Numerical Simulations of the 2D Ising Model

(Summer Project Report)

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Abstract

We study the two-dimensional Ising model by simulating it using Metropolis algorithm. We measure the observables such as the average energy, magnetization, specific heat, susceptibility, and spin-spin correlator. Our results indicate the occurrence of a second-order ferromagnetic phase transition. We find the critical temperature for the phase transition. We also simulate the one-dimensional Ising model but no indication of phase transition is found from the simulations. Overall, our computed results are in excellent agreement with the analytical results.

Acknowledgements

I would like to thank Dr. Anosh Joseph for giving me the opportunity to work on this project. His guidance through regular meetings and discussions were of immense help and I sincerely appreciate the time he spent to help me.

I would also like to thank Navdeep Singh Dhindsa for his help throughout the project. I would like to thank the IISER Mohali Library for providing the resources whenever needed.

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1 Introduction

It may be extremely difficult to find analytical solutions, sometimes even impossible, for many physical systems. We can take the help of numerical simulations to study many such systems. In the method of numerical simulations we start with an initial state and let the rules (usually some mathematical model) of the system work on it to generate further states. Computers are used to carry out this process. Then we can measure the observables on these states and understand the behavior of the system. Sometimes, directly simulating systems in this way can take thousands of years for even the best computer available to complete. In such cases, we resort to algorithms made for fast and efficient numerical simulations.

In this project, we simulate the 2D Ising model using the Metropolis algorithm and measure the observables such as energy $\langle E \rangle$, magnetization $\langle M \rangle$, specific heat C_V, and susceptibility χ for various values of the temperature T. We will also study the 2nd order ferromagnetic phase transition that occurs in the 2D Ising model and find the critical temperature T_c. All the simulation codes are written in C++.

2 Markov Chain Monte Carlo

In this section, we briefly discuss the method and algorithms used for the numerical simulations in this project.

2.1 Markov Chains

Markov chain is a mathematical model of random process, which describes a sequence of states in which probability of attaining each state depends only on the immediate previous state. It was introduced by the Russian mathematician Andrey Markov.

In this process, we can make predictions regarding the future outcomes solely based on its present state without needing to know the full history of the process (*memorylessness* property). The change from one state of the system to another is called the *transition* and the probability associated with it is called the *transition probability*.

2.2 Markov Chain Monte Carlo

Markov Chain Monte Carlo (MCMC) is a method of random sampling.

> The goal in this method is to visit a point x with probability proportional to some given distribution function, say $\pi(x)$ [1].

It is not necessary for $\pi(x)$ to be a normalized probability distribution function and it is sufficient for it to be proportional to some probability. This method gives greater *importance* to points for which $\pi(x)$ is large. This results in points of less importance (or contribution) being less visited and makes the method much more efficient compared to uniformly visiting all possible points in the space.

We first start with an initial distribution and then jump from one point to the next with the help of the *transition probability function*. Since it is a Markov chain, the probability of visiting a point x_i depends only on the immediate preceding point x_{i-1}. The transition probability function is completely defined as a function of two variables x_i and x_{i-1} as $p(x_i \mid x_{i-1})$, which is the *conditional probability* of x_i given x_{i-1}. This dependence results in a sequence of these points being *locally correlated* and because of this, later when we take measurements on a system simulated using this method, we need to take measurements after some gap to get independent measurements.

A Markov chain with stationary distribution has the property of *irreducibility* and *aperiodicity*. According to the property of aperiodicity, a state does not repeat after a given time period. According to the property of irreducibility, the probability to go from any state to every other state, in one or more steps, is greater than zero. This ensures that we explore as much of the space as possible and naturally visit closer to the points x_i with greater probability $\pi(x_i)$ in some finite steps. In a physical system, such points with greater probability would be close to the equilibrium states of the system.

2.3 Pseudo Random Number Generators

The random numbers used in Monte Carlo simulations are usually generated using a deterministic algorithm. They exhibit sufficiently random-like properties and are called *pseudo-random numbers* [1].

In the simulations of this project, the UNIX function **drand48()** is used, which is a pseudo-random number generator (PRNG) using Linear congruential generator (LCG) algorithm and 48-bit arithmetic. It gives us a pseudo-random number uniformly distributed in the range [0,1). We used the time of running the code to get different seed (which can be set using srand48()) for each run.

2.4 Metropolis Algorithm

Metropolis-Hastings algorithm is an algorithm for Markov Chain Monte Carlo (MCMC) which is used to get random samples from a probability distribution $\Pi(x)$ given that

we have a probability distribution $\pi(x)$, which is proportional to $\Pi(x)$ and the values of $\pi(x)$ can be calculated. We use this method when it is difficult to calculate the values of $\Pi(x)$ itself.

Metropolis algorithm is a special case of the Metropolis-Hastings algorithm with the condition that the transitional probability function is symmetric, that is $p(x \mid y) = p(y \mid x)$ where $p(x \mid y)$ is probability of the next sample x given the previous value y. Since the probability of the next sample depends only on the current sample, this algorithm forms a Markov chain.

The Metropolis algorithm proceeds in the following way

1. **Initialization:** Initial point x_0 is arbitrarily chosen as a first sample.

2. **Generation:** A candidate x' is generated for the next sample according to the transition probability $p(x' \mid x_i)$.

3. **Accept/Reject:** Metropolis ratio r is calculated. The candidate x' is accepted for the next sample with probability r. Otherwise, it is rejected.

   $$r = \frac{\pi(x')}{\pi(x_i)}$$

   Since $\pi(x)$ is proportional to $\Pi(x)$, the ratio r is

   $$r = \frac{\pi(x')}{\pi(x_i)} = \frac{\Pi(x')}{\Pi(x_i)}.$$

4. Steps **2** to **3** are repeated to accept new samples and continue the chain. After sufficient number of iterations, we will move closer to the target distribution $\Pi(x)$. The initial part of the chain before getting closer to the target distribution is called the *thermalization steps* (or burn-in). These initial samples are not close to the target distribution and are discarded from the result.

