic spins within the material. When current is passed through a closed loop it produces some magnetism. Similarly, when electrons in an atom rotate around the nucleus a small magnetism is produced. These atomic magnets are just like normal magnets and have 'magnet vectors' that point up or down (from south to north pole or vice-versa). In normal materials these atomic magnets are aligned randomly and hence cancel each others magnetic field. However, in some materials these atomic magnets can align in a particulate direction and add up to give rise to magnetism. A good example of such a material would be iron. In the Ising model we can choose any type of geomtry we want (e.g. simple cubic lattice) and assign a spin value to each lattice site. However, in this paper we stick to a 2-D Ising model as depicted in Fig.1.

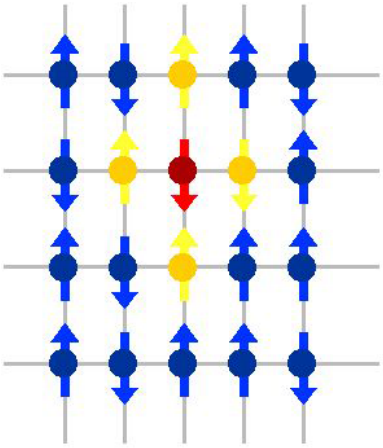

FIG. 1: A 2-D lattice model. The red spins only interacts with the yellow spins

The spin can only take a +1 or -1 value. Also, in real systems these spins interact with each other. So in order to compensate for the interactions the ising model includes a term proportional to the product of two spins,$s_i s_j$, in its Hamiltonian. However, it does assume that all spins interact with the same strength J (units of energy) and only spins on the nearest neighbor lattice sites are allowed to interact with each other. The Hamiltonian for such a system then becomes:

$$H = -J \sum_{\langle ij \rangle} s_i s_j, \quad (3)$$

where $\langle ij \rangle$ indicates site i and j in the sum are neighbors. The minus sign is conventional and dictates the choice of sign of J. A positive value of J makes the spins want to line up and makes the material ferromagnetic and a negative value makes it anti-ferromagnetic. In the Ising model, at high temperatures all the spins are random and uncorrelated, but as the temperature is lowered the interactions between them encourages nearby spins to point in the same direction, giving rise to correlation in the system. This also results in the formation of clusters which is a group of spins all pointing in the same direction. As we approach the critical temperature (T_c) the size of these clusters diverges, such that precisely at the transition we may encounter arbitrarily large areas in which spins are pointing mostly up or down. Then, as we pass below the transition temperature the system spontaneously chooses to have majority of its spins either point up or down. The direction it picks solely depends on the random detail of the thermal fluctuations it was going through as it was moving through T_c. In this way the system undergoes a order-disorder phase transition or a paramagnetic to ferromagnetic phase transition.

IV. METROPOLIS ALGORITHM

It is a widely used algorithm that generates a sequence of microscopic states. Suppose we were trying to calculate $\langle A \rangle$ by random sampling i.e. generate n states at random then we would have:

$$\langle A \rangle = \frac{\sum_{i=1}^{n} A(s_i) e^{-H(s_i)/kT}}{\sum_{i=1}^{n} e^{-H(s_i)/kT}} \tag{4}$$

This would lead to poor convergence of estimate of $\langle A \rangle$ because for many of the n states the P_{eq} would be small. An alternative to this approach would be to sample states in such a way that they occur with a non-random distribution ($P(s_i)$) giving:

$$\langle A \rangle = \frac{\sum_{i=1}^{n} A(s_i) e^{-H(s_i)/kT}}{p(s_i) \sum_{i=1}^{n} \frac{e^{-H(s_i)/kT}}{p(s_i)}} \tag{5}$$

The best choice is to choose $P(s_i)$ equal to the Boltzmann's probability distribution function or equilibrium distribution. With this choice we get:

$$\langle A \rangle = \frac{\sum_{i=1}^{n} A(s_i)}{n} \tag{6}$$

This choice leads to a rapidly converging estimate of $\langle A \rangle$. Metropolis algorithm helps generate a sequence of states according to a transition probability,

$$W(S(t_l) \rightarrow S(t_{l+1})) = W_{l,l+1}, \tag{7}$$

where W is the probability of going from state $S(l)$ to $S(l+1)$. The states are generated stochastically according to the above probability. These sequence of states is called 'Markov chain' i.e the subsequent state is only dependent on the previous state. However, $W_{l,l+1}$ has to obey detailed balance i.e the number of states transforming from s_l to $s_{l'}$ has equal to the number of states transforming back from $s_{l'}$ to s_l.

