The Ising model and the Metropolis Algorithm

Kosar Nozari Mirarkolaei

November 2018

Abstract

The aim of this project is to determine the Curie temperature T_c, of a system undergoing phase transitions. When the temperature is raised above this critical level a ferromagnetic material will change into a paramagnetic material. The aim is to solve the problem employing the Metropolis-Hastings algorithm and Monte Carlo methods. The source code for this project can be found at my github[1].

1 Introduction

This study is both an exercise in the use of Monte Carlo methods and an analysis of the very popular Ising model. Monte Carlo methods are applicable in several situations where many other methods are too computationally heavy. They are a broad class of methods that rely on random sampling to obtain numerical results. The Ising model is a mathematical model of ferromagnetism in statistical mechanics. The Ising model and Monte Carlo methods go hand in hand as we shall see in this study.

I will start by giving a very brief description and definition of the two-dimensional Ising model. This general model will be simplified by assuming zero extern field which leads to a simple energy equation. Then I will present the Metropolis-Hastings algorithm and how it is implemented using Monte Carlo methods. Lastly, several simulations are presented, and I will try to uncover the Curie temperature where the ferromagnetic model transitions into a paramagnetic one.

2 Theory

The model we will employ in this study of phase transitions at finite temperature for magnetic systems is the Ising model, named after Ernst Ising who solved a one-dimensional variant of the model. The two-dimensional square lattice model, employed herein, was given an analytic description much later by Lars Onsager.

[1] `https://github.com/Kosarnm/FYS4150`

2.1 The general Ising model

Let Λ be a set of lattice positions, each with adjacent positions, forming a d-dimensional lattice. For each lattice site, $k \in \Lambda$, there is a discrete variable $\sigma_k \in \{+1, -1\}$, representing the spin of the site, $\uparrow$ and $\downarrow$, respectively. A spin configuration σ is a specific spin configuration of the lattice.

For two adjacent sites, $i, j \in \Lambda$, one has an interaction J_{ij}. A site $j \in \Lambda$ will also have an external magnetic field h_j interacting with it. The energy of a specific system is given by the following Hamiltonian

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j\sigma_j, \tag{1}$$

where the first sum is over pairs of adjacent spins. The notation $\langle ij \rangle$ indicates that sites i and j are nearest neighbours. In the second sum, μ is the magnetic moment.

The probability of a certain configurations is given by the Boltzmann distribution

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta} \tag{2}$$

where Z_β is the partition function acting as a normalization constant, and $\beta = (k_B T)^{-1}$. This would mean that by increasing the temperature T, finding the system in one particular configuration decreases. It must be so, because with a relatively higher temperature, one would expect previously unfavourable configuration to become more feasible.

There are two important expected values that are important in order to characterize a magnetic system. The *mean energy* of the system is

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_\beta(\sigma) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}, \tag{3}$$

and the *mean magnetisation* is

$$\langle \mathcal{M} \rangle = \sum_{i=1}^{M} \mathcal{M}_i P_\beta(\sigma) = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{\beta E_i}, \tag{4}$$

where $\mathcal{M}_i = \sum_{j \in \Lambda} \sigma_j$ for all configurations σ, and M denotes the number of possible configurations. Another quantity of interest is *magnetic susceptibility* χ which tells us how much an extensive parameter changes when an intensive parameter increases. It is given by

$$\chi = \frac{1}{k_B T}(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2). \tag{5}$$

The *heat capacity*, at constant volume, is given by

$$C_V = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

The minus sign on each term of the Hamiltonian $H(\sigma)$ in equation 1 is conventional. By this sign convention, the Ising model can be classified according to the sign of the interaction. If, for all pairs i, j:

- $J_{ij} > 0$, the interaction is ferromagnetic,
- $J_{ij} < 0$, the interaction is anti-ferromagnetic,
- $J_{ij} = 0$, the spins are non-interacting.

In a ferromagnetic Ising model, spins desire to be aligned: the configurations in which adjacent spins are of the same sign have higher probability. In an anti-ferromagnetic model, adjacent spins tend to have opposite signs.

