Computational Studies of the Ising Model

Summer Project Report

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Abstract

We conducted a study of the two-dimensional Ising model implemented using the Metropolis Algorithm to observe parameters such as Energy, Net Magnetization, Specific Heat Capacity, Magnetic Susceptibility etc. and determined the existence of a phase transition in the model. Using Finite size scaling and the Binder Cumulant, we determined the Critical Temperature of the phase transition which was in agreement with the analytical value. We further briefly analyzed the 2D model under an external magnetic field and the three-dimensional Ising Model to find an increase in the Critical Temperature. Using results from above we attempted to incorporate non reciprocal interactions to observe an increase in Critical temperature which reduces with reciprocity, and applied a random field to the model and obtained an invariance in critical properties with the distribution.

Acknowledgements

I would like to express my gratitude to Dr. A. V. Anil Kumar for providing me the opportunity to work on this project. The guidance he provided through our numerous conversations and meetings was invaluable, and I deeply value the time he dedicated to support me and my project. I would like to thank the NISER Library for providing the resources to aid me in this project. I would also like to thank Jacob Binu Abraham for allowing me to bounce ideas off of one another as a peer. Last but not least, I'd like to express my gratitude to everyone who directly or indirectly assisted me in completing this project.

Contents

1 Introduction

The Ising model is a classic illustration of a basic yet highly insightful system in the field of condensed matter physics. The Ising model, which was originally developed to describe the behaviour of magnetic materials, has grown beyond its origins to become an essential tool in understanding phase transitions and key phenomena across numerous scientific disciplines. Applications of the ising model range from study of ferromagnetism and spin glasses to large neural networks and neuroscience. It functions as a paradigmatic model for studying phase transitions. Because of its intrinsic simplicity and ability to monitor complicated behaviours, it has proven to be an excellent tool for testing theories and techniques.

This project uses proficient computational methods to not only recreate existing results but also to push the boundaries of our understanding by examining the model's behaviour under various circumstances and dimensions. We shall first understand the framework of the model and its properties, choose a suitable Monte Carlo Algorithm for its implementation and then write a program for the simulation and data collection. We will proceed to analyze the observed data to recognize any phase transition and find the critical temperature of the transition using various methods. We further test our model under varying conditions and dimensions and correlate the observations with theory to further ensure the feasibility of the model. Once verified, we shall attempt to study nonreciprocal interactions and random fields using the Ising model.

In the parts that follow, we will look into the theoretical foundations of the Ising model, explain the computational approaches used, present the acquired results, and engage in important discussions about the implications of these findings. Ultimately this project serves to illustrate the simple computational models which can be used to recreate and study complex real life phenomena.

2 The Ising Model

The Ising model (or Lenz-Ising model), named after the physicists Ernst Ising and Wilhelm Lenz, is a mathematical model of ferromagnetism in statistical mechanics. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins" that can be in one of two states (+1 or -1). The spins are arranged in a graph, usually a lattice (where the local structure repeats periodically in all directions), allowing each spin to interact with its neighbors.

2.1 Definition

The Ising Model consists of a Lattice **L** (typically taken to be a square) where for every lattice site k $\in$ L, there exists a discrete *spin variable* $\boldsymbol{\sigma_k}$ $\in$ {-1,1}. [$\boldsymbol{\sigma_k}$] for all k$\in$L is called the *spin configuration* of the system.

Between the spin variables of two adjacent lattice sites, there exists an *interaction constant* **J**. Hence the energy[1] of the spin configuration is given by

$$\boldsymbol{H = -J \sum_{<i,j>} \sigma_i \sigma_j} \tag{1}$$

Here <i,j> denotes a pair of nearest neighbours

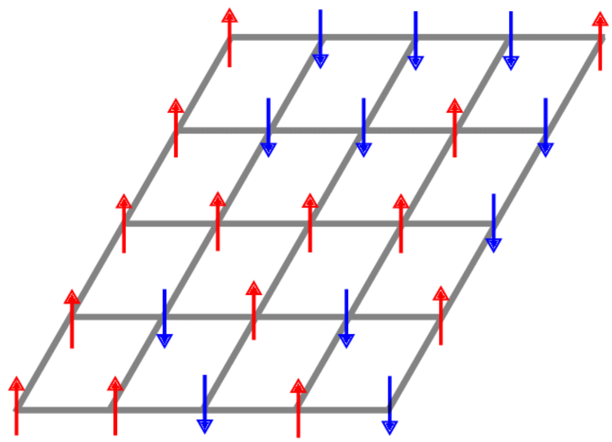

Figure 1: Schematic Representation of the Ising Model

Periodic boundary conditions are applied on the lattice as in the bulk of the system shall be assumed to be isotropically made up of this lattice in-order to extent the scope of the simulation. Thus, lattice sites at two opposite edges of the lattice are considered to be nearest neighbours.

The main aspect of interest of the model is in its equilibrium state. At temperature T, the probability $\boldsymbol{p_\mu}$ of a spin configuration $\boldsymbol{\mu}$ is given by the Boltzmann Distribution at inverse temperature $\boldsymbol{\beta}$ = 1/$\boldsymbol{k_b}$T as

$$\boldsymbol{p_\mu = \frac{e^{-\beta H(\mu)}}{\sum_\nu e^{-\beta H(\nu)}}} \tag{2}$$

Let P($\boldsymbol{\mu \to \nu}$) denote the probability of transitioning from a spin configuration $\boldsymbol{\mu}$ to another spin configuration $\boldsymbol{\nu}$. Hence, at equilibrium, the following criterion must hold

$$\boldsymbol{\sum_\nu p_\mu P(\mu \to \nu) = \sum_\nu p_\nu P(\nu \to \mu)} \tag{3}$$

[1]This is the Hamiltonian for the simplest case of the Ising Model

In-order to maintain this criterion the **detailed balance condition** is imposed which goes as follows

$$p_\mu P(\mu \to \nu) = p_\nu P(\nu \to \mu) \tag{4}$$

Rearranging Equation 4 and substituting Equation 2, we get

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{p_\nu}{p_\mu} = e^{-\beta(H(\nu)-H(\mu))} \tag{5}$$

This shall be the principal equation around which the Monte Carlo Algorithm for the model will be constructed.

2.2 The Metropolis Algorithm

In-order to obtain the equilibrium spin configuration of the Ising model, the **Metropolis Algorithm** shall be used. The Metropolis Algorithm or the Metropolis-Hastings algorithm is an **MCMC (Markov Chain Monte Carlo)** algorithm used to generate samples from a given probability distribution. A Markov chain process is a process where at each state there exists a transition probability for the system to transition to a new state. Given the condition of detailed balance, a Markov chain is guaranteed to have unique stationary (equilibrium) distribution.

The Metropolis algorithm will be applied to the Ising Model by adhering to the following procedure

1. Initialize the lattice L to a random spin configuration μ
2. Change the spin configuration by picking a random lattice point and flipping its corresponding spin variable (+1 $\to$ -1 , -1 $\to$ +1). Let the new configuration be ν
3. - If H(ν) > H(μ) : set $P(\nu \to \mu)$ to 1 and so, $P(\mu \to \nu)$ = $e^{-\beta(H(\nu)-H(\mu))}$
   - If H(μ) > H(ν) : set $P(\mu \to \nu)$ = 1

   Observe that both conditions satisfy detailed balance
4. Generate a random value r between 0 and 1
5. - If r < $P(\mu \to \nu)$: move the lattice to config. ν
   - If r > $P(\mu \to \nu)$: keep the lattice in config. μ

6. Repeat this process for a large number of iterations until the lattice reaches the equilibrium configuration

Equilibrium can be ensured by keeping track of observables such as the **energy of the system (E)** and the **net magnetization (S =** $\sum_i \sigma_i$**)**

2.3 Packages and Modules

The Model was implemented in *Python3.10*. *Numpy* package was used for all major mathematical computations and data structures. The *Numba* module was used to optimize and speed up the code in synergy with *Numpy*. *Matplotlib* Library was used for all plots and diagrams. *Scipy* package was used for a few instances of curve fitting over data points. All code used in this project can be found in the following GitHub page https://github.com/AKR211/ising_model

3 The Critical Temperature

The Ising model at equilibrium can be in two different phases. An **ordered phase** characterised by minimal energy, high net magnetization and a spin configuration composed of several clusters of identical spins. This phase can be observed at low temperatures. The **disordered phase** is characterized by higher energy, near zero net magnetization and a scattered spin configuration. This phase is typically observed at high temperatures. The transition of the Lattice from one phase to the other is called a **Phase Transition**. The temperature at which this transition occurs is known as the **Critical Temperature (**T_c**)**.