2.5 Jackknife Method of Computing Errors

We will use the Jackknife method to calculate errors of the observables measured in the simulated system. If our observable is an average over N samples, we can use the Jackknife method to calculate the error in the following way:

1. We create N new datasets from the original dataset of N samples.

2. For i^{th} sample among the N samples of original dataset, we create a new dataset containing all N samples except the i^{th} sample. That is, the new dataset will have $N-1$ samples.

3. Now we calculate the mean of the $N-1$ samples ($\mu_i^{'}$) in each of the newly created datasets. This will give us N values of the mean.

4. Then we can calculate the variance of these N new means ($\mu_i^{'}$) from the mean of the original dataset (μ_0). Taking square root of it will give us required error. We have
$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(\mu_0 - \mu_i^{'})^2.$$

3 The Ising Model

The Ising model is a simple system of arrangements of spins in an n-dimensional lattice. The spins have two possible states: up or down. This model can be used to study the ferro-magnetic behavior of certain systems. The neighboring spins interact with each other and contribute to the energy term of the system.

The Hamiltonian of the model is given by

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} s_i s_j, \tag{1}$$

where s_i and s_j denote the spins. Mathematically we assign up as $+1$ and down as -1. $\langle i,j\rangle$ in the summation denotes nearest neighbors. J is called the *coupling constant* and it affects the strength of the interaction among spins. The form of the Hamiltonian in Eq. (1) suggests that parallel spins lower the energy and thus are favored. This leads us to predict that the lowest energy state will have all the spins aligned in one direction. However, we cannot predict whether the direction will be up or down, and that is the symmetry inherent in the system. We can have an external magnetic field (H) such that the spins experience an upward magnetic field. Then, we have

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}(s_i s_j) - H\sum_{i}^{N} s_i. \tag{2}$$

In this case, at the lowest energy state, even with the slightest external magnetic field H, will bias the spins to align upwards ($H > 0$) and we will have all spins

pointing up. We will consider no external magnetic field to be present in this model for this project.

We would like to study the behavior of this system for various temperature T. One way is the statistical mechanics approach of the canonical ensemble.

3.1 The Canonical Ensemble

We consider the physical system to be in contact with a large heat bath (the environment) whose temperature remains constant. When the system comes in thermal equilibrium with the environment, it can be described by the canonical ensemble [2].

Then the probability to find a system in microstate v with energy E_v at temperature T is given by

$$P(v) = \frac{1}{Z} e^{-\beta E_v}, \tag{3}$$

where, $\beta = \frac{1}{k_B T}$. We will work with natural units ($k_B = 1$) and thus we have $\beta = \frac{1}{T}$. Z in Eq. (3) is called the *partition function* and it is defined as

$$Z = \sum_v e^{-\beta E_v}, \tag{4}$$

where the summation is over all microstates v of the system, assuming all the microstates have discrete energies E_v.

The Helmholtz free energy, F of the system is then given by

$$F = \frac{1}{\beta} \ln Z. \tag{5}$$

All the other thermodynamic quantities of the system can now be calculated once we know F.

3.2 The 1D Ising Model

We consider N spins arranged in a one-dimensional lattice. Each spin has 2 nearest neighbors. We consider periodic boundary conditions such that the n^{th} spin interact with the 1^{st} spin. The Hamiltonian of this system is given by

$$\mathcal{H} = -J \sum_i^N s_i s_{i+1}, \tag{6}$$

where, s_{N+1} is identified by s_1 because of the periodic boundary condition.

The analytical expression for average energy per spin is given by

$$\langle E \rangle = -J \tanh(\beta J). \tag{7}$$

3.3 The 2D Ising Model

We consider an $(n \times n)$ arrangement of spins in a 2-dimensional square lattice. Each spin has 4 nearest neighbors. We consider periodic boundary conditions such that the spins on the n^{th} row interact with the spins on the 1^{st} row and the spins on the n^{th} column interact with the spins on the 1^{st} column.

The Hamiltonian of this system is given by

$$\mathcal{H} = -J \sum_{i}^{n} \sum_{j}^{n} s_{(i,j)} s_{(i+1,j)} - J^* \sum_{i}^{n} \sum_{j}^{n} s_{(i,j)} s_{(i,j+1)}, \tag{8}$$

where $s_{(i,j)}$ represents the spin at i^{th} row and j^{th} column. J is the *horizontal coupling* and J^* is the *vertical coupling*. We will study the isotropic case in which $J = J^*$.

The partition function of this system is given by

$$Z = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_n} e^{-\beta \mathcal{H}}. \tag{9}$$

The partition function Z in this case is extremely difficult and time consuming to calculate. We will instead use the method of Metropolis algorithm to simulate the 2D Ising model.

3.4 The Algorithm

The probability to find the system in a microstate v is given by

$$P(v) = \frac{1}{Z} e^{-\beta \mathcal{H}_v}, \tag{10}$$

where $\mathcal{H}$ is given in Eq. (8) and Z is given in Eq. (9). We will use Metropolis algorithm to sample $P(v)$ with the proposed distribution $\pi(v)$, where $\pi(v)$ is given by

$$\pi(v) = e^{-\beta \mathcal{H}_v}. \tag{11}$$

We will proceed in the following way:

1. **Initialization:** We generate an $(n \times n)$ matrix of spins with each spin assigned the value $+1$ or -1, randomly.

2. **Generation:** We choose a spin at random from the 2D lattice of spins and flip it to generate a candidate sample v'.

Metropolis ratio r in this case is given by

$$r = \frac{\pi(v')}{\pi(v_i)} = \frac{e^{-\beta \mathcal{H}_{v'}}}{e^{-\beta \mathcal{H}_v}} = e^{-\beta \Delta \mathcal{H}_v}, \tag{12}$$

where $\beta = \frac{1}{T}$ is in natural units. It is clear that after generating a new candidate sample by flipping a spin, we just need to calculate the change $\Delta\mathcal{H}$.

3. **Accept/Reject:** There are two possible cases:

   (a) If $\Delta\mathcal{H} < 0$, we accept the candidate sample.

