Simulating the phase transition of the Ising model using Markov chain Monte Carlo

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Abstract

By simulating the Ising model which uses the Markov chain Monte Carlo to sample spin-configurations **s**. We calculated $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_V and χ numerically for 10^3 up to 10^7 Monte Carlo cycles for a 2×2 lattice. In the case of 10^7 cycles the numerical values for $\langle\epsilon\rangle = -1.99594J$, $\langle|m|\rangle = 0.99865$, $C_V = 0.03242J/K$ and $\chi = 0.00402$, gave a good conjecture with the analytical values $\langle\epsilon\rangle = -1.99598J$, $\langle|m|\rangle = 0.99866$, $C_V = 0.03208J/K$ and $\chi = 0.00401$ for a 2×2 lattice. The higher the Monte Carlo cycles the closer the numerical values approached the analytical results. The ϵ distribution for $T = 1J/k_b$ has more configurations states with energy -1.9995 J. For $T = 2.4J/k_b$ the distribution looks more like a Gaussian with the most common energy of any configuration was -1.26 J. The plots of C_V and χ clearly peaked around $T_c = 2.25\ J/k_b$ and $2.30\ J/k_b$ respectively. These result are a clear sign of a phase transition, and corresponds well with the analytical value for $T_c(L = \infty) = \frac{2}{\ln(1+\sqrt{2})} J/k_B \approx 2.269J/k_B$ calculated by Lars Onsager.

Contents

1 Introduction

In this article we studied the Ising model and it's finite temperature dependence in ferromagnets in two dimensions. The system were modeled as a $L \times L$ lattice with 2^N total spin-states[5]. Such a large system motivated us to use Monte Carlo methods to simulate the Ising model. With our simulations we numerically estimated the critical temperature where our system underwent a phase transition, which led to our material no longer having any net magnetization. Our numerical estimations of the temperature were compared to the analytical values found by Lars Onsager, in 1944.

On the more methodological side, the specific Monte Carlo method we utilized is the method known as Markov chain Monte Carlo, from which we implemented the metropolis algorithm to sample from the Boltzmann distribution. These samples were used to approximate probability distributions and expectation values, from which we used to anticipate what the next state would be in.

2 Theory

2.1 The two dimensional square lattice Ising model

The two dimensional square lattice Ising model[3] which will be the focus of this article, consists of discrete variables, where each variable represent a binary spin state, "up" or "down". These different spin-states is located on a two dimensional $L \times L$ square lattice, where each spin s_i can either be +1(up) or -1(down). The energy of this system can be expressed as[4]:

$$E = -J \sum_{<kl>}^{N} s_k s_l - \mathscr{B} \sum_{k}^{N} s_k, \tag{1}$$

where J is the coupling constant between two neighboring spins. We assume this coupling constant to be the same between every single spin, but we still emphasise in the equation with $\langle kl \rangle$ that the sum goes over neighboring spins only. Also since the spins are unit-less, J has units of energy N is the number of lattice sites, $s_{k,l} = \pm 1$ and $\mathscr{B}$ is an external magnetic field which interacts with the magnetic moment created by the spins. For this model, there will be no external magnetic field acting on our ferromagnetic. Therefor the total energy of our system is given by just the interaction between neighboring spin pairs:

$$E = -J \sum_{<kl>}^{N} s_k s_l. \tag{2}$$

By neighboring spins, it is only the spins located on the nearest north, south, west and east lattice sites that can effect each-other, see figure 1:

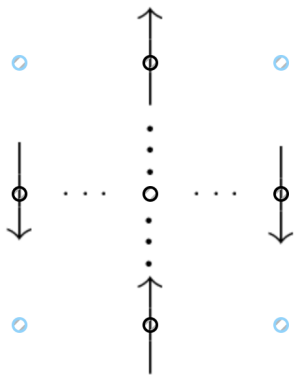


Figure 1: An illustration highlighting only the neighboring spins which would affect the center lattice site spin.

With the energy clearly defined, we also need a way to calculate the mean energy of the system $\langle E \rangle$ and magnetization $\langle m \rangle$. To be able to calculate these values, we need a probability distribution which tells us the probability of a certain state **s**.