For a lattice of finite size, the critical temperature can be obtained using the cumulants of the observables collected throughout the simulation.

The equilibrium energy of the system is taken to be the mean of the energy of all states divided by the size of the lattice after equilibrium was attained

$$E = \frac{\langle H \rangle}{N} \tag{6}$$

The equilibrium magnetization of the system is taken to be the mean of the net magnetization of all states divided by the size of the lattice after equilibrium was attained

$$M = \frac{\langle S \rangle}{N} \tag{7}$$

The heat capacity of the system is taken to be the variance of the energy divided by the square of the temperature for all states after equilibrium was attained

$$C_v = \frac{\langle H^2 \rangle - \langle H \rangle^2}{T^2} \tag{8}$$

The susceptibility of the system is taken to be the variance of the net magnetization divided by the temperature for all states after equilibrium was attained

$$\chi = \frac{\langle S^2 \rangle - \langle S \rangle^2}{T} \tag{9}$$

Heat capacity and susceptibility are supposed derivatives of energy and magnetization respectively, and must attain maximum when energy and magnetization transitions between states.

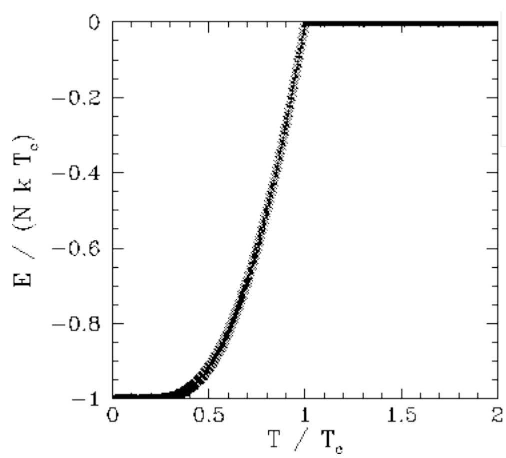

Figure 2: Ideal Energy vs Temperature plot

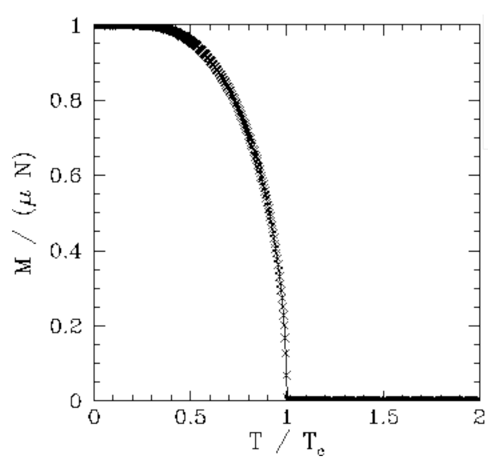

Figure 3: Ideal Magnetization vs Temperature plot

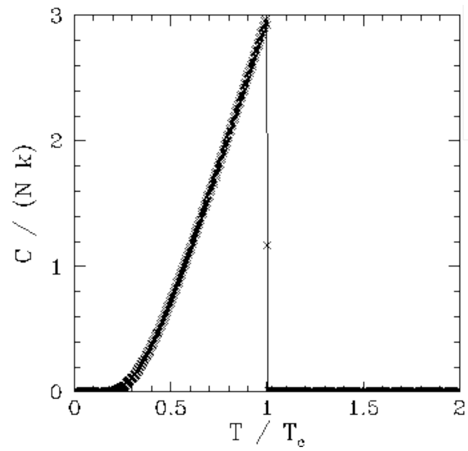

Figure 4: Ideal Heat Capacity vs Temperature plot

From these quantities the value of the critical temperature for a particular lattice size can be obtained. However, due to periodic boundary conditions, this value will be slightly different from the actual value of the critical temperature T_c. To obtain the true value, extrapolation of critical temperatures for finite sizes to that for infinite size must be done. Extrapolation can be done using **Finite Size Scaling** as well as using the **Binder Cumulant**.

3.1 Finite Size Scaling

Most phase transitions can be described by an order parameter. Most transitions are of two types: first order or continuous. They are characterized by the number of derivatives of Free energy it takes to get a discontinuity. The Ising model without any external field has a continuous transition. Continuous transitions are classified by their critical exponents which show the behaviour around the critical point.The relation which we are interested in is the following

$$\xi \propto |\beta_c - \beta|^{-\gamma} \tag{10}$$

where ξ is the correlation length, β is the inverse temperature, β_c is the inverse temperature at the critical point and γ is the critical exponent. Correlation length, in simple terms, is the length between two spin cluster in configuration. It peaks around the critical temperature. If we have a finite lattice of length **L**, then around the critical temperature $\xi \approx$ L. This gives us the equation,

$$\beta = \beta_c - c.L^{-1/\gamma} \tag{11}$$

Once we have values for β for enough values of L, we can use a power law fit to find both β_c and γ

3.2 Binder Cumulant

The Binder Cumulant is the 4^{th} order cumulant or kurtosis of the order parameter. It was introduced by Kurt Binder as a way to determine the critical temperature. Denoted as U_L, it is given by the equation

$$U_L = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2} \tag{12}$$

As L $\rightarrow \infty$, the Binder Cumulant behaves as follows

$$U_L = \begin{cases} 2/3 & T < T_c, \\ 0 & T < T_c. \end{cases} \tag{13}$$

The intersection of various Binder Cumulants (or Binder Ratios) for various sizes must give the value of the Critical Temperature

4 Variations of Ising Model

So only the simplest case of the two dimensional Ising model has been discussed, which is the model with uniform interactions and no external field. The simulation can be further challenged by incorporating further parameters and observing the changes to the observables and the critical temperature.

4.1 Ising Model with an External Field

An external field is a bias of the system to one specific spin variable (either +1 or -1). This field tries to align the system in a particular spin configuration according to the bias. The Hamiltonian of the ising model with an external field is given by

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{14}$$

Here the assumption is that the field is uniform throughout the Lattice in both magnitude and direction. The constant B denotes the strength of the magnetic field. If B > 0, the field is biased towards +1, if B < 0, the field is biased towards -1

4.2 The 3D Ising Model

The 3D Ising model is a three dimensional realization of the Ising model with the same criteria and principles. The square lattice is changed to a cubical lattice and the Hamiltonian remains the same. However, instead of 4 nearest neighbours, a lattice point in a 3D ising model will have 4 nearest neighbours for interaction. This increases the scope of interaction and that of spin configurations.

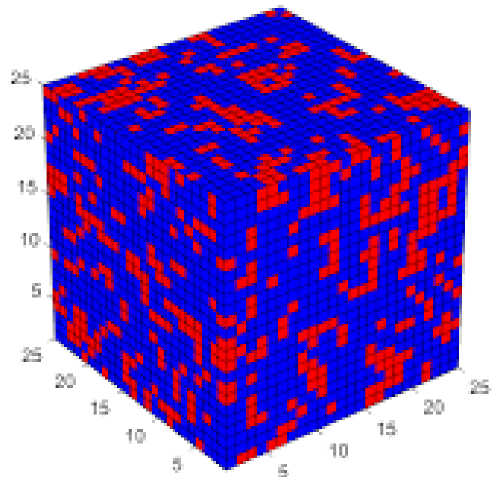

Figure 5: Visualization of the 3D Ising Model

4.3 Nonreciprocal Interactions

According to Newton's third law, when two objects come in contact with each other, the forces they produce on each other are equal in magnitude. While this always holds true for an isolated system, due to interactions with the environment being neglected. Certain systems (mainly bio-systems) exhibit **non-reciprocal interactions** where Newton's third law appears to be violated.