2.2 Simplified ferromagnetic Ising model

The general Ising model, as described above, will not be used in this study, but a much simpler version of it. Firstly, we will examine a system with no external magnetic field, as was originally solved analytically by Onsager[3]. Because the second sum in the Hamiltonian in equation 1 is zero, and we are left with

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij}\sigma_i\sigma_j. \tag{7}$$

Secondly, we assume that the coupling constant J_{ij}, that describe the interaction of a spin with its neighbour, to be constant. That is $J_{ij} = J \forall i, j \in \Lambda$ and equation 7 is simplified further to

$$E = H(\sigma) = -J\sum_{\langle ik \rangle} \sigma_i\sigma_j \tag{8}$$

In this study, we will assume that we have a ferromagnetic ordering, id est $J > 0$. This means that neighbouring spins are aligned, because it would lead to lower energy. It is easy to see why it must be so, as $\sigma_i\sigma_j = 1$ whenever spin i and j have the same sign.

2.3 The Onsager Limit

The critical temperature T_C of the system is the temperature below which the system becomes spontaneously magnetized, and above which is doesn't. At T_C we then get a phase shift. It has been shown that the mean magnetization of the system as $T \to T_C$ scales as[2]

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta}$$

[2] J. Cardy, Scaling and Renormalization in Statistical Physics (Cambridge University Press, 1996)

where $\beta = 1/8$ is called the critical exponent. Similarly for the heat capacity and magnetic susceptibility:

$$C_V \sim |T_C - T|^{\alpha}$$
$$\text{and} \qquad \chi \sim |T_C - T|^{\gamma}$$

where $\alpha = 0$ and $\gamma = 7/4$ are the corresponding critical exponents.

As mentioned, the system experiences no net magnetization at $T > T_C$. That is $\langle \mathcal{M} \rangle = 0$ in this limit. However, any spin can only interact with it nearest neighbours only, but in some way, the system as a whole will tend to a specific state. This gives rise to another important quantity called the correlation length, and it describes how far from a specific spin i one have to go before there will not be any correlation between the spin at the current position and the spin at position i. In other words the length within which there is a reasonable probability that a change in spin i will cause a change in any other spin within the correlation length.

For smaller temperatures, a change in one spin will have a small probability of changing any of its nearest spins, and hence the correlation length is small, possibly on the order of the lattice spacing. As the temperature increases, however, the correlation length increases and as it approaches T_C. This behaviour can be expressed as another power law

$$\xi \sim |T_C - T|^{-\nu}$$

For any finite lattice, the correlation length will be of the order of the lattice size L, $\xi = a'L$ where a' is a constant. Assume we approaching the critical temperature T_C with increasingly larger $T < T_C$ for 1) a finite lattice and 2) an infinite lattice. Since the correlation length is proportional to the size of the lattice we have

$$\xi \sim (T_C(L) - T)^{-\nu} = a'L \Rightarrow T_C(L) - T = aL^{-1/\nu}$$

and similarly for the infinite lattice:

$$T_C(L = \infty) - T = aL^{-1/\nu}$$

Using the exact result $\nu = 1$ we get

$$T_C(L) = aL^{-1} + T \text{and} \qquad T_C(L = \infty) = T$$

which leads to the so-called finite size scaling relation

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} = aL^{-1} \tag{9}$$

Onsager showed that the exact result is $kT_C/J = 2/\ln\left(1 + \sqrt{2}\right) \approx 2.269$ with $\nu = 1$. This limit is hereby referred to as the Onsager limit.

Table 1: All possible configurations of a 2×2 Ising model

No of spins↑	Degeneracies	E_i	$\mathcal{M}_i$
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

2.4 Analytical Solution for 2×2 Ising model

It would be beneficial to test the waters of the ocean of the vast ocean that is the Ising model, by a two-dimensional model with lattice dimension $L = 2$ and periodic boundary conditions. This model has $s = 2^4 = 16$. different configurations σ. The energy of a given configuration would be

$$E_i = -J \sum_{\langle kl \rangle}^{4} \sigma_k \sigma_l.$$

Figure 1 shows an arbitrary configuration of a 2×2 spin lattice. The energy for this configuration is

$$E_i = -J((+1)(-1) + (+1)(-1) + (+1)(-1) + (+1)(-1)) = 8J$$

which happens to be the highest energy possible for the system. When all spins are parallel we see that $E_i = -8J$ which is the lowest energy possible. If only one spin would differ from the others, the energy would be $E_i = 0$ and so on. Of the 16 possible configurations, several will have degeneracies ($\Omega(E_i)$), which corresponds to the number of configurations with the same energy. Moreover, the magnetization of a particular configuration is simply the sum of the spins and is easy to calculate. All the possible configurations of this system can be found in table 1.