V. APPLICATION TO CODE

1. Apply periodic boundary conditions to the system so that all the spins have the same environment. Periodic images are obtained by translating the system by assing multiples of n.

2. Pick a site at random by calling two random numbers r_1 and r_2 and setting $[x, y] = [r_1, r_2]$.

3. Attempt a Monte-Carlo move consisting of change of spin. So if earlier the site has spin-up it would be changed to spin-down and vice-versa.

4. Compute the change in the value of the Hamiltonian by using,

$$\Delta E = -2J \sum_{\langle ij \rangle} s_i s_j \tag{8}$$

5. Determine wheter to accept or reject the move according to the following rules:

   (a) if $\Delta H \leq 0$, accept the move.

   (b) if $\Delta H \geq 0$,pick a random number r between 0 and 1.

      i. if $r \leq e^{-\Delta H/kT}$, accept the move.

      ii. if $r \geq e^{-\Delta H/kT}$, reject the move.

6. Update your data.

   (a) if accepted, change the lattice occupation else leave lattice unchanged.

   (b) if accepted, update energy else leave energy unchanged.

   (c) update the counter for 'time' by 1.

7. Repeat all the steps.

VI. RESULTS

This Ising model was run at 11 different temperature between 0.5 and 3.0 for a total of 3000 Monte Carlo steps. The value of J was -4.0 eV. We started with a system where all the lattice sites were spin up. By Monte Carlo steps I mean: When we perform N Monte Carlo steps –one for each spin in the system on average - we have complete one sweep of the lattice. The x axis in all the following plots will correspond to this 'time'. Another important concept in Monte Carlo calculations is the idea of an equilibration time. It means that we have to run our system for a suitably long time until it has come to equilibrium and then we measure the quantities we are interested in over another long period of time and take an average to estimate the quantity. Equilibrium means that the average probability of finding our system in any particular state is proportional to the Boltzmann's probability

distribution as discussed in Section II. So if we start our system in any random state at a certain temperature eventually the system will reach an equilibrium state. The following energy vs. monte carlo time plots depict this behavior. The energy of the system increases steadily until it reaches the equilibrium state and then simply oscillates around an average value. The equilibration time was 200 mcs on average.

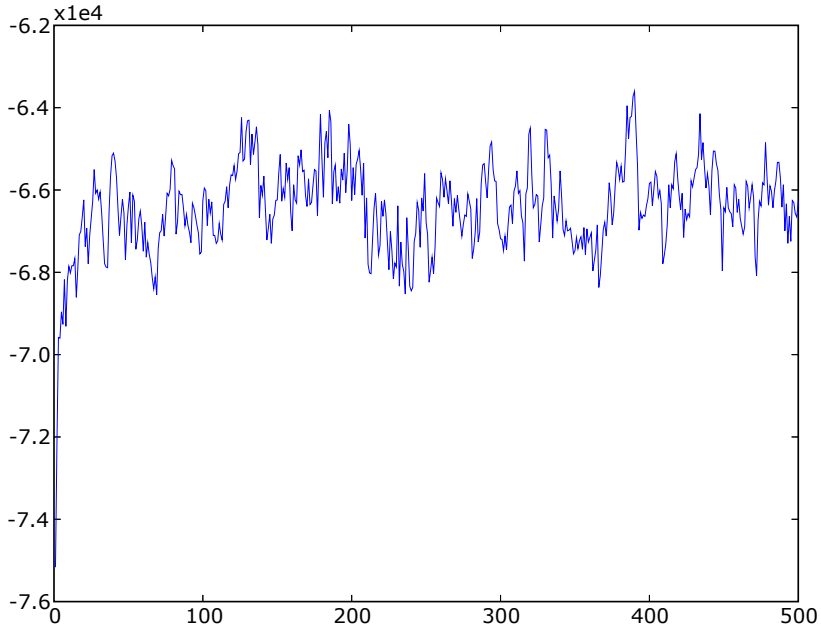

FIG. 2: A Energy vs Timestep plot for Temperature 2.1. The equilibration time was 200 mcs