A model example of non-reciprocal interactions occur in the collective behaviour animal groups such as locusts, fish etc. These interactions can have an effect on the phase behaviour and the motion of flocking objects.

To use the ising model to simulate non-reciprocal interactions, the Hamiltonian is modified in the following way

$$H = -\frac{1}{2}\sum_i \sigma_i \sum_j J_{ij}\sigma_j \tag{15}$$

where J_{ij} is representative of the magnitude of interaction of σ_i on σ_j. [2] We can see that here $J_{ij} \neq J_{ji}$.

[2] Note that σ_i and σ_j need not be nearest neighbours here

This is a more generalized form of the Hamiltonian for the Ising Model. The Hamiltonian for the traditional Ising Model can be recovered from this by taking our $\boldsymbol{J_{ij}}$ as the following

$$\boldsymbol{J_{ij} = J[\delta_{i-e_x,j} + \delta_{i+e_x,j} + \delta_{i-e_y,j} + \delta_{i+e_y,j}]} \tag{16}$$

where i+$\boldsymbol{e_x}$ represents a neighbour on the right of i and i+$\boldsymbol{e_y}$ represents a neighbour above.

To incorporate non-reciprocity, we modify this $\boldsymbol{J_{ij}}$ with an **offset vector $\boldsymbol{\Delta}$**. Where $\boldsymbol{\Delta = \Delta_x e_x + \Delta_y e_y}$. Therefore our $\boldsymbol{J_{ij}}$ transforms to

$$\boldsymbol{J_{ij} = J[\delta_{i+\Delta-e_x,j} + \delta_{i+\Delta+e_x,j} + \delta_{i+\Delta-e_y,j} + \delta_{i+\Delta+e_y,j}]} \tag{17}$$

In this project, we confined $\boldsymbol{\Delta}$ to the form $\boldsymbol{\Delta}$ = $\Delta \boldsymbol{e_x}$ where Δ is a constant throughout the Lattice. Δ = 0 represents the traditional Ising model and we shall increment Δ in steps of two. [3]

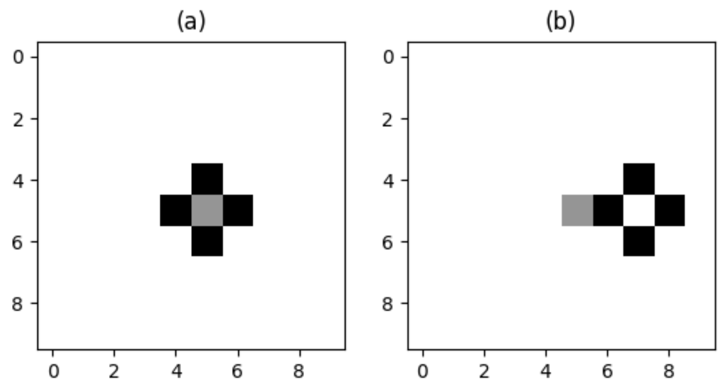

Figure 6: (a)Interactions for a spin variable in the traditional ising model. (b)Interactions for a spin variable in the non reciprocal ising model with offset=2

4.4 Random Field Ising Model

Section 4.1 dealt with the behaviour of the Ising Model in a uniform external field. However in some materials such as colloid-polymer mixtures and relaxor ferro electrics, the magnitude of the external field varies at each lattice site. The value of the field at each point is unequal with varying distributions. The Hamiltonian of the Ising Model in external field can be further modified to the following to represent random fields

$$\boldsymbol{H = -J \sum_{<i,j>} \sigma_i \sigma_j - \sum_i B_i \sigma_i} \tag{18}$$

Here the value of $\boldsymbol{B_i}$ depends on the distribution of the field.

[3]Step size is chosen to be 2 since Δ = 1 results in self-interaction which is not possible

We observed the behaviour of the model for three different distributions, constant, Gaussian and uniformly random to determine the effect of the field distribution in observables.

Furthermore, we can incorporate non-reciprocal interactions into the Random Field Ising Model to study the combined effect of both in a system. The Model will have the following Hamiltonian.

$$H = -\frac{1}{2}\sum_i \sigma_i \sum_j J_{ij}\sigma_j - \sum_i B_i\sigma_i \tag{19}$$

This is the most general Hamiltonian which incorporates all variations of the 2 dimensional Ising Model.[4]

5 Results and Discussion

5.1 The Metropolis Algorithm

The following graphs represent the results of the system subject to the Metropolis algorithm. The energy and the magnetization of the system after each Monte Carlo step is plotted along with the lattice before and after subject to the Metropolis Algorithm. Note that a white lattice point indicates $\sigma_i = -1$ and black indicates $\sigma_i = +1$. The algorithm was run on a 500x500 lattice for 10^7 steps for both high (T = 5) and low (T = 1) temperatures. Two different initial lattice configurations were also used where one configuration had nearly equal distribution of both spins whereas the other had a 3:1 ratio of -1 to +1.

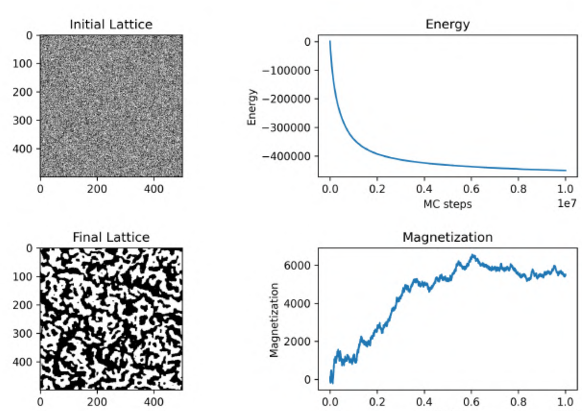

Figure 7: Low Temperature with equal distribution

[4]Note that this system is not studied in this project. The mention serves just to illustrate the further scope of the project

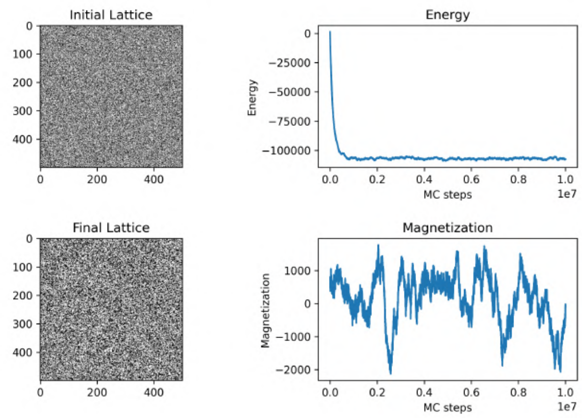

Figure 8: High Temperature with equal distribution

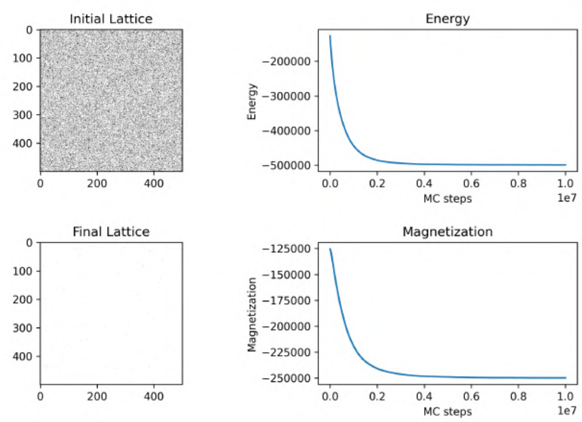

Figure 9: Low Temperature with unequal distribution

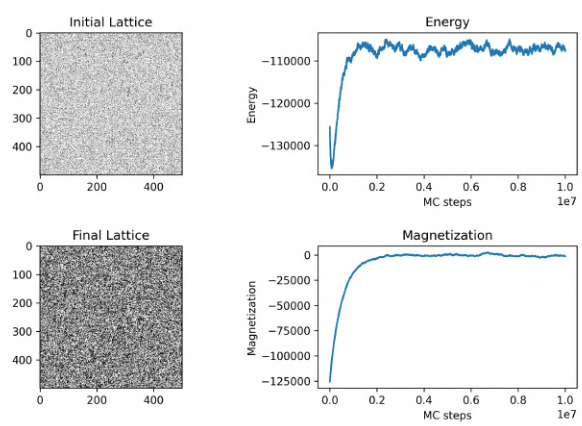

Figure 10: High Temperature with unequal distribution

We observe that the energy of the system decreases with the number of steps and attains equilibrium at a particular point beyond which there is minimal variation in the system energy. Although the magnetization fluctuates much more, it too appears to oscillate about an average point after equilibrium.