   (b) If $\Delta\mathcal{H} > 0$, we generate a uniform random number u between 0 and 1.
   If $u < r$, then we accept the candidate sample.
   If $u > r$, then we reject the candidate sample.
   Here r is given in Eq. (12).

4. Steps **2** to **3** are repeated to accept new samples and continue the chain. After a sufficient number of iterations, we will move closer to the target distribution $P(v)$.

5. Measurements of the observables are taken at a fixed gap of iterations.

4 Results

4.1 The 1D Ising Model

First, we show some results obtained by simulating the 1D Ising model using the Metropolis algorithm as a test before moving on to the 2D Ising model.

We note that in Fig. 3 the magnetization is zero for most of the temperature ranges and it slightly starts to deviate from zero as the temperature decreases. The deviation is very small considering that the analytical value of the magnetization can range from -1 to $+1$.

4.2 The 2D Ising Model

We have simulated the Ising model with 50×50 spins arranged in a square lattice. As discussed in Sec. 2.2, the measurements made on our simulation of the 2D Ising model can be correlated. To check it, we plot the *autocorrelation* for the observable $\langle E \rangle$.

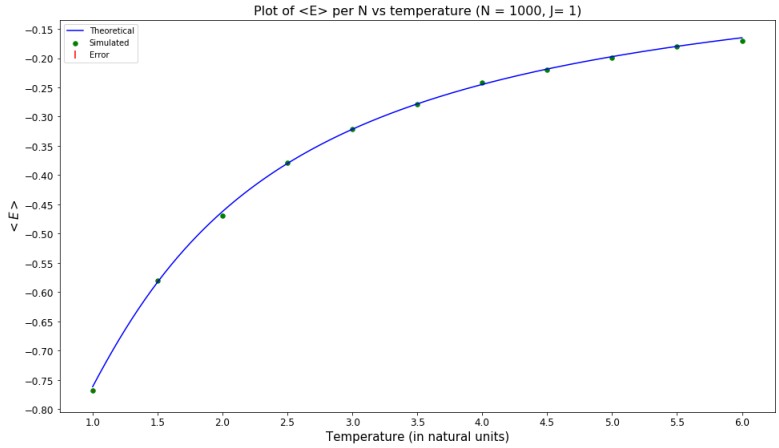


Figure 1: Average energy per spin plotted against the temperature. The simulated results are in great agreement with theoretical values. Errors were calculated using the Jackknife method and the error bars are too small to be visible in the plot.

From the autocorrelation plot given in Fig. 4, we note that we should make measurements of energy with a gap of at least 250 iterations for them to be uncorrelated.

After starting the simulation from a random configuration, the system requires some iterations to reach equilibrium as evident from Fig. 5. This is called the *thermalization* (or burn-in) stage and it needs to be excluded from the results before calculating the observables (see Fig. 6).

The number of times a candidate sample is accepted compared to the number of candidates generated gives us the *acceptance rate*. We have plotted the acceptance rate after every 250^{th} iteration for $T = 3$ in Fig. 7. The acceptance rate can give us an idea about the efficiency of the simulation. If the rate is too low, then the time spent on generating the many rejected candidates is just wasted. If the rate is too high, we might be accepting too many samples that are aways from the equilibrium states. From Fig. 8, it can be noted that the acceptance rate is very low for lower temperatures.

4.2.1 Average Energy

We can now look at the measured observables. In Fig. 9, we have plotted the average energy per spin, $\langle E \rangle$ as a function of temperature. It decreases with decreasing temperature and approaches $\langle E \rangle = -2$, which is the lowest possible value for this model (with $J = J^* = 1$).

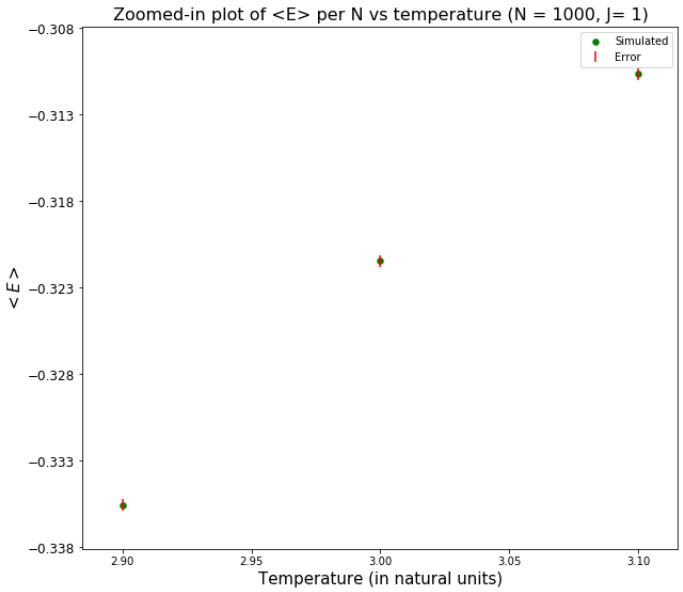


Figure 2: A zoomed-in plot of $\langle E \rangle$ vs T to show the scale of the error bars.

4.2.2 Average Magnetization

Figure 10 shows the average *magnetization* $\langle M \rangle$ as a function of temperature. The analytical result, given by Eq. (13), is also shown on the plot. Note that the equation

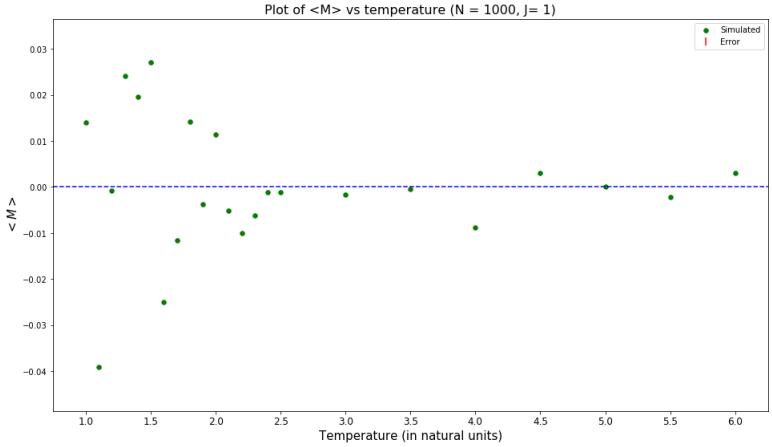


Figure 3: Plot of magnetization against temperature. Errors were calculated using Jackknife method and the error bars are too small to be visible in the plot.