At a given temperature T, the probability of a state **s** exists, is given by the Boltzmann distribution:

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})} (12).$$

β is the inverse temperature $\beta = \frac{1}{k_b T}$, and Z is the partition function given by:

$$Z = \sum_{s} e^{-\beta E(s)} (10). \tag{3}$$

Where s is all possible states, Z is the partition function for the canonical ensemble, meaning Z represents the possible states of a system in thermal equilibrium at a fixed temperature. Such a canonical ensemble assigns the probability for a spin configuration P_i[6]

The total magnetization of the system is given by:

$$M(s) = \sum_{<i>}^{N} s_i. \tag{4}$$

With the probability of a certain configuration of the $L \times L$ lattice given by $P(s, T)$, we can begin to calculate the quantities $\langle E \rangle$ and $\langle \mathscr{M} \rangle$. $\langle E \rangle$ and $\langle \mathscr{M} \rangle$ here will be defined *per spin*:

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N} (18).$$
$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N} (26).$$

Where $E(s)$ represents the total energy of a certain configuration given by equation (4). $M(s)$ represents total magnetization and is simply defined as the sum over all spins.

To build intuition, lets first consider a simple case where L = 2. This yields a 2×2 lattice, with 4 different lattice sites as in the figure 2:

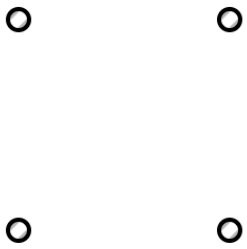


Figure 2: Empty 2×2 lattice.

Each of these lattice sites can be filled with either a spin-up or a spin-down state. Allowing for degeneracy, then from straight forward combinatorics there are 2^4 different ways to arrange the different spin states. The first two configurations are shown in figure 3

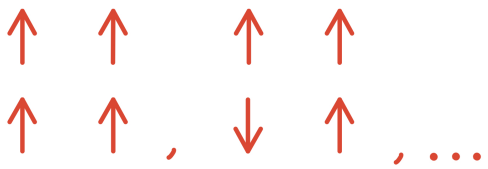


Figure 3: Caption

Table 1 shows the total energy, magnetization as-well as the degeneracy in energy and magnetization for each of the different configurations.

Number of up-states	Total E	Total M	Degeneracy
0	-8J	-4	1
1	0	-2	4
2	0	0	4
2	8J	0	2
3	0	2	4
4	-8J	4	1

Table 1: Table showing total energy E_i, total magnetization M_i and the degeneracy in energy and magnetization for different configurations of a 2x2 lattice. [1]

See 6 for derivations of the different energies values found in table 1. The different values in Table 1 were calculated by assuming there are other lattice sites outside the 2×2 grid which affects each spin-state that we can not see. This condition is implemented in the form of periodic boundary conditions. The low

variance in energy will come in handy when we need to define the acceptance rule in our Monte Carlo algorithm.

2.2 Phase transitions and critical temperature

The $2D$ Ising model undergoes what is known as a phase transition of second order.[4] Second order phase transitions are under a collective group known as critical phenomena. For a ferromagnetic system the critical phenomena we want to study, is the system when it approaches a critical temperature T_C. Below this critical temperature our Ising model exhibits spontaneous mangetization $\langle \mathscr{M} \rangle \neq 0$[4] The closer and closer the system gets to the critical temperature, the mean magnetization would approach zero infinitely fast. If we could somehow create an infinitely large lattice, then quantities like heat capacity C_V, and the magnetic susceptibility χ would be discontinuous or diverge when we move from a finite magnetization $\langle \mathscr{M} \rangle \neq 0$ to a paramagnetic phase $\langle \mathscr{M} \rangle = 0$.[4] With a discontinuous or diverging C_V and χ there will be a discontinuous or diverging variance in both energy and magnetization.

Since we are not able to simulate an infinitely large lattice, a finite lattice of size L, would have to be adequate. For a finite lattice the variance will scale as $\frac{1}{\sqrt{M}}$ where M is the number of ways to rearrange the lattice, i.e configurations. In this finite lattice, we will use specific heat capacity and susceptibility which are normalized to number of spins.

$$C_V = \frac{1}{N}\frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right) \quad (33)$$

$$\chi = \frac{1}{N}\frac{1}{k_B T}\left(\langle M^2 \rangle - \langle |M| \rangle^2\right) \quad (35)$$

In a finite size lattice, C_V and χ will not show diverging behaviour. However for increasing L, we will begin to see a sharpening of an initial broad maximum in C_V and χ around T_C. The sharpening indicates a critical temperature is approaching, which leads to a phase transition in the ferromagnetic system resulting in a para-magnetic phase.