At low temperature, the energy either reaches or gets very close to the absolute minimum energy possible[5] by the equilibrium point. As the simulation runs, the lattice tends to partition the two spins into separate groups to minimize the interaction energy. At high temperatures, the energy does not reach a minimum and maintains a particular level after equilibrium. The magnetization eventually tends to zero regardless of its initial state. The lattice appears chaotic with no distinct boundaries or patterns between spins.

There are differences observed between the equilibrium configurations for different initial configurations. At low temperature, when starting with an equal distribution of both spins, the equilibrium configuration tends to form clusters of spins. From the magnetization graph, we can see that there is only a small difference between the number of each spin in the lattice. When starting with an unequal distribution, the equilibrium configuration is dominated by the majority spin and attains maximum absolute magnetization[6].

Note: All quantities mentioned have been multiplied and divided by appropriate constants so that they remain unit-less

$$\boldsymbol{E \rightarrow E/J} \tag{20}$$

$$\boldsymbol{T \rightarrow K_b T/J} \tag{21}$$

etc.

5.2 The 2D Ising Model

In this section we shall analyze the equilibrium spin configuration of the model. The main focus shall be in the variation of observables such as energy, magnetization, heat capacity etc. Variation in the final lattice by changing other parameters such as lattice size, number of MC steps etc. are also analyzed

5.2.1 Variation with Temperature

The Metropolis Algorithm was run for 100 temperatures between 0 and 5 at equal intervals. The lattice size was 250x250 and the initial lattice was taken with a 3:1 distribution. The

[5] Min energy possible = $-\frac{\boldsymbol{4*500*500}}{\boldsymbol{2}} = \boldsymbol{-500000H/J}$

[6] Max abs magnetization = $\boldsymbol{500*500 = 250000}$

algorithm ran for 10^7 steps and the variation in Energy per lattice point,negative of absolute magnetization per lattice point, heat capacity and susceptibility was measured.

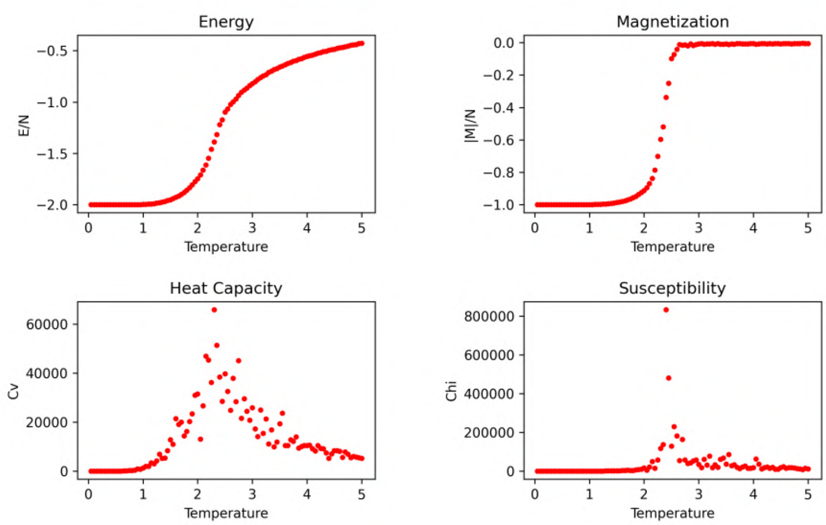

Figure 11: Variation of equilibrium quantities with Temperature

Adhering to results in section 5.1, the energy of the system is minimum at low temperatures and higher at higher temperature. From the energy vs temperature plot, it is observed that the transition occurs between T=2 and T=3. This is even more evident from the magnetization vs temperature plot where the transition is more sharp. Both the heat capacity and susceptibility peak at T=2.3 suggesting that the critical temperature is very close to 2.3. There are considerable inconsistencies in both the heat capacity and the susceptibility plots which most likely originate from probabilistic noise in the metropolis algorithm which gets amplified when calculating the variance.

5.2.2 Variation in other parameters

The equilibrium spin configurations were observed for various values of parameters such as lattice size, number of steps and initial distribution, and the variations were studied. This allowed for better choices of mentioned parameters for future simulations.

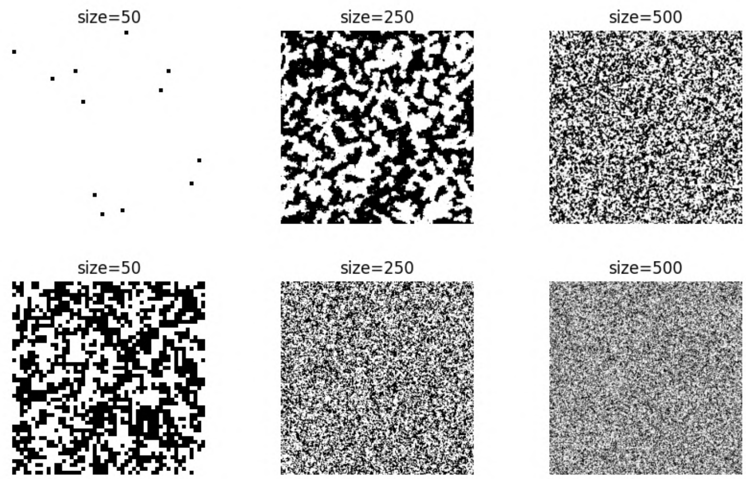

Figure 12: Variation with lattice size (size = side length) for $\mathbf{10^6}$ steps and equal initial distribution for low temperature(above) and high temperature(below)

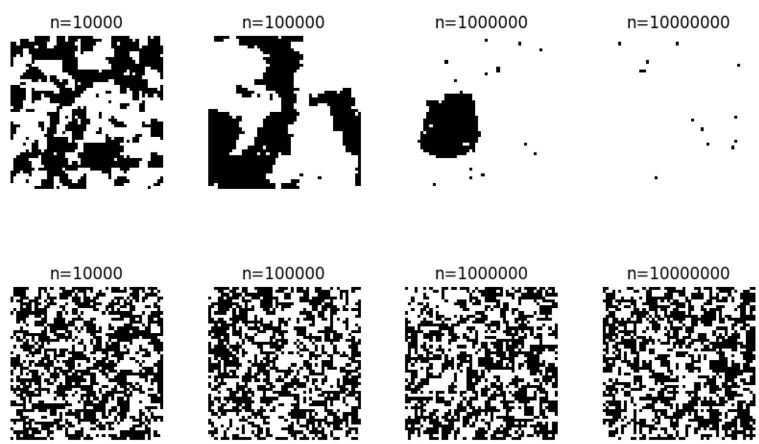

Figure 13: Variation with number of steps (n) for a 50x50 lattice with equal initial distribution for low temperature(above) and high temperature(below)