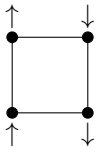

Figure 1: Sample 2×2 spin lattice.

Now to compute the physical quantities as discussed above, expected value for energy $\langle E \rangle$, expected value for magnetization $\langle \mathcal{M} \rangle$, expected value for specific heat $\langle C_V \rangle$, and susceptibility χ. For the 2×2 Ising model these quantities

have closed form expressions. The partition function for the system is given by

$$Z = \sum_{i=1}^{1} 6e^{-\beta E_i} = e^{\beta 8J} + 12 + 2e^{-\beta 8J} + e^{\beta 8J} = 4\cosh(\beta 8J) + 12 \tag{10}$$

The expected energy is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln(4\cosh(\beta J) + 12) = -8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3}. \tag{11}$$

The mean magnetization for this system is easiest to compute with equation 4, merely adding all possible states and dividing by the partition function.

$$\langle \mathcal{M} \rangle = \frac{1}{Z}(-4e^{8\beta J} - 8e^{0} + 8e^{0} + 8e^{8\beta J}) = 0 \tag{12}$$

the expected absolute magnetization, on the other hand, becomes

$$\langle |\mathcal{M}| \rangle = \frac{1}{Z}(4e^{8\beta J} + 8e^{0} + 8e^{0} + 4e^{8\beta J}) = \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J) + 3}. \tag{13}$$

The expected value for specific heat is

$$\langle C_V \rangle = \frac{1}{k_b T^2} \frac{\partial^2}{\partial \beta^2} \tag{14}$$

inserting equation 11 gives

$$\begin{aligned}
\langle C_V \rangle &= -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta} \left(-8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3} \right) \\
&= \frac{1}{k_B T^2} \left(\frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3} - \frac{64J^2 \sinh^2(8\beta J)}{(\cosh(8\beta J) + 3)^2} \right) \\
&= \frac{1}{k_B T^2} \frac{64J^2}{\cosh(8\beta J) + 3} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right)
\end{aligned}$$

The susceptibility χ of a thermodynamic system is easy to compute if one knows what the variance of magnetization, $\sigma^2_{\mathcal{M}}$), is. Rewriting equation 5 gives

$$\chi = \frac{1}{k_B T} \sigma^2_{\mathcal{M}}. \tag{15}$$

Using equations 12 and 13 one can deduce that the variance of the magnetization must be

$$\sigma^2_{\mathcal{M}} = \left\langle \mathcal{M}^2 \right\rangle - \langle \mathcal{M} \rangle^2 = \frac{32}{Z}(e^{8\beta J} + 1) - 0 = \frac{8(e^{8\beta J} + 1)}{\cosh(8\beta J) + 3}. \tag{16}$$

Inserting 16 into 15 yields the susceptibility for the system

$$\chi = \frac{8(e^{8\beta J} + 1)}{k_B T(\cosh(8\beta T) + 3)} \tag{17}$$

Bear in mind that $\beta = \frac{1}{k_B T}$, and that all the quantities computed are functions of T. The results computed here can be used as comparison for numerical computations.

3 Algorithm

The algorithm for solving the Ising model consists of several parts and interesting aspects. The path to a steady state for the Ising mode can be seen as a Markov chain, which justifies the use of the Metropolis-Hastings algorithm, which again can be seen as one cycle in a Monte Carlo solver.

3.1 Markov chains

A Markov chain gives a good description for a system that moves towards a steady state given an initial configuration. A Markov process is a random walk with a a set of probabilities for making a set of moves. Such a process is usually represented by a stochastic matrix containing probabilities of transitioning from one state to another. In physics Markov chains can by used to study diffusion because it gives a framework for the rules of Brownian motion - the behaviour exhibited by small parts of any system when exposed to random fluctuations of the medium.