The physics around critical phenomena is still to this day poorly understood . Simplified theoretical models may even predict the wrong physics.[4] One brief example of this is the one dimensional Ising model predicting a second order phase transition, although this is only possible for multi-dimensional models. We resort to using power laws to more accurately describe the specific heat capacity, susceptibility and mean magnetization. For an infinite lattice, these power laws are defined as:

$$\begin{aligned}\langle|m|\rangle &\propto |T - T_c(L=\infty)|^{\beta} \\ C_V &\propto |T - T_c(L=\infty)|^{-\alpha} \\ \chi &\propto |T - T_c(L=\infty)|^{-\gamma}\end{aligned}$$

These power laws are valid only for temperatures near T_C. The exponents in the above expressions are known as critical exponents. These critical exponents are constants that depend only on the dimension of the system, the range of interaction and the spin dimension. [1]. For a ferromagnetic transition in the Ising model, these critical exponents are equal to $\beta = \frac{1}{8}$, $\alpha = 0$, and $\gamma = \frac{7}{4}$.[2] For an Ising model of an infinite lattice, the power laws are not dependent on ξ, however when looking at the power laws we need to describe our finite lattice, we need to introduce yet another critical exponent. This new critical exponent ν is logarithmic proportional to the correlation length:

$$\xi \propto |T - T_c(L=\infty)|^{-v}$$

ν is equal to 1 for our Ising model of a finite lattice. Since our lattice is finite, the largest possible correlation length is $\xi = L$, which is when the system has reached critical temperature $T = T_C(L)$. Inserting $T = T_C(L)$ into the ξ relation and using the scaling relation $T_C(L) - T_C(L=\infty) = aL^{-1}$, our new power laws describe our finite lattice as:

$$\begin{aligned}\langle|m|\rangle &\propto |T_C(L) - T_c(L=\infty)|^{\beta} = \left|aL^{-\frac{1}{\nu}}\right|^{\beta} = L^{-\frac{\beta}{\nu}} \\ C_V &\propto |T_C(L) - T_c(L=\infty)|^{-\alpha} = \left|aL^{-\frac{1}{\nu}}\right|^{-\alpha} = L^{\frac{\alpha}{\nu}} \\ \chi &\propto |T_C(L) - T_c(L=\infty)|^{-\gamma} = \left|aL^{-\frac{1}{\nu}}\right|^{-\gamma} = L^{\frac{\gamma}{\nu}}\end{aligned}$$

Where the constant a is a proportionality factor which is absorbed by the proportionality symbol.

With the power laws of a *finite* lattice defined, we will try to numerically estimate the critical temperature and compare it to the analytically result found by Lars Onsager in 1944. The analytical result were:

$$T_c(L=\infty) = \frac{2}{\ln(1+\sqrt{2})} J/k_B \approx 2.269 J/k_B$$

2.3 Markov chain Monte Carlo: Metropolis Algorithm

Monte Carlo methods are a wide range of computational algorithms typically used for simulating systems with, among others, uncertain variables, random systems, and or high dimensional systems. Simulations are performed via utilization of repeated random sampling. The physical process of a system is simulated directly by randomly sampling from a probability distribution function which describes our system, in our 2D Ising model case the probability for a system state $\vec{s}$ given a system temperature T is given by the Boltzmann distribution 2.1.

These samples' stationary distribution is a given probability distribution in the Markov chain Monte Carlo method. In other words we generate samples from a probability density function by recording samples in a Markov chain.

Markov chains are a random sequence of states for which the probability of the next state depends only on the current state. Via the Markov property

$$p(x_{i+1}|x_i, x_{i-1}, ...x_0) = p(x_{i+1}|x_i)$$

we generate a new candidate x' using a pdf that only depends on the current state x_i. We then apply some acceptance rule which in this case is the Metropolis rule, and repeat the process.

For the list of the samples $(x_1, x_2, ...)$ to end up being distributed according to a probability density function $p(x)$, the Metropolis rule algorithm ensures both ergodicity and a specific balance between the probabilities of changing states, proposal probability, and acceptance probability such that

$$Prob(x_i \to x') = T(x_i \to x')A(x_i \to x').$$

Thereby, we generate candidates x' according to the proposal probability $T(x_i \to x')$. Assuming the proposal probability is symmetric, that is to say

$$T(x' \to x_i) = T(x_i \to x')$$

the Metropolis rule for acceptance probability is thus given by

$$A(x_i \to x') = min(1, \frac{p(x')}{p(x_i)}) \tag{5}$$

3 Method

3.1 Energy in a system

In the Markov chain Monte Carlo Metropolis Algorithm, the probability of acceptance is equivalent to the ratio the probability of the proposed state and the probability of the current state(5).