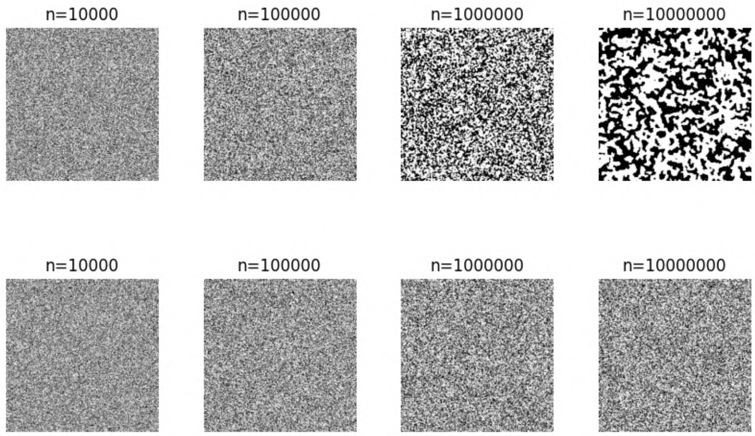

Figure 14: Variation with number of steps (n) for a 500x500 lattice with equal initial distribution for low temperature(above) and high temperature(below)

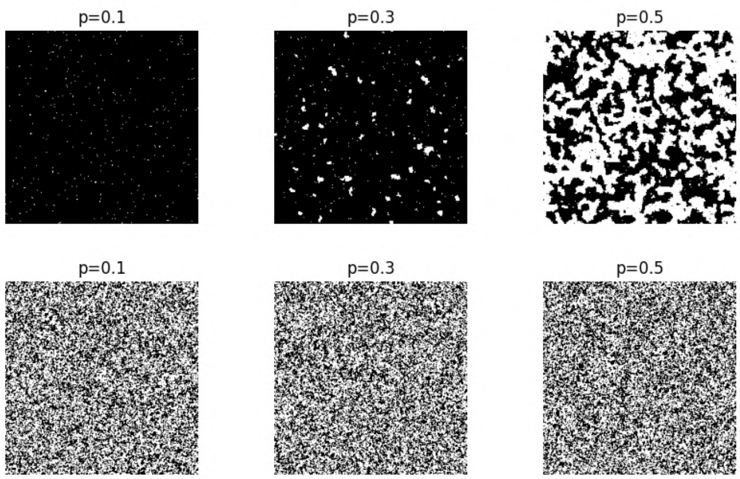

Figure 15: Variation with initial distribution (p = relative number of -1 spins) for 10^7 steps and a 250x250 lattice for low temperature(above) and high temperature(below)

We observe that lattices of smaller size tends to equilibrium much faster than larger lattice sizes. This is expected as smaller lattice sizes requires less number of steps to sweep the entire lattice. Also as expected, more the number of steps run for, closer the system is to equilibrium. lattice of size 50 takes about $10^5 - 10^6$ steps to reach equilibrium while lattice of size 500 takes about $10^6 - 10^7$ steps. Verifying the previous observation, if the initial configuration is close to equal for both spins, the system tends to form clusters whereas if it is biased to a spin, it tends to be align itself homogeneously to that particular spin at low temperatures.

5.3 Finite Size Scaling

In section 5.2, it was observed that the value of the critical temperature must be close to 2.3. In order to accurately determine the value of T_c independent of periodic boundary conditions, we shall use finite size scaling. The approximate critical temperature for lattices of size ranging from side length 4 to 12 were determined using the susceptibility vs temperature plot for each size. The temperature range used was trimmed down to (2,4) for more accurate results.[7]

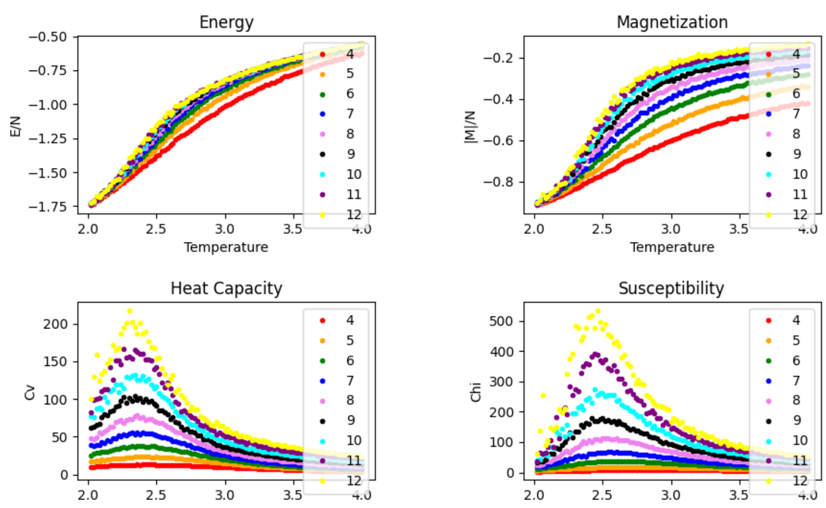

Figure 16: Evolution of observables for variously sized lattices

Using the values of the critical temperature at various lattice sizes, the inverse of the lattice size (1/L) vs the inverse temperature (β) plot was constructed and a power law fit (11) was applied.

[7]Therefore Least count for the temperature = 4-2/100 = 0.02

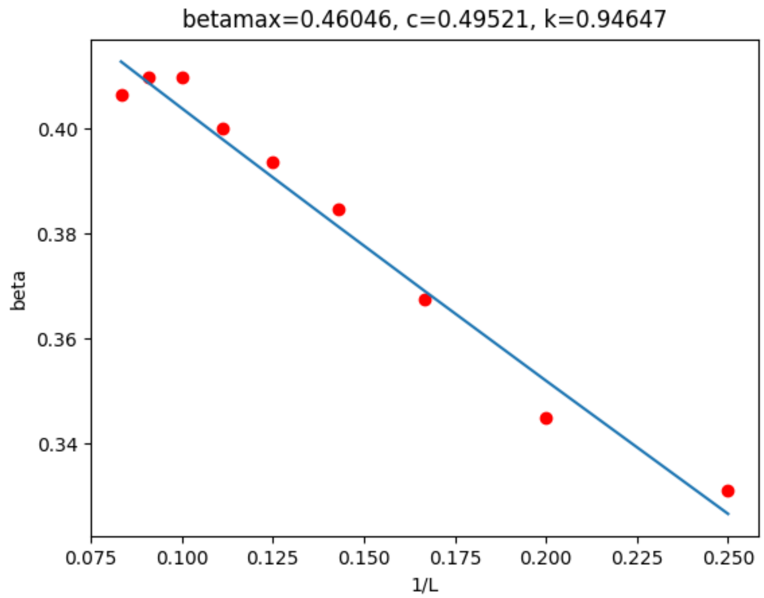

Figure 17: 1/L vs β with values of the fit parameters obtained at the top

The following values were obtained

$$\beta_{max} = 0.46 \pm 0.04 \quad k = 0.94 \pm 0.08 \tag{22}$$

$$T_c = 1/\beta_{max} = 2.18 \pm 0.18 \tag{23}$$

The true value value of k is 1 and it does fall in the range of values of k obtained. The value of T_c obtained from the value of β_{max} is very close to the approximate value in section 5.2. However, the error in the value is around 8-9% and the range of values of T_c is from 2.00 to 2.36. This is only slightly better than the range obtained from the plot in section 5.2.

The large error is likely due to the aforementioned probabilistic error when computing the values of susceptibility. This is especially enhanced due to the trimming down of the temperature range, reducing the temperature difference between two successive plot points. lattices of reduced sizes and the average of multiple simulations were used to obtain the critical temperatures in order to reduce the error. However, the error produced is still too large for accurate assessment of the critical temperature.

5.4 Binder Cumulant

The Binder Cumulant was calculated for Energies at each temperature in the range of 0-5 for 100 points and was plotted alongside other Observables. This was done for lattice sizes of 4,8,12 and 16. In-order to identify a sharp intersection, the ratios of binder cumulants were also plotted alongside.