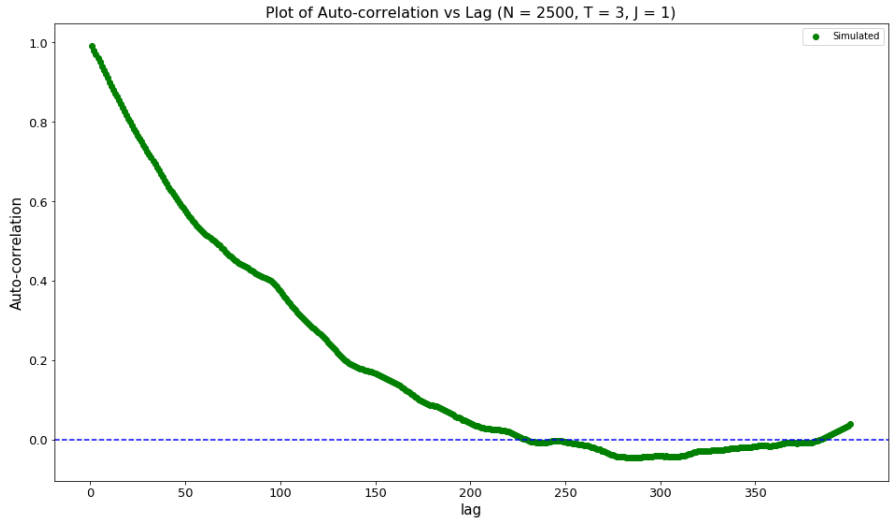


Figure 4: The autocorrelation for the observable $\langle E \rangle$.

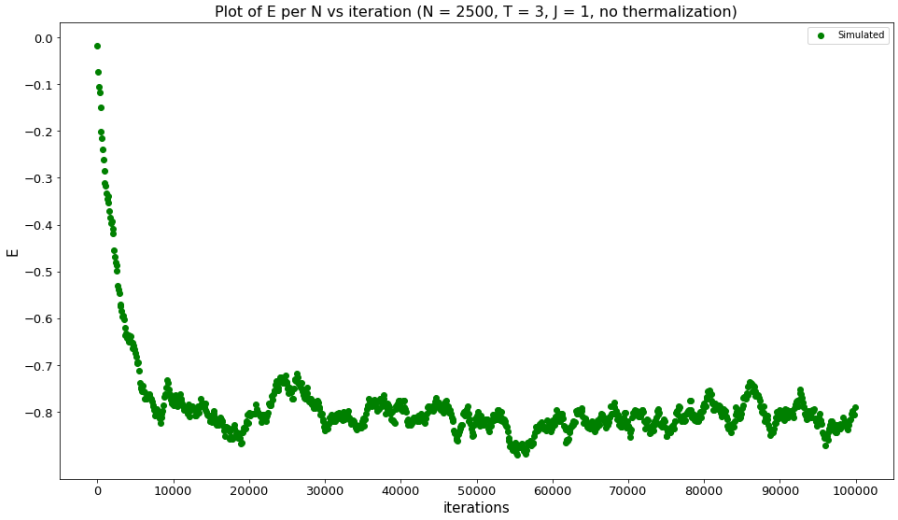


Figure 5: E per N plotted against iterations without excluding thermalization steps.

is valid only for zero external magnetic field and T less than the critical temperature. (We will discuss the critical temperature later.)

We have

$$M = [1 - \sinh^{-4}(2\beta J)]^{1/8}. \tag{13}$$

This equation only gives us positive values of M and has been mirrored in the plot

to account for possible range of magnetization from -1 to $+1$.

We observe a notable change in the values of $\langle M \rangle$ in Fig. 10 as we decrease the temperature below $T = 2.4$. This indicates the possibility of a *phase transition* in between at the *critical temperature* T_c. For temperatures greater than T_c, we note that the magnetization is close to zero, which indicates uniform randomness (disor-

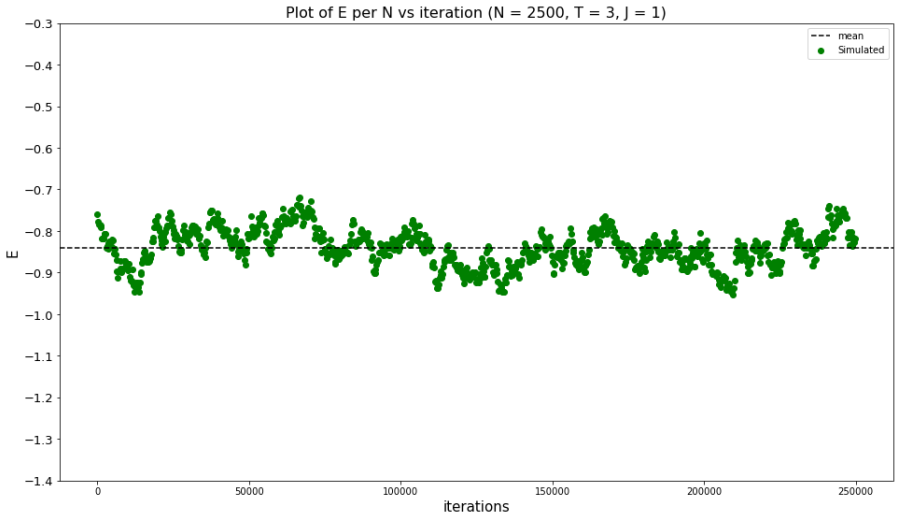


Figure 6: E per N plotted against iterations after excluding the thermalization steps.