For our 2D Ising model this acceptance probability can be expressed as

$$\frac{p(\vec{s'})}{p(\vec{s_i})} = \frac{e^{-\beta E(\vec{s'})}}{e^{-\beta E(\vec{s})}} = e^{-\beta \Delta E}$$

where $\Delta E = E_{\text{after}} - E_{\text{before}}$ for the energy shift due to flipping one random spin.

In an arbitrary 2D lattice of our spin configuration, when only one random spin is flipped it locally affects its four neighbouring spins. This results into only five possible values for ΔE. Table 2 below displays the change in energy in the case of a spin flipping:

E_{before}	E_{after}	ΔE
-4J	4J	8J
-2J	2J	4J
0	0	0
2J	-2J	-4J
4J	-4J	-8J

Table 2: Energy change of a single spin flip

By calculating all possible value for the change in energy of flipping one spin once and refer to that variable in memory rather than unnecessarily calling the exponential function every time, we are able to make our code more effective. As we change the size of the lattice the run time duration changes drastically. This then becomes very important and useful in our code.

3.2 Boundary Conditions

The boundary conditions are defined to mimic an infinite lattice. When reaching the end of the lattice in any direction, the spin on the opposite side will be used as a neighbouring spin. It would be like connecting the ends of all sides to each other.

For all position (i, j) in the lattice, the spin will effect the neighbours $(i, j+1)$ and $(i+1, j)$ such that calculating the energy $E(\vec{s})$ of the system will only count the energy of neighboring spins once.

However, for the spins near an edge or boundary of our lattice or matrix to call to the correct neighbouring spin, a function for correct index referencing is implemented, such that for example calling to an upper neighboring spin to a spin near on the boundary is technically calling to the spin at the end of the same column.

This function takes in an input integer and returns

$$\text{correct index} = (i + L + \rho) mod L.$$

The correct position of any neighbouring spin can be achieved by using the modulo operator, thus taking the remainder of the sum of the length of the lattice L, the distance to the next neighbouring spin ρ, and the spin position itself i when divided by L.

3.3 The Metropolis Algorithm

When a random spin is chosen to be flipped, we calculate the energy on the original spin, as well as the energy on the spin when it is flipped. We then must calculate the change in energy ΔE in the proposed new $\vec{s'}$ spin configuration and call to the correct value for the transitional probability $T(\vec{s_i} \rightarrow \vec{s'})$.

However, based on Table 2, we can simplify the change in energy ΔE as $2E(\vec{s_i})$ where $\vec{s_i}$ is the original spin. This makes the run time duration shorter by reducing the number of floating point operations, as well as making it easier to refer to the correct value of the transitional probability for the proposed change.

When a proposed new spin configuration is accepted, the energy needs to be updated by adding in the difference in energy, i.e. ΔE. The magnetization also needs to be updated by adding $2\vec{s'}$.

- We choose a random spin configuration and calculate its energy E_{before}.
- We suggest a new spin configuration by flipping a random spin and calculate the new energy E_{after}
- We calculate the change in energy:
  $\Delta E = E_{\text{after}} - E_{\text{before}} = 2E(\vec{s_i})$.
- if:
  - $\Delta E < 0$:
    We accept the new spin configuration and update the physical quantities. The system will go towards the lowest energy.
  - $\Delta E >= 0$
    We give the system a chance to still transition to the new spin configuration by generating a random number r uniformly distributed between [0,1].
    if: $r \leq e^{-\beta \Delta E}$ We accept the new spin configuration and update the physical quantities.
- Else: Keep the current configuration

- We repeat this process for N times for 1 Monte Carlo cycle.