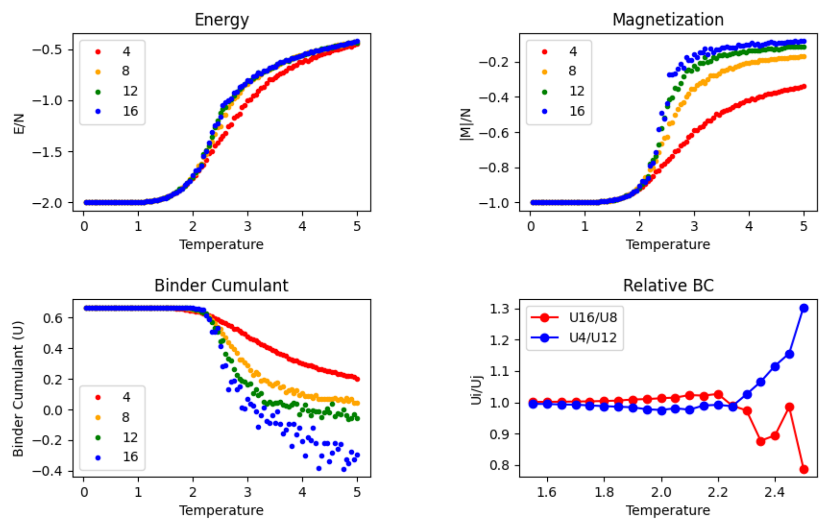

Figure 18: Binder Cumulant vs Temperature for various lattice sizes (bottom left) and Binder ratio of size 4:12 and 16:8 (bottom right)

In the plot of relative Binder Cumulants,we can see that one ratio increases with temperature and the other decreases. This is expected for the ratios used. Their intersection point is sharp and has a y-value of 1 indicating equal value for all Binder Cumulants which occurs at the critical temperature. The intersection occurs at T = 2.25 with a least count of 0.05

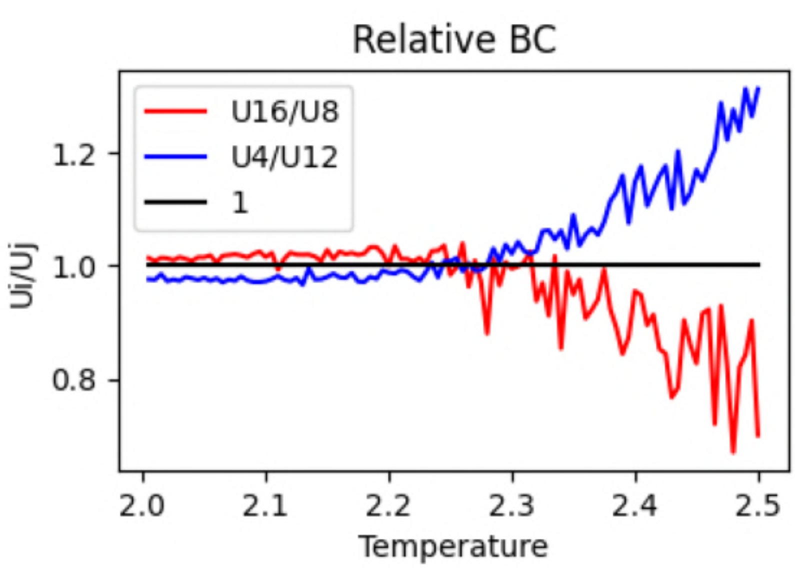

Figure 19: Relative Binder Cumulants for shorter temperature range 2-2.5 (least count = 0.005

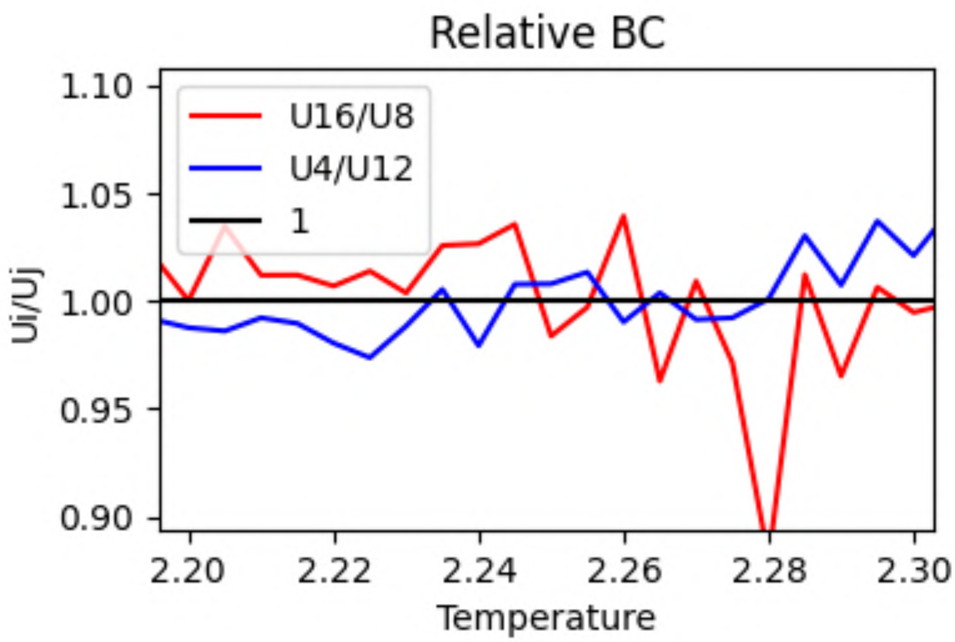

Figure 20: fig:19 zoomed in

From fig.20 we can observe that the ratios both ratios intersect with $U_i/U_j = 1$ at **T = 2.265**. However, since at this small temperature scales the values oscillate rapidly, it was safer to assume the value of the Critical Temperature to be between **T = 2.24 and T = 2.28** where both ratios intersect with each other multiple times, with values very close to 1. Although it is difficult to establish the exact amount of error for the value, it is almost certainly lesser compared to the error obtained using the Finite Size Scaling method.

Lars Onsager analytically determined the value of the critical temperature for the 2D Ising Model in 1944. The value he gave was

$$T = \frac{2}{ln(1+\sqrt{2})} \approx 2.269 \tag{24}$$

The value of the critical temperature obtained using the Binder Cumulant method is extremely close to this (considering the least count) and is well within the range of values estimated.

5.5 Ising Model with an External Magnetic Field

For a 10x10 Lattice, with initial distribution of 3:1, the metropolis was run for 10^6 steps with varying values of B from 0.5 to 2.5 (relative to J). The critical temperature for each value was noted using the susceptibility curve. The temperature range was expanded to (0,10) in-order to incorporate all values.

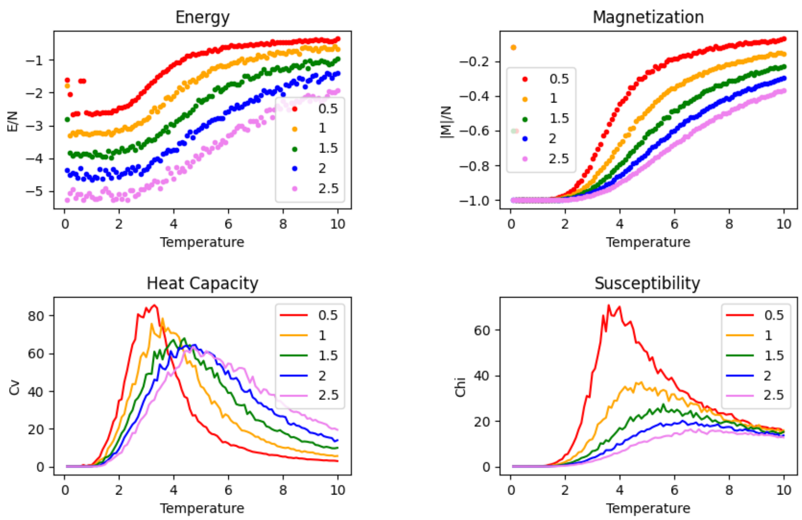

Figure 21: Evolution of observables for various values of B

The energy curve is offset in the y-direction due to the external field, increasing the total energy. The magnetization is equal at low temperatures for all values of B but at high temperatures, lower values of B creates more disorder (near zero net magnetization).