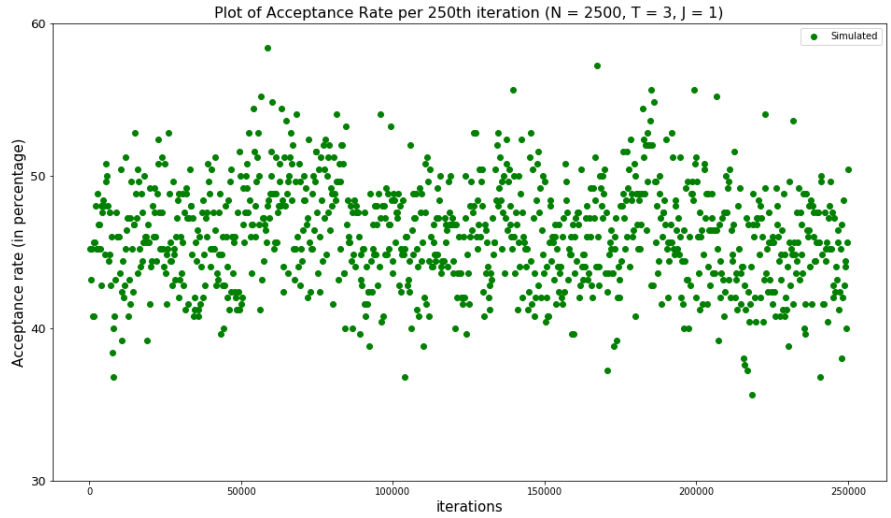


Figure 7: Plot of acceptance rate for $T = 3$.

der) in the system with almost equal number of up and down spins. At temperatures below T_c, the magnetization is close to either -1 or $+1$. This indicates that the majority of the spins are aligned in one direction (either up or down). This continuous change in the behavior of the system from disorder ($\langle M \rangle = 0$) to order, with the operation $s_{ij} \to -s_{ij}$ resulting in $\langle M \rangle \to -\langle M \rangle$, is characteristic of a *second order*

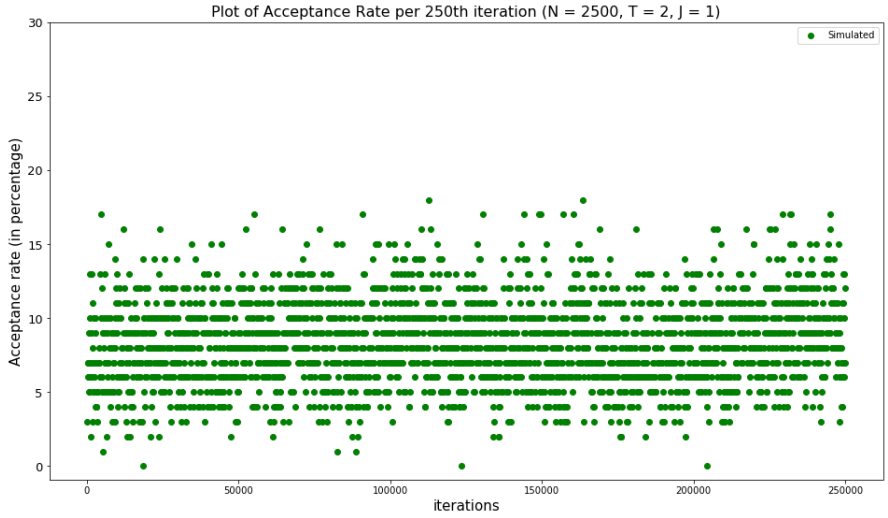


Figure 8: Plot of acceptance rate for $T = 2$.

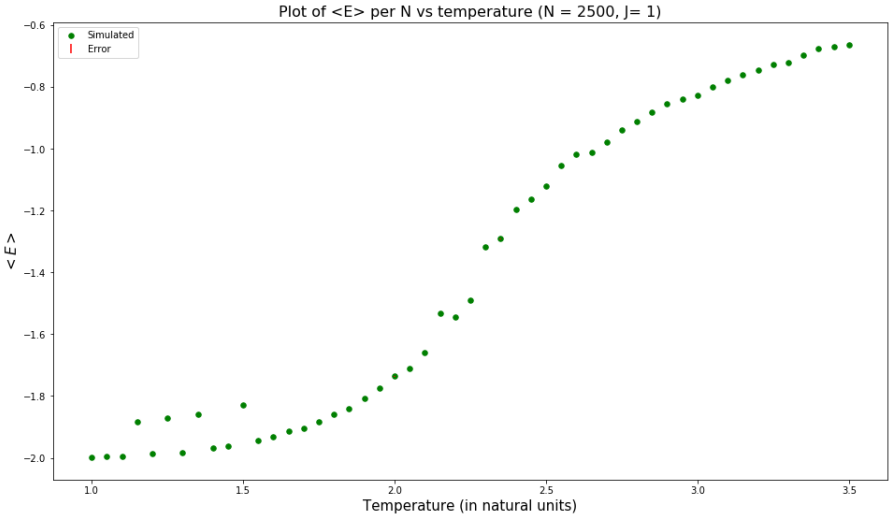


Figure 9: Plot of $\langle E \rangle$ vs T.

phase transition.