4 Results

4.1 Numerical analysis: 2×2 Lattice

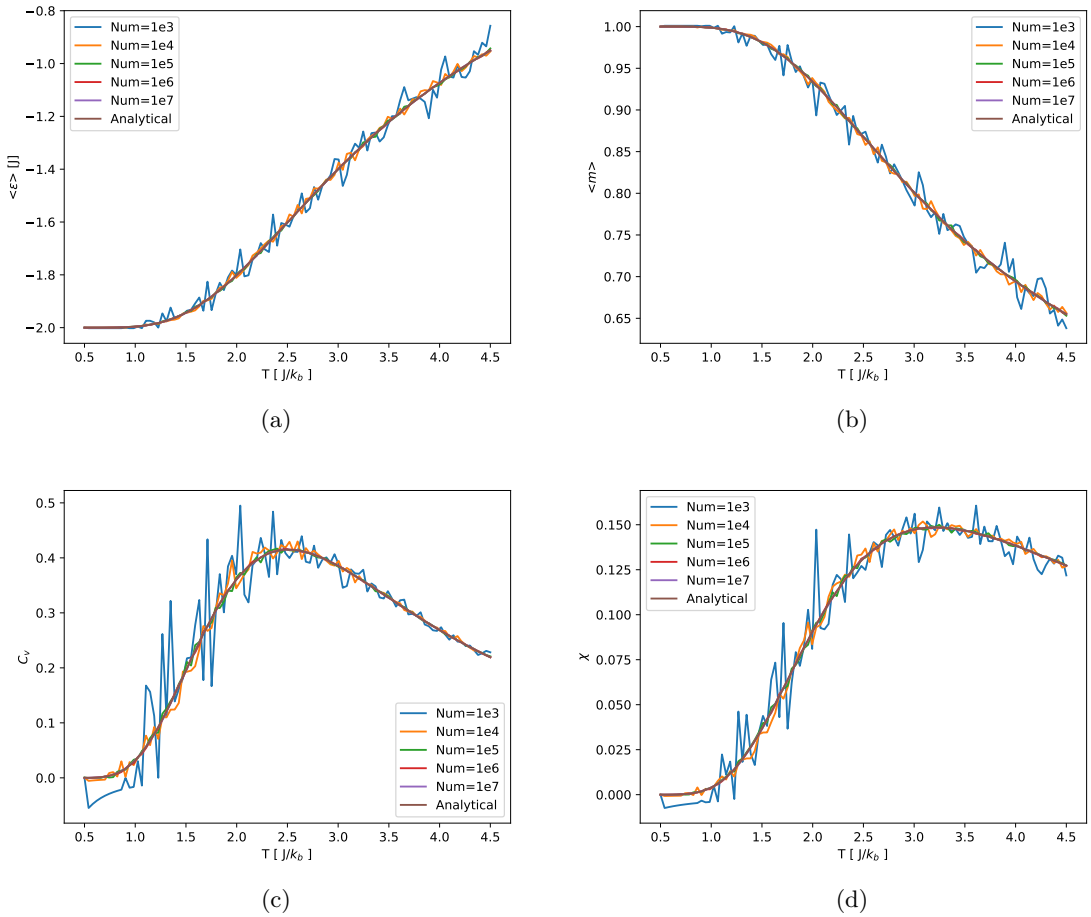


Figure 4: These plots shows us the different physical quantities as function of temperature; Mean energy in (a), mean absolute magnetization in (b), specific heat capacity in (c) and magnetic susceptibility in (d) are all plotted as a function of temperature from [0.5, 4.5]J/k_b. We plot and compare the analytical solution to these physical quantities to 5 numerical solutions with 5 different Monte Carlo cycles. We are observing these physical quantities for a temperature equal to 1 J/k_b and comparing these values with the analytical values, shown in table(3) and (4).

	$\langle\epsilon\rangle$	$\langle\lvert m\rvert\rangle$	C_v	χ
Analytical values	-1.99598	0.99866	0.03208	0.00401

Table 3: This table show us the analytical values for the mean energy, mean magnetization, heat capacity and the susceptibility. These values are calculated from a 2 x 2 Lattice when the temperature is equal to 1 J/k_b.

Monte Carlo cycles	$\langle\epsilon\rangle$	$\langle\lvert m\rvert\rangle$	C_v	χ
10^3	-1.98200	0.99400	0.14270	0.01786
10^4	-1.99480	0.99815	0.04149	0.00589
10^5	-1.99608	0.99875	0.03130	0.00357
10^6	-1.99627	0.99876	0.02977	0.00373
10^7	-1.99594	0.99865	0.03242	0.00402

Table 4: This table shows us the numerical values for the mean energy, mean magnetization, heat capacity and susceptibility for 5 different Monte Carlo cycles. These physical values are calculated for a 2 x 2 Lattice when the temperature is equal to 1 J/k_b.