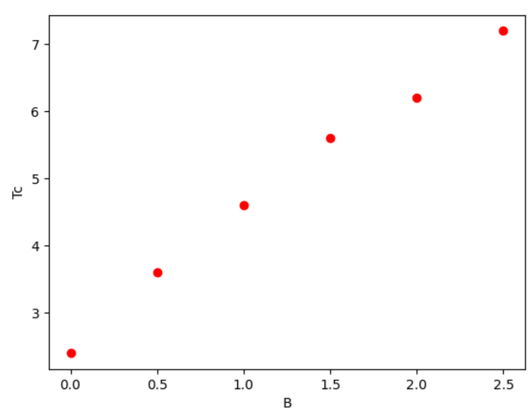

Figure 22: B vs T_c for fig.21

Critical temperature appears to have a linear relationship with magnetic field. for every 0.5 increase in B, the critical temperature increases by around 1(± 0.2). This is expected since Magnetic field aligns the Lattice in the ordering phase along its own direction while Temperature disorients the lattice to the disordered phase. They act as opposing agents and must have a directly proportional relationship.

5.6 The 3D Ising Model

A 50x50x50 Lattice with 3:1 initial distribution was used to run the metropolis algorithm for 10^6 steps. The temperature range was initially chosen to be (0,10).

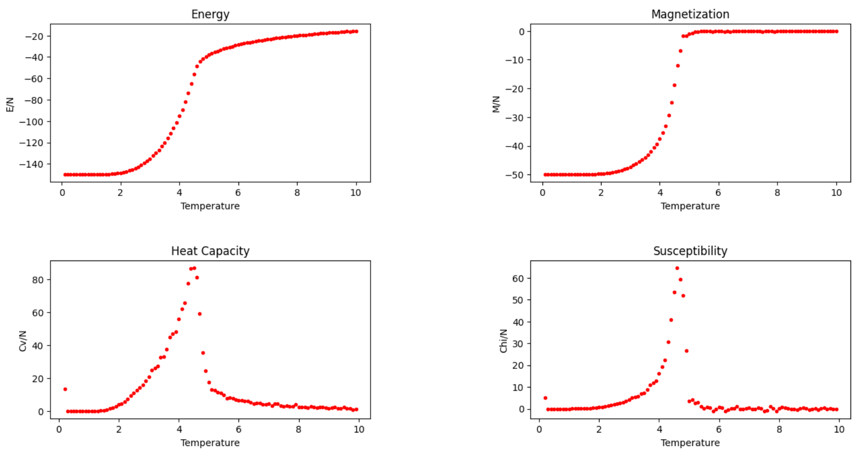

Figure 23: Observables for 100 temperatures in the range (0,10)

The observables appear to behave in a similar way to the 2 dimensional Ising model with the exception of the critical temperature which is higher than that of the 2D ising model. The susceptibility curve peaks at T=4.7 and the value seems to be in the range of (4,6).

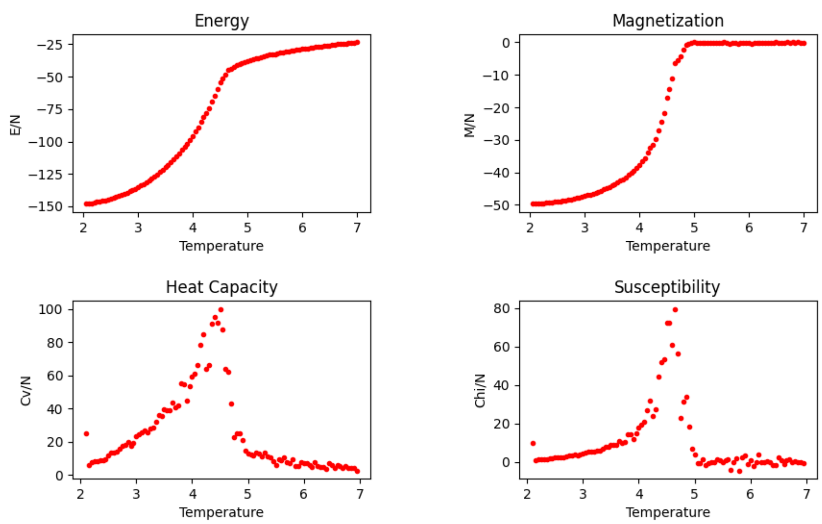

Figure 24: Observables for 100 temperatures in the range (2,7)

After trimming the temperature range down to (2,7), the critical temperature obtained is $\boldsymbol{T = 4.55(\pm 0.05)}$. Although this value was not scaled for finite size, it should be close enough considering the larger size of the lattice used. The 3D ising model is not yet solved analytically and the current accepted value of the critical temperature solved numerically is $T = 4.512$. This is very close to the value obtained from the simulation.

5.7 Nonreciprocal Interactions

The simulation was run on a 100x100 Lattice for 10^6 steps with initial distribution of 3:1. Observables were plotted for values of Δ = 0,2,4,6,8 for the initial temperature range of (0,5)

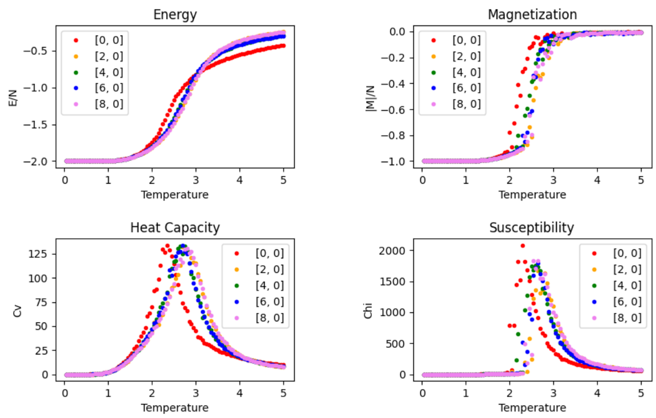

Figure 25: Observables for 100 temperatures in the range (0,5)

The plots for Δ = 0 and 2 are the only distinguishable plots while all other plots appear similar.

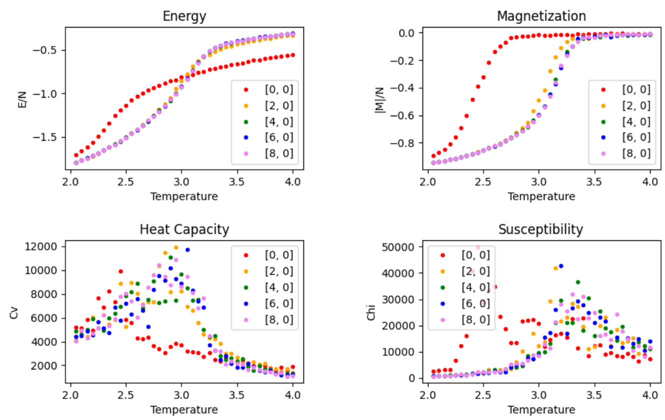

Figure 26: Observables for 40 temperatures in the range (2,4)

Using the susceptibility plots, the Critical temperature for each Δ value was obtained.