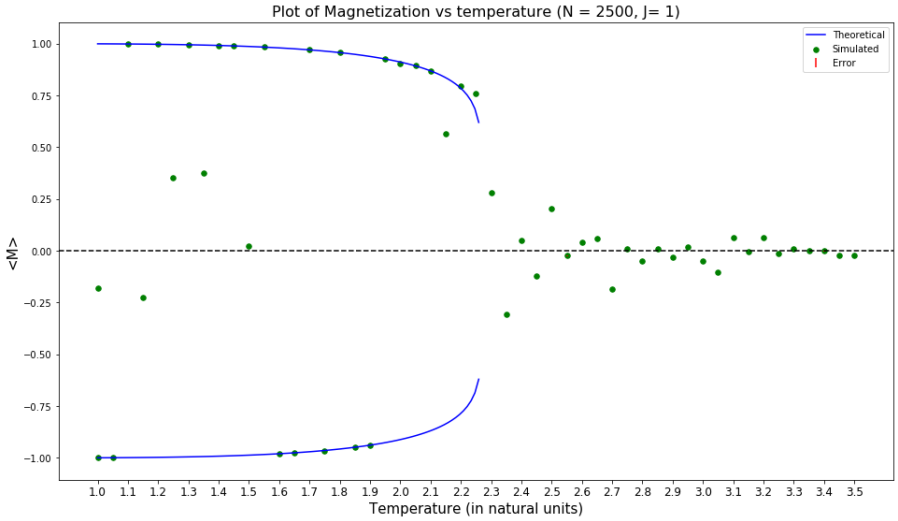


Figure 10: Plot of $\langle M \rangle$ vs T.

We now look at the behavior of $\langle M \rangle$ at temperature range close to the critical temperature in more detail in Fig. 11. We can suggest the critical temperature T_c to be 2.3 ± 0.1.

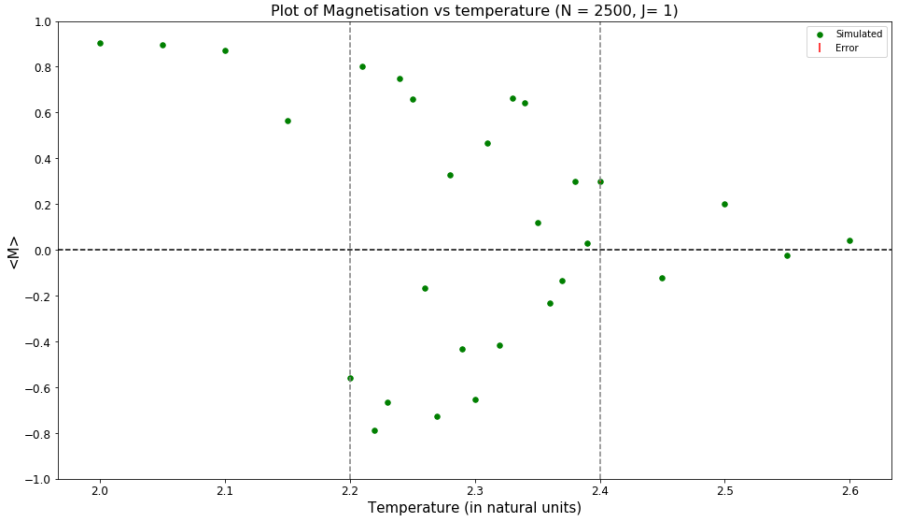


Figure 11: A closer look at the plot of $\langle M \rangle$ vs T with more data points.

4.2.3 The Specific Heat Capacity

The specific heat capacity C_V was calculated from the observable, energy, using Eq. (14) and error was calculated by doing error propagation.

We have

$$C_V = \frac{1}{T^2}(\langle E^2 \rangle - \langle E \rangle^2). \tag{14}$$

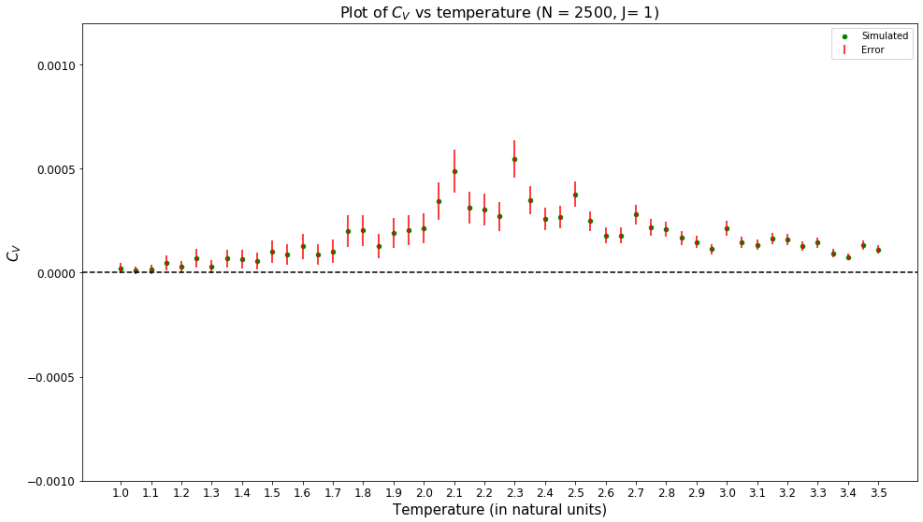


Figure 12: Plot of the specific heat vs T.

In Fig. 12, we have plotted the *specific heat capacity*, C_V as a function of the temperature. We note that around the temperature range 1.9 to 2.7 (where we suggest the critical temperature lies), we see a positive deviation from zero.

4.2.4 Magnetic Susceptibility

Magnetic susceptibility χ is plotted as a function of temperature in figure (13).

We note that there is a peak at $2.2 < T < 2.7$ and that below temperature 2.2, $\chi = 0$. This can be understood by considering how we calculated the susceptibility (see Eq. (15)).

$$\chi = \frac{1}{T}(\langle M^2 \rangle - \langle M \rangle^2). \tag{15}$$

First of all, it is clear from our observation of the magnetisation and the specific heat that a phase transition takes place around 2.3 ± 0.1 where for $T < 2.2$, where we have the most of the spins aligned in one direction. This makes the fluctuation