In order to simulate how the system in this study evolves towards a steady state, Markov chains are used repeatedly in Monte Carlo simulations. From Markov chains one gets two conditions needed for reaching a steady state, detailed balance and ergodicity. These properties governs our choice of algorithm, the Metropolis-Hastings algorithm.

3.2 The Metropolis-Hastings algorithm

In this project we need random samples from a probability distribution $P_\beta(\sigma)$ associated with the physical system we wish to model. Regrettably, direct sampling can be incredibly difficult, as we need to compute the partition function in order to express the probability distribution in its entirety. The Metropolis-Hastings algorithm is circumvents this problem because it only requires a function f proportional to the distribution density.

The Metropolis-Hastings algorithm can be condensed down to the following steps.

1. The system is initialized by an initial state which can be randomly generated. The energy E_b of this configuration is computed.

2. The initial configuration is changed by flipping the spin of an arbitrary site. One then computes the energy of this new trial state E_t.

3. The difference in energy between the two states $\Delta E = E_t - E_b$ is calculated. For the two-dimensional Ising model there are only five different possible values for ΔE.

4. If $\Delta E < 0$ the new configuration is accepted, meaning that the energy is lower than it was, and the system is progressing towards an energy minimum.

5. If $\Delta E > 0$ one computes $w = e^(\beta \Delta E)$ and compares w to a random number r. If $r < w$ the state is accepted, else the initial state is kept.

6. The expectation values are updated. And the steps are repeated until a sufficiently good steady state is reached.

As stated above, the possible different energy changes for a two-dimensional Ising model are finite. The possible changes are $\Delta E = 8J, 4J, 0, -4J, -8J$. An array containing these values is constructed which contains the possible values before doing the Metropolis sampling. One can compare the possible energy changes against elements of this array instead of computing w for every other iteration. This should vastly increase computing speed.

The algorithm determines whether a proposed move is implemented based on a transition probability and an acceptance probability. The strength of the algorithm is that the transition probability need not be known.

4 Implementation

The Ising model is implemented in Python in the class Ising.py contains all the methods necessary for a simulation of the model. The full program which can be found by following the link at the front page of this article.

4.1 Ising class

An object-oriented approach was picked in order to increase flexibility and tidiness. I implement different methods in order to easier approach to the result.

Of the various methods incorporated in the Ising class, iterate_metropolis and metropolis are the most important ones. The method iterate_metropolis calls the metropolis for every Monte Carlo cycle. Denoting L as the spin lattice dimension and M the number of Monte Carlo cycles, each call of metropolis constitutes a complexity of $\mathcal{O}(L^2)$.

5 Results

5.1 Code verification on the 2×2 lattice

For the 2×2 case, the analytical solution is given by equations 11, 13 , 14 and 17. To verify the program, I compared the analytical solutions with the numerical ones for $T = 1$ in units of kT/J. Table 2 shows such comparison.

It is immediately evident that by increasing the Monte Carlo cycles we could get closer to the analytical values. All quantities are given per spin.

5.2 20×20 Ising model

I switch now to a larger lattice size in order to get a more representing model of reality.

Table 2: Comparison between Monte Carlo simulations at different length and the analytical solution for a 2×2 system.

M	$\langle E \rangle$	C_V	χ	$\langle \lvert \mathcal{M} \rvert \rangle$
100	-2	0	0	1
1000	-1.85	0.1439	0.09	0.95
10000	-1.998	0.028748	0.011963	0.995
100000	-1.994	0.04785	0.002990	0.9985
1000000	-1.995	0.0383	0.005987	0.9982
Analytical	-1.99598	0.03208	0.00401	0.9986

A good way of determining the stability of the system over time is to decide at which point various expectation values are sufficiently stable. The Onsager limit for critical temperature is $T_C \approx 2.269$. The time dependence corresponds here to the total number of Monte Carlo cycles.

Figure 3 shows such a plot for one temperature above and below T_C and a clear pattern occurs. If we choose a uniform starting position, there are little or no fluctuations in the expectation values for $T = 1 < T_C$, which is the expected result because the system is now starting with all its spins pointing up which is the most likely situation at this temperature. When changing to a random starting position, however, the situation is somewhat different. The system is now in a very *unlikely* state and it needs some time to reach the state with the highest probability.