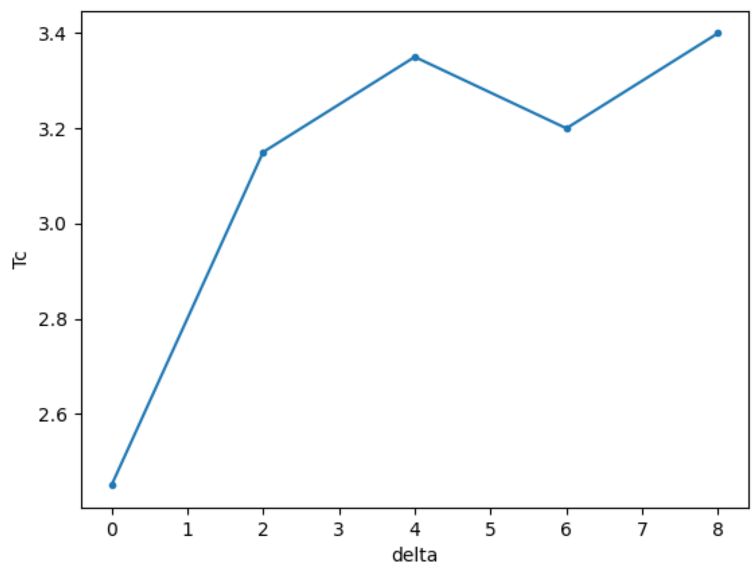

Figure 27: Δ vs T_c from fig.26

The Value of T_c appears to increase from Δ = 0 to 2 then remain stable. More data points were obtained and plotted for further clarity

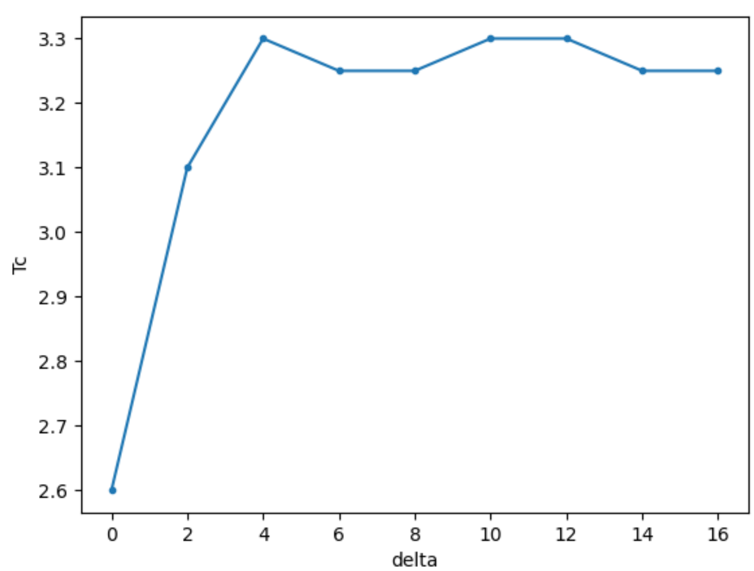

Figure 28: Δ vs T_c for Δ from 0 to 18

Fig.28 shows a large jump from Δ = 0 to 2 then a smaller jump from Δ = 2 to 4 following which is remains nearly constant. It appears that critical temperature are dependent on the distance between the interacting spins. Although it initially increases dramatically, with enough distance, the it stops influencing the critical temperature. Using large lattice size results in a considerable error when finding the critical temperature and furthermore, scaling for finite size cannot be done due to the lack of precision in the temperature range. Unfortunately, using lower lattice sizes would result in a high periodicity which can alter the results.

5.8 Random Field Ising Model

The simulation was run on a 50x50 lattice for 10^6 steps with an initial distribution of 3:1. The observables for 3 different distributions of external field were considered. The uniform field, the Gaussian field and a uniformly random field.

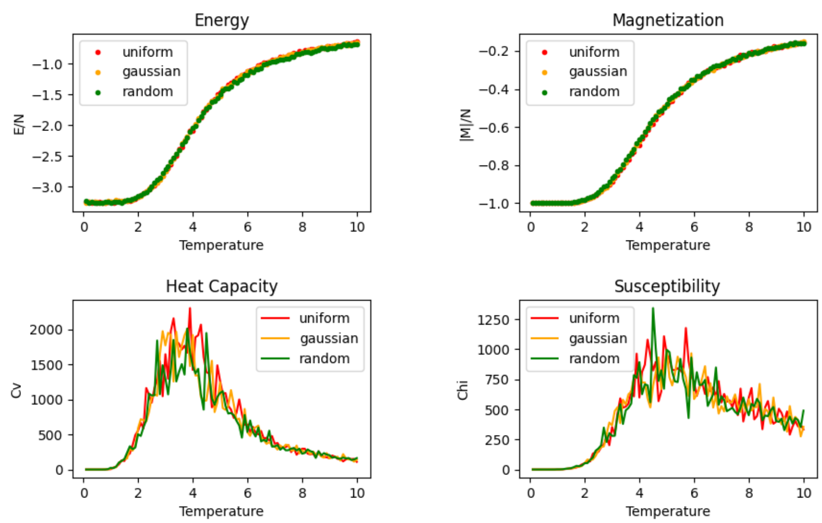

Figure 29: Observables for 100 temperatures in the range (0,10)

Surprisingly, the distribution does not appear to have any effect on the observables. The distributions were all normalized to have the average value for the magnetic field at each lattice point be 1.

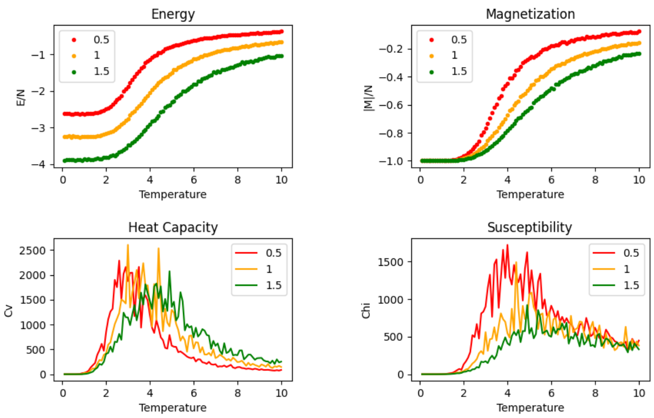

Figure 30: Observables under various magnitudes of a random magnetic field

Furthermore, the observables behave the same way for various magnitudes of a random field in the same way as they behave for the corresponding magnitude of a uniform field.

This suggests that the effect of an external field on the observables of an Ising model is only dependent on the total sum of magnetic fields of every lattice point and has little dependence on the values at individual points.

6 Conclusions

In this project, we have analyzed the two dimensional Ising Model and its behaviour at equilibrium using the Metropolis Algorithm. We illustrated the existence of an ordered and a disordered state for the Ising Model at high and low temperatures respectively, indicating the presence of a phase transition. We were able to observe the evolution of observables such as energy, magnetization, heat capacity and susceptibility for varying temperatures. Although a small amount of noise was present in the plots, they were principally in agreement with the theory. The value of the critical temperature was found using both finite size scaling and the binder cumulant methods. The Binder Cumulant appears to be the superior method for calculating the Critical temperature due to reduced error (<1%) as well as being very much closer to the theoretical value given by Onsager. The effects of an external field in the Model were studied and matched the expectations from the theory. The 3d dimensional Ising Model was also studied with the same algorithm and provided matching results to other simulation studies.

We further used the model to investigate non-reciprocal interactions originating from an offset in the interaction pairs. We observed an initial increase in the critical temperature with the offset which gradually stabilizes at higher offsets. No finite size scaling could be applied due to the larger size of the lattice. The selection of lattice size for all simulations was done by balancing the counteracting effects of periodicity and noise reduction. Random field Ising Model was also studied with uniform, Gaussian and random distribution of an external field. We proved that the effect of an external field on the Ising model is dependent solely on the magnitude of interaction with no dependence on the distribution of the field. This result is in agreement with similar studies on the Ising Model [9, 10].

Overall, we were able to create an accurate model to study phase transitions which satisfies the theory and is in agreement with the literature. We were also able to establish the usefulness of the model to study the effects of advanced phenomena such as non-reciprocal interactions and random fields. We further intend to improve the model to incorporate and study the effects of further factors and combinations of them.

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