Notice how the system's equilibration time decreases with temperature. However, just to be safe I excluded 200 time steps from all the data. We also obtained snapshots of the final state at different temperatures of the Ising model (fig. 5, 6, **??**). We notice that at low temperatures most of our spins are still up however as the system aproaches the critical temperature we see the formation of spin up and down clusters.

Finally we calculated the mean magnetisation (fig. 8) and the specific heat per spin (fig. 9) for the Ising model. Both properties show the right behavior. The magnetisation of the system goes from 1 to 0 as the temperature is increased and the spins start aligning randomly. However, the magnetisation curve is not very smooth due to lack of enough data. I should have run the code at more temperatures. But we do see the phase transition very clearly at the critical temperature of 2.269. The specific heat also shows the right behavior.

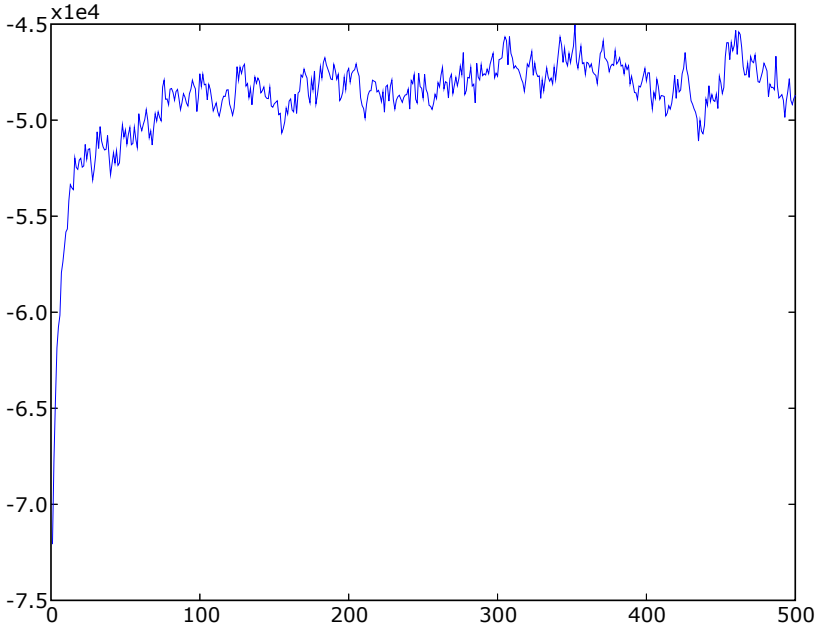

FIG. 3: A Energy vs Timestep plot for Temperature 2.4. The equilibration time was 200 mcs

It steadilt increases till it reaches the critical temperature and then decreases back again.

VII. SUMMARY

The Ising model was run at 11 different temperatures between 0.5 and 3.0 for 3000 Monte Carlo steps. The J value was -4 eV. The equilibration time was found to be 200 mcs. The data from the runs was used to construct magnetisation and specific heat per spin plots. The Ising model code reproduced the expected behavior as discussed in section III. We were able to see the phase transition in the Ising model at the critical temperature of 2.269. The magnetisation went from 1 to 0 as the temperature increased. The specific heat reached a maximum at the critical temperature and then decreased. The statistical error was not calculated in this paper. However, since it is a Monte Carlo is a statistical model there is always some error associated with all the calculations.