4.2 Numerical analysis: 20×20 Lattice

4.2.1 Mean energy vs. Monte Carlo cycles

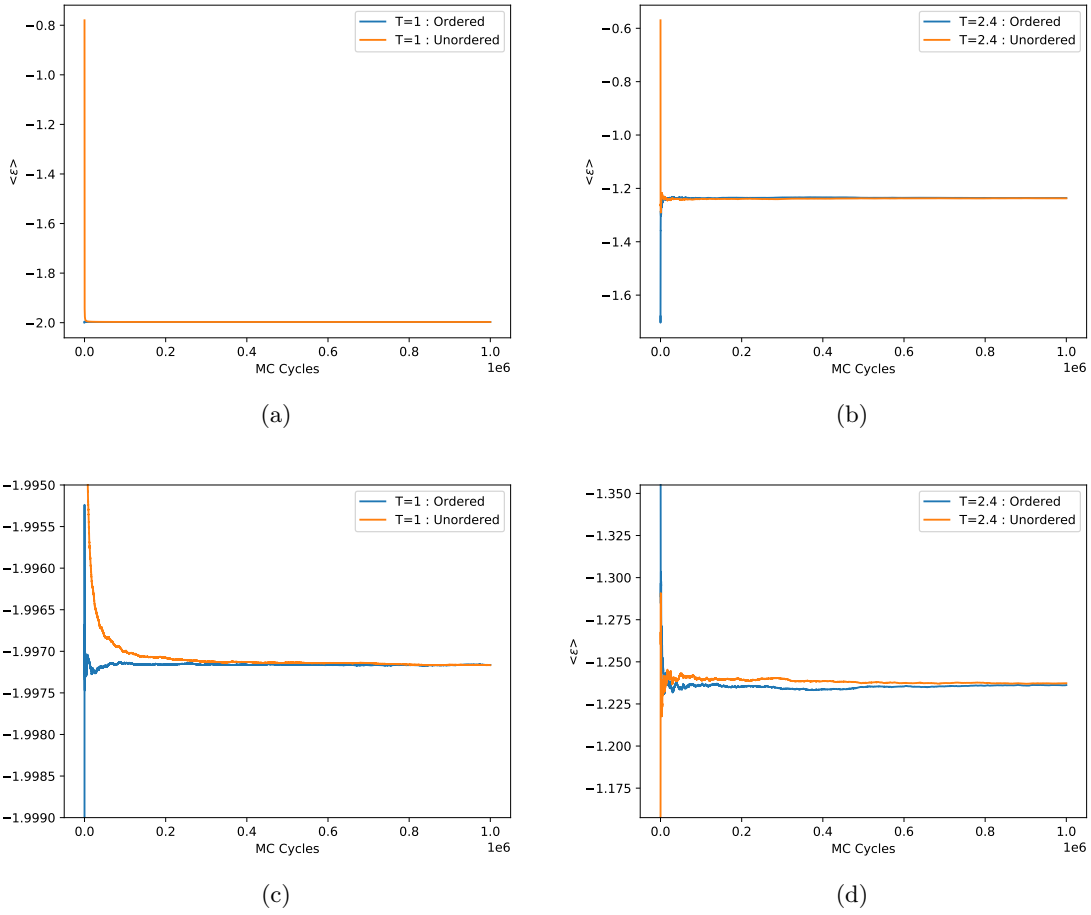


Figure 5: These plots shows the mean energy as a function of Monte Carlo cycles. The evolution of both, an originally ordered and unordered system is shown in each plot. (a) mean energy vs. Monte Carlo cycles for $T = 1.0\ J/k_b$, (b) mean energy vs. Monte Carlo cycles for $T = 2.4\ J/k_b$, (c) is a zoomed in plot of (a), (d) is a zoomed in plot of (b).