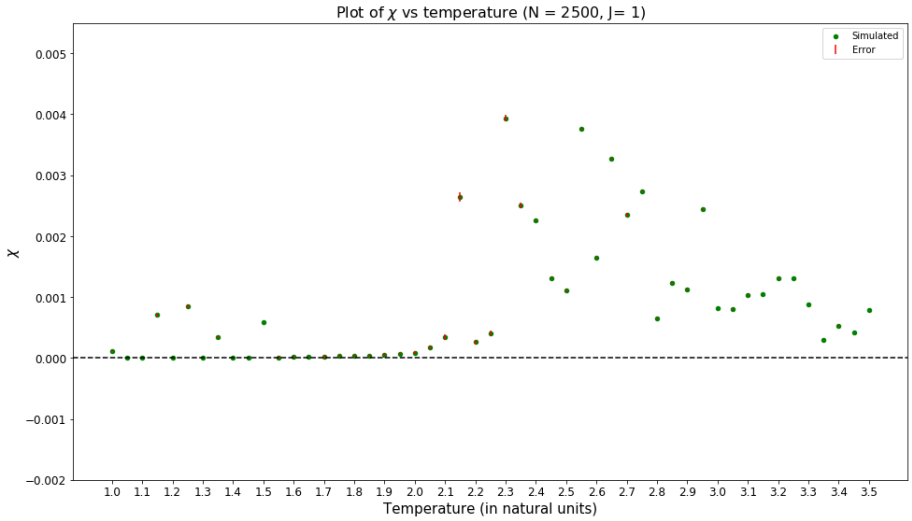


Figure 13: Plot of susceptibility vs T.

of M term in the numerator of Eq. (15) very small which outweighs the decrease in T and overall makes χ close to zero.

4.2.5 Spin-spin Correlator

Spin-spin correlator, C_{ij} can be used to understand how the spins interact with each other over the entire lattice. It shows how spins s_i and s_j separated by distance d are related. Fig. 14 plots the spin correlator over lattice distance for $T = 3$, which is a temperature greater than critical temperature ($T > T_c$).

The fit used for Fig. 14 is an exponential fit given by $y = ae^{-bx}$ where $a = 0.9793 \pm 0.0908$ and $b = 0.6355 \pm 0.1113$.

We observe that for $T > T_c$, the spin-spin correlation exponentially falls to zero as the distance between the two spins increases. This suggests a greater disorder in the system as the correlation is very short ranged. This distance was calculated only in horizontal direction in the lattice and since our model is isotropic, we would get same results in vertical direction as well. Our model has 50 spins in one direction and we note that since we are using periodic boundary conditions, the spin-spin correlation begins to rise again after we move a distance greater than 25 lattice points (Fig. 14). This is because we start approaching the same spin as the one we are measuring the correlation from and thus the correlation begins to rise again. We will ignore this effect and consider the values only till 25 lattice distances.

In Fig. (15) we plot the spin-spin correlator over lattice distance for $T \leq T_c$.

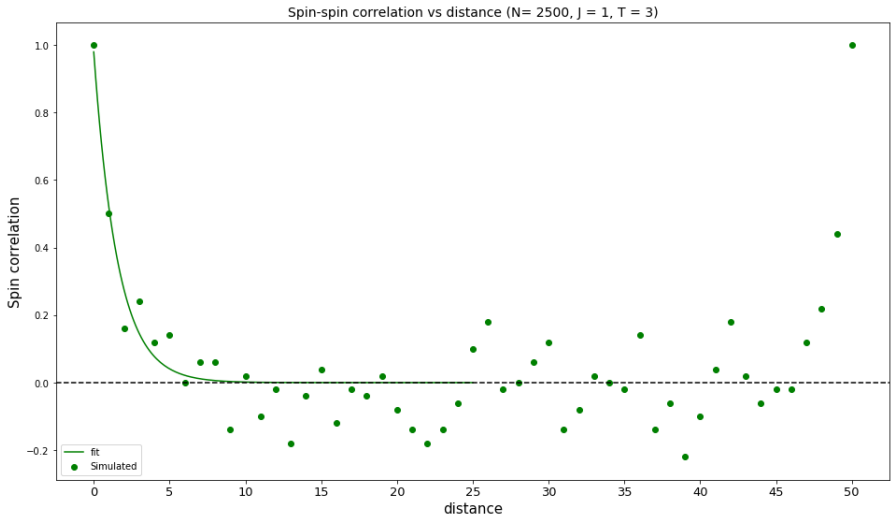


Figure 14: Plot of spin-spin correlator for $T > T_c$.

The fit used for Fig. 15a is a polynomial fit of the form $y = a(x-b)^6 + c$ where $a = 4.9071 \pm (5.5260 \times 10^{-08})$, $b = 14.5489 \pm 2.5818$ and $c = 0.4989 \pm 0.0185$.

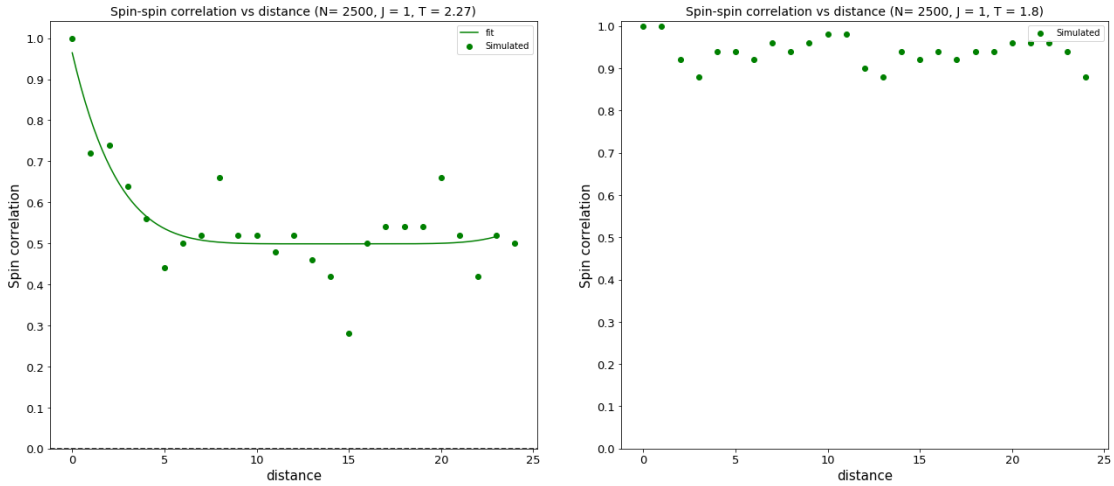
We observe that for temperature close to the critical temperature, the spin-spin correlator has a polynomial decay to about 0.5 and never reaches zero. From Fig. 15b, we observe that for $T < T_c$ there is very high correlation between the spins over all distances. This indicates increased order in our system, which is true as we expect almost all the spins to be aligned in one direction after the phase transition. In this state of the system, let us say we know that one of the spins is down. Due to the high spin-spin correlation, there is a very high probability that the majority of the spins at any distance from this spin also has to be down.