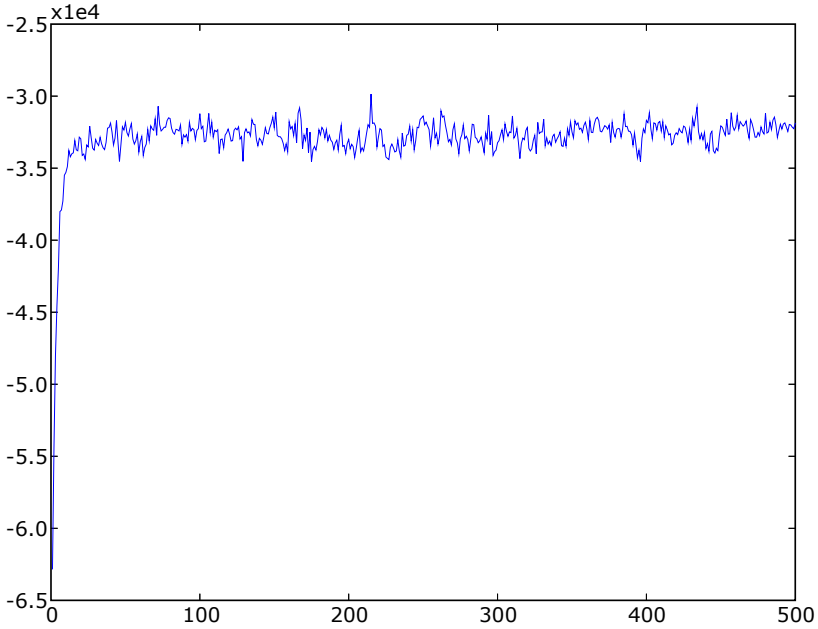

FIG. 4: A Energy vs Timestep plot for Temperature 3.0. The equilibration time was 200 mcs