A similar discussion applies for $T = 2.4 > T_C$. Now, the uniform starting position is closer to the most likely position and the expectation values settle faster for the random starting position.

The settling is, however fairly quick no matter which temperature or starting position and it looks like they have settled after around 5000 Monte Carlo cycles.

5.2.1 Accepted states

It would also be interesting to see how many spin changes of the Metropolis-Hastings algorithm are accepted at this higher temperature. A plot for accepted configuration changes as a function of cycles for the two temperatures $T = 1$ and $T = 2.4$ is shown in figure 4. When the steady state has been reached, we expect the rate of accepted configurations to remain unchanged. One can clearly see that for the higher-temperature system the number of accepted states linearly proportional to the number of cycles in the simulation which is reasonable, because For higher values temperatures, one would expect more chaos, and thus more accepted configurations. While for the lower-temperature system the number of accepted states stay the same after the steady state is reached.

5.2.2 Probability Distribution

Figure 5 shows a histogram of the probability distribution of total energy of the system. The energies are sampled after the steady state situation was reached

Table 3: Computed critical temperatures for the different lattice sizes.

L	$T_C(C_V)$	$T_C(\chi)$
20	2.18	2.25
40	2.1	2.18
60	2.251	2.225

and the corresponding variances are

$$\sigma_E(T=1) = 1.435 \qquad \text{and} \qquad \sigma_E(T=2.4) = 1.074$$

We see that the system will cluster around a certain value for the specific temperature, and for $T = 1$ this is, not surprisingly, at the lowest possible energy.

5.3 Phase Transition

So long I have only looked at finite lattice sizes, and indeed infinite sizes are not possible to simulate. However, I try to make an approximation to the infinite lattice by gradually increasing the size of the lattice.Unfortunately, because of hardware issue I can not get accurate data for larger lattice size and Monte Carlo cycles(I've got overflow encountered in long scalars warning and it causes the negative value for $\langle E \rangle^2$) Figure 6 shows a comparison of the different interesting quantities for lattice sized 20, 40 and 60. The critical temperature of the system is, as we know, where the heat capacity and magnetic susceptibility diverges. We see that as the lattice size increases, the computed critical temperature approaches the true critical temperature in the Onsager limit $kT_C/J = 2.269$.

Table 3 shows the critical temperatures for the heat capacity and magnetic susceptibility. I used this data to compute the constant of proportionality in eq. (9) by letting

$$T_C(L_1) - aL_1^{-1} = T_C(L_2) - aL_2^{-1}$$

then comparing all combinations of L_1 and L_2 in table 3. By taking the average a, then inserting back in eq. (9), I obtained the following for the critical temperature:

$$T_C(C_V) = 2.062 \qquad \text{and} \qquad T_C(\chi) = 2.232$$

6 Conclusion

In this project I employed the Ising model and the Metropolis algorithm to model a phase transition from ferromagnetic to para-magnetic material. I tried to obtain the Curie temperature, T_c at which such a phase transition happens, but was only partly successful in this endeavour. Despite this I feel that I have demonstrated to a great extent how the Ising model functions and the benefit of Monte Carlo methods.

References

[1] Hjort -Jensen Morten, *Computational Physics*,
Lecture notes fall 2015, 2015.

[2] Ising, E., Beitrag zur Theorie des Ferromagnetismus, *Z. Phys.,* 31, pp. 253-258 (1925).

[3] Onsager, L., Crystal statistics. I. A two-dimensional model with an order-disorder transition, *Physical Review,* Series II, 65 (3-4), pp. 117-149 (1944).