4.2.6 Visualization of the Spins

In this section, we show a visual representation of the 2D Ising model in a 50×50 square lattice at equilibrium state for various temperatures. The up and down spins are represented by white and grey color, respectively.

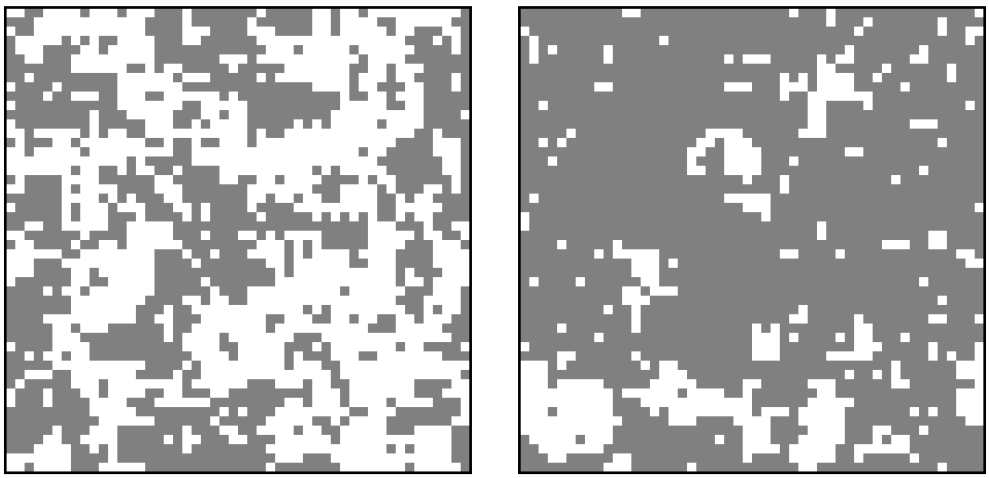
For $T > T_c$, the spins are randomly up and down (Fig. 16a) and as we approach the critical temperature, we note an increase in order in the system (Fig. 16b).

Below the critical temperature, the order is greatly increased in the system with majority of the spins aligned either up (Fig. 17a) or down (Fig. 17b).



(a) $T \approx T_c$. (b) $T < T_c$

Figure 15: Plot of spin-spin correlator for $T \leq T_c$.

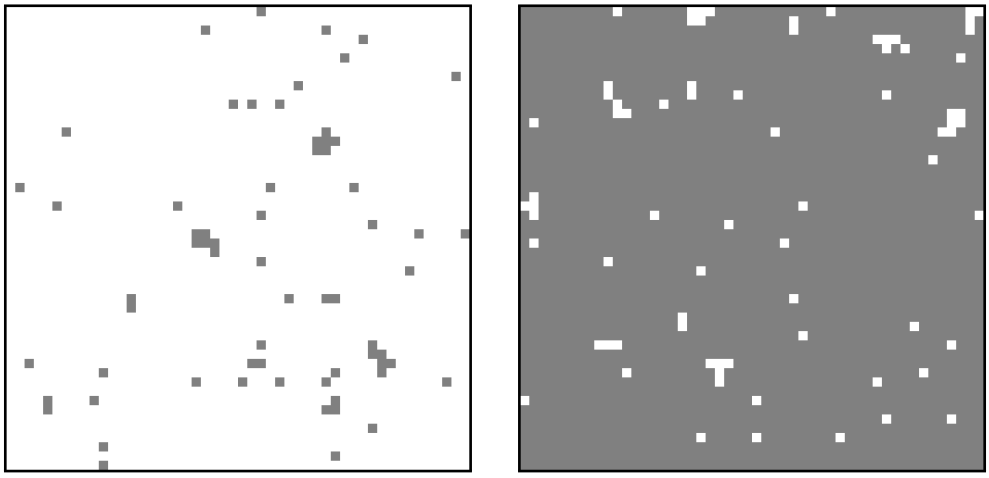


(a) $T > T_c$. (b) $T \approx T_c$.

Figure 16: A visual representation of the spins for $T \geq T_c$.

5 Conclusions

We have simulated the 1D and 2D Ising models using Metropolis Monte Carlo algorithm and made measurements on the observables of the system. We have also calculated the errors using the jackknife method. We tracked the auto-correlation



(a) Majority of spins aligned up. (b) Majority of spins aligned down

Figure 17: A visual representation of the spins for $T < T_c$.

of the data points and took measurements in the required gaps to minimize the correlation. We have also made sure that the system had reached equilibrium before making measurements and discarded the iterations required for thermalization.

In the 1D Ising model, we did not observe any special behavior of the system as we decreased the temperature, suggesting the lack of a phase transition. The simulated values of $\langle E \rangle$ were in excellent agreement with the analytical solution. Our system had no external magnetic field and the simulated $\langle M \rangle$ was close to zero for the entire temperature range.

For the 2D Ising model, we observed a characteristic change in the behavior of the system below a certain temperature as we decreased the temperature. This indicates that a second order ferromagnetic phase transition took place and we suggested $T = 2.3 \pm 0.1$ to be the critical temperature based on our results. This is in agreement with the analytical result, $T_c = 2.2692$ ($J = 1$). We noted that the acceptance rate is very low for lower temperatures and no tweaking of the simulation could fix it. This might indicate that the Metropolis algorithm might be inefficient to study this model at low temperatures and some other method with higher acceptance rates could be much faster. Nevertheless, the Metropolis algorithm was able to simulate the 2D Ising model with excellent results.

References

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