4.2.2 Mean magnetization vs. Monte Carlo cycles

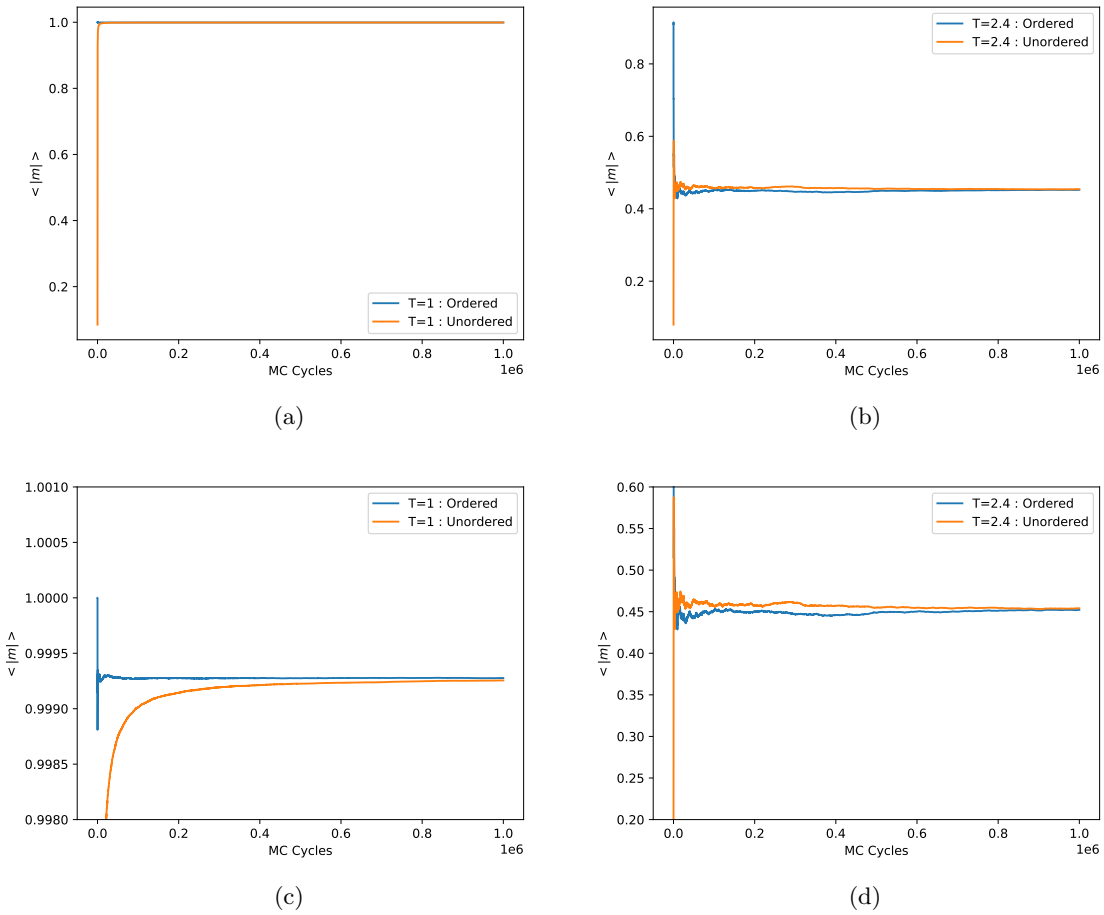
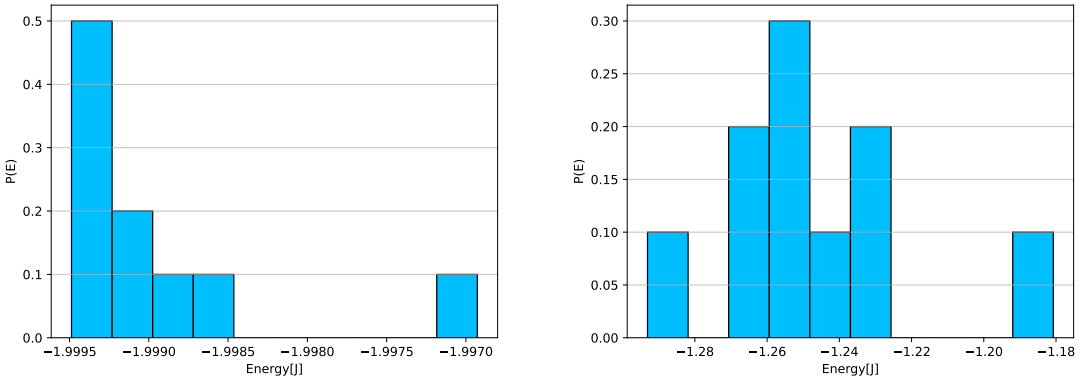


Figure 6: These plots shows the mean magnetization as a function of Monte Carlo cycles. The evolution of both, an originally ordered and unordered system is shown in each plot. (a) mean magnetization vs. Monte Carlo cycles for $T = 1.0\ J/k_b$, (b) mean magnetization vs. Monte Carlo cycles for $T = 2.4\ J/k_b$, (c) is a zoomed in plot of (a), (d) is a zoomed in plot of (b).

4.2.3 Probability distribution



(a) (b)

Figure 7: These plots shows us a probability distribution for a 20 x 20 Lattice as a function of the energy, E, for $T = 1\ J/k_b$ in (a) and $T = 2.4\ J/k_b$ in (b).