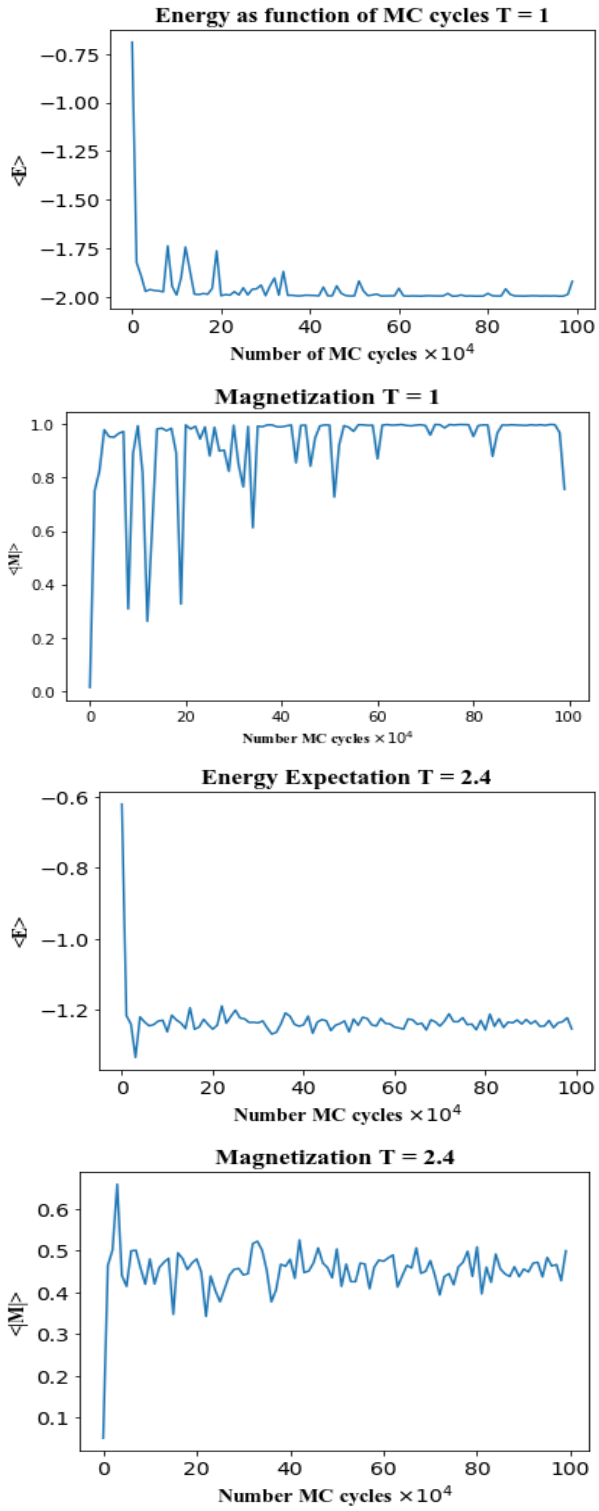

Figure 2: Mean Energy and Mean magnetization for a 20×20 spin lattice with temperatures $T = 1$ and $T = 2.4$.