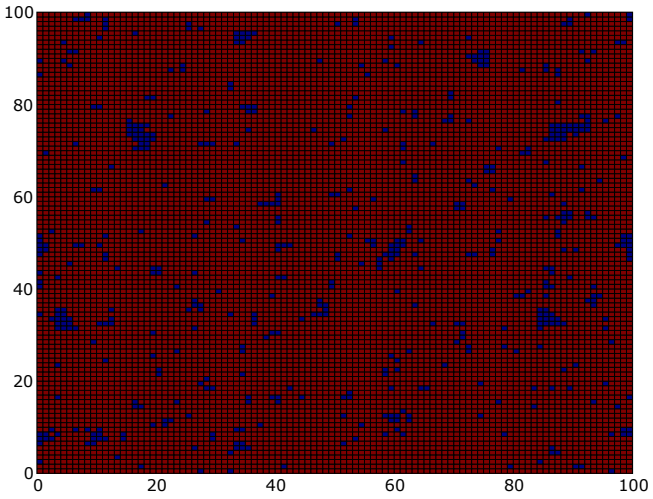

FIG. 5: Snapshot of a 100×100 ising model at a temperature of 2.1

VIII. REFERENCE

M. E. J. Newman and G. T. Barkema, Monte Carlo Methods in Statistical Physics, Clarendon press, 2001

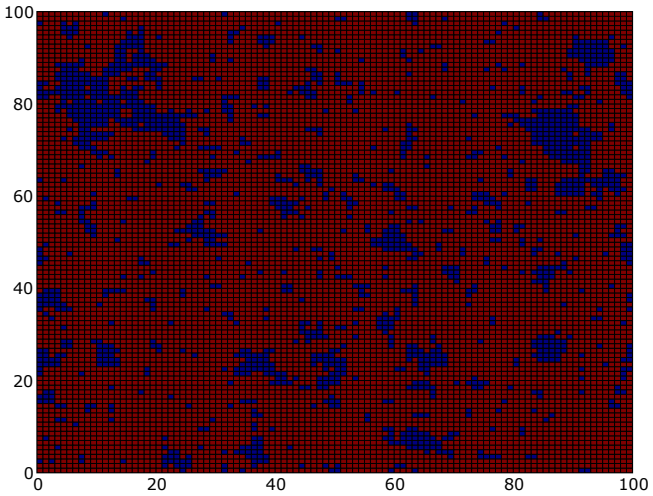

FIG. 6: Snapshot of a 100×100 ising model at a temperature of 2.268

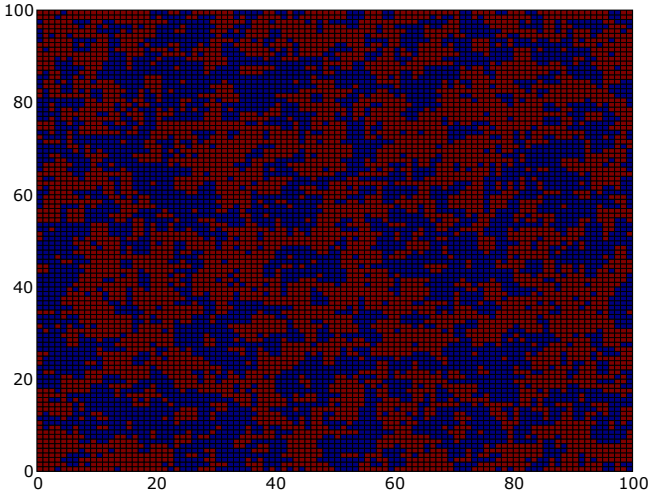

FIG. 7: Snapshot of a 100×100 ising model at a temperature of 3.0

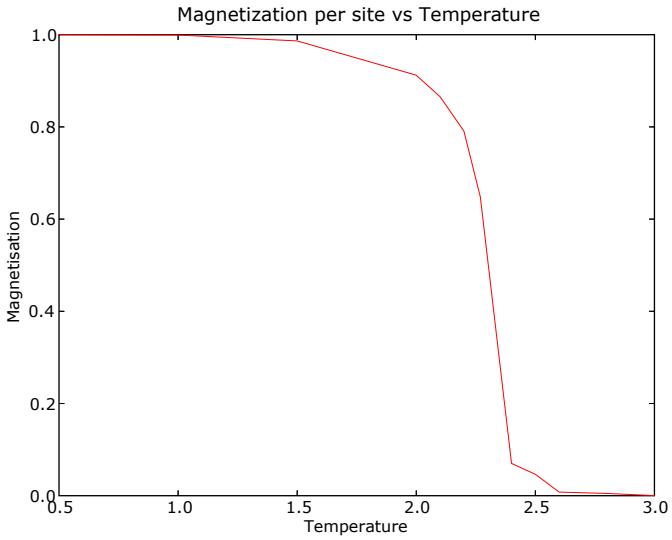

FIG. 8: The magnetisation per spin of a 100×100 2D Ising model

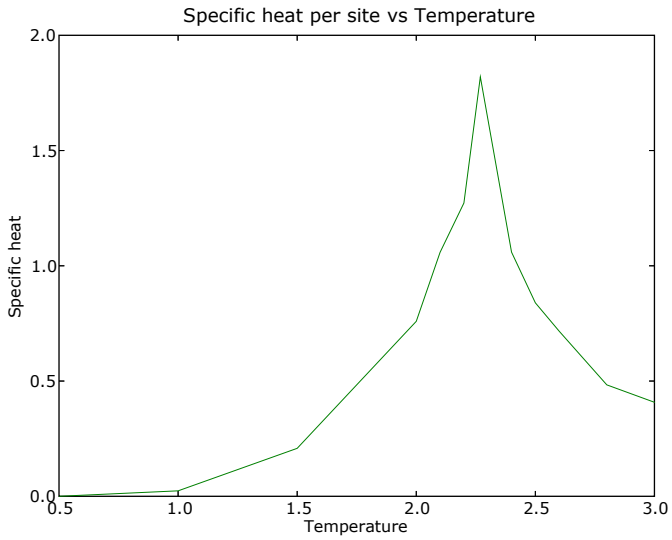

FIG. 9: The specific heat per spin of a 100×100 2D Ising model