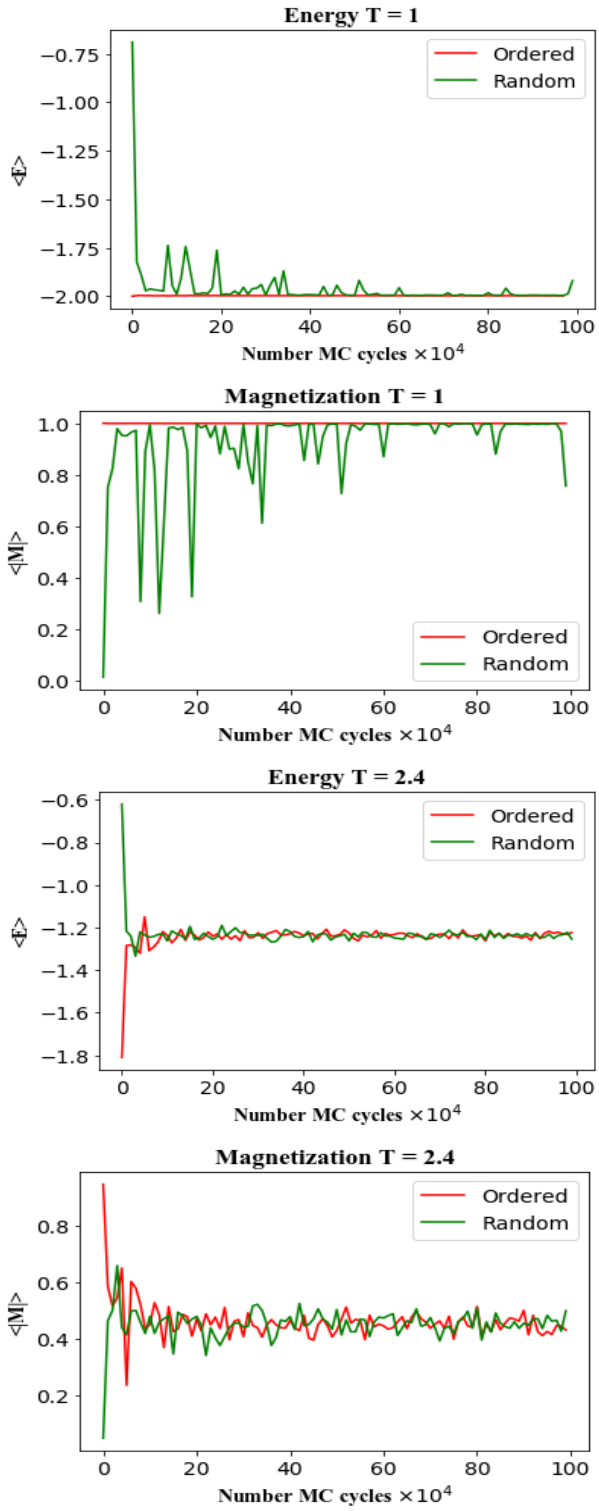

Figure 3: Mean Energy and Mean magnetization for a 20×20 spin lattice with ordered spin configuration ,temperatures $T = 1$ and $T = 2.4$.

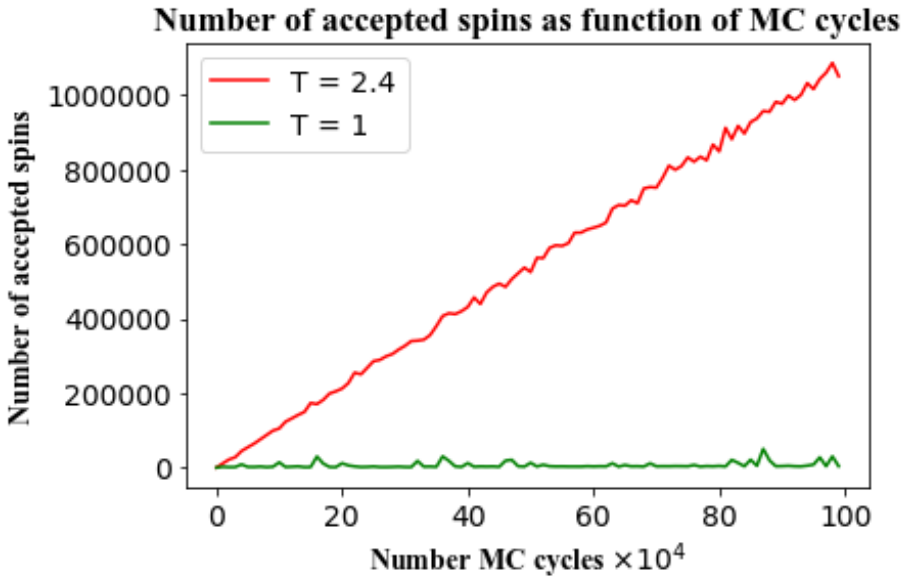

Figure 4: Figure showing that the number of accepted states for a higher-temperature system ($T = 2.4$) rises linearly, while the accepted states for for a lower-temperature system ($T = 1$) stays the constant at equilibrium.

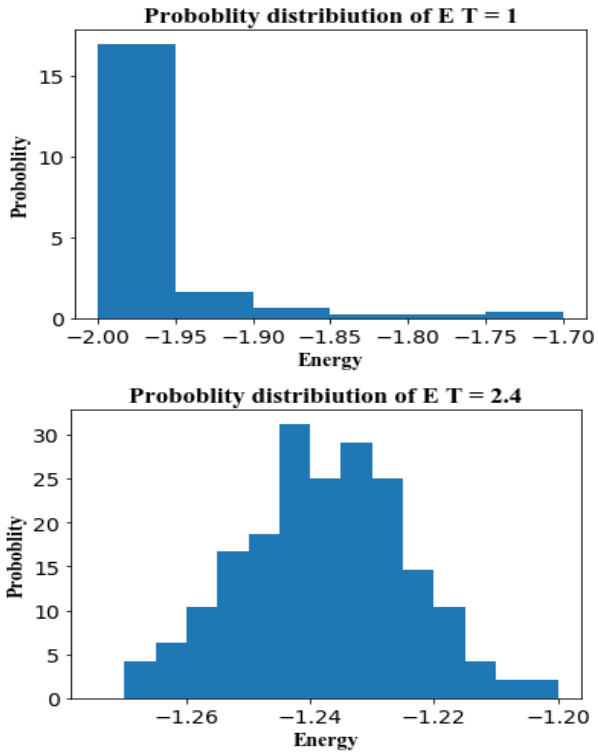

Figure 5: Mean Energy and Mean magnetization for a 20×20 spin lattice with ordered spin configuration ,temperatures $T = 1$ and $T = 2.4$.

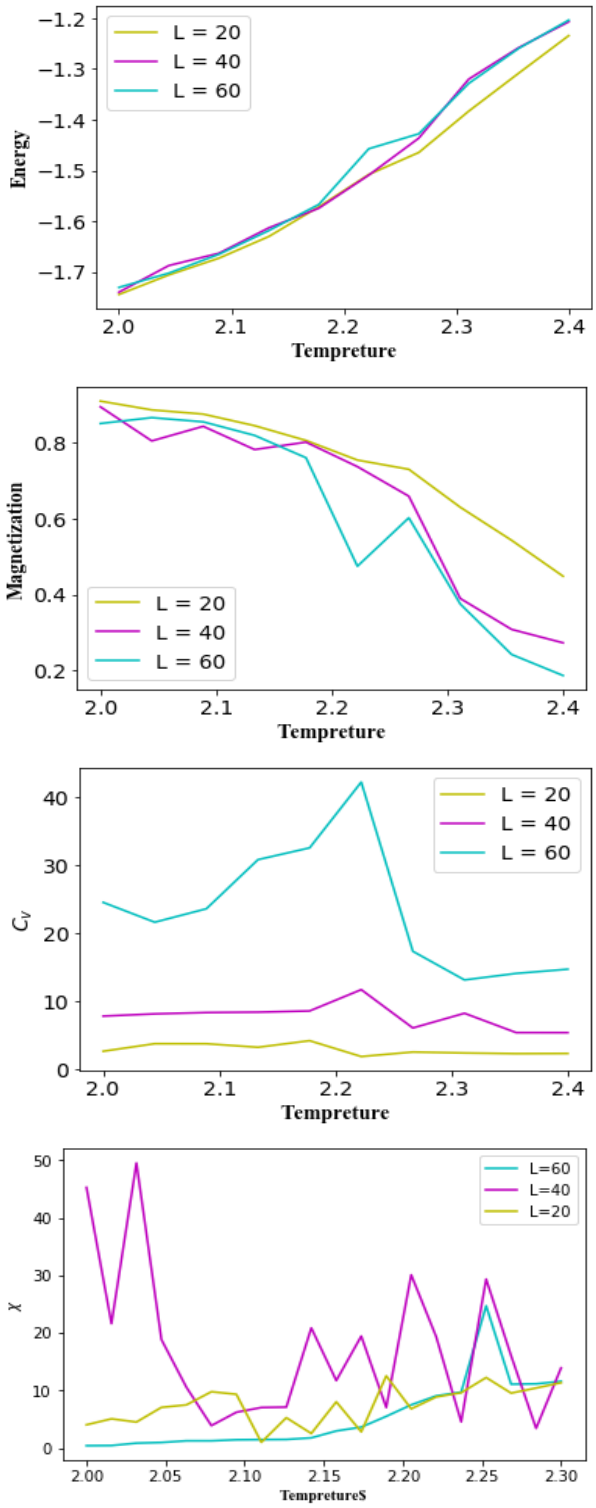

Figure 6: Mean Energy and Mean magnetization for a 20×20 spin lattice with ordered spin configuration ,temperatures $T = 1$ and $T = 2.4$.