4.3 Phase transition of higher Lattice order

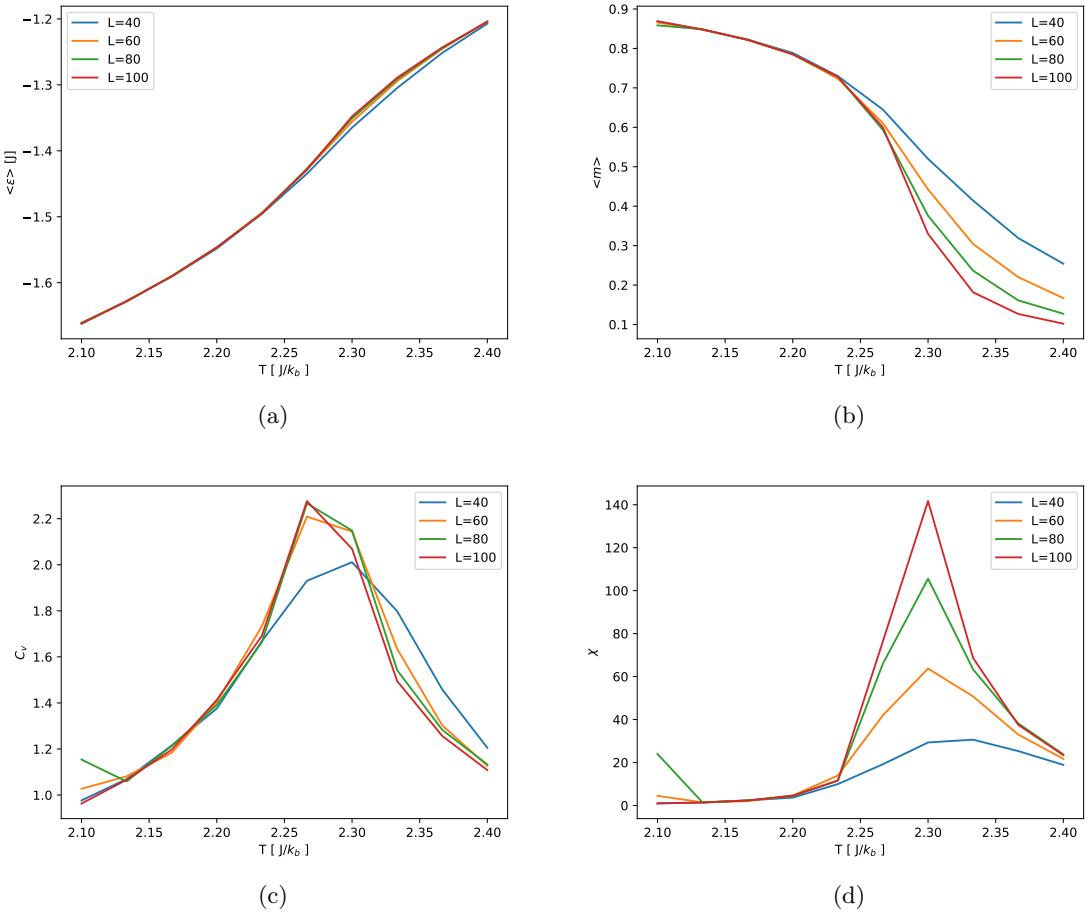
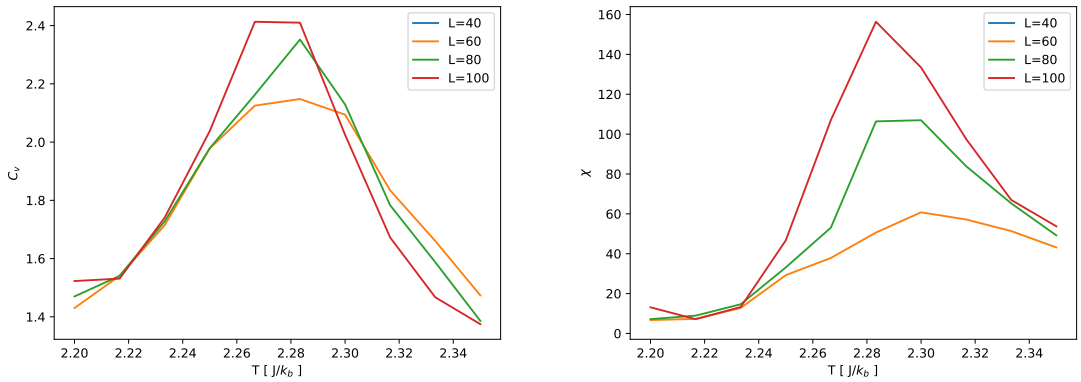


Figure 8: These plots shows us mean energy(a), mean magnetization(b), heat capacity(c) and susceptibility(d) as a function of temperature $[J/k_b]$ for four different Lattice sizes with given $\Delta T = 0.33$.



(a) (b)

Figure 9: These plots shows heat capacity(a) and susceptibility(b) as a function of temperature $[J/k_b]$ for four different Lattice sizes with given $\Delta T = 0.33$ for T = [2.2, 2.35].

4.3.1 Critical temperature

L	$T_c(L)$ for $\Delta T = 0.33$
40	2.2000
60	2.2833
80	2.2833
100	2.2666

Table 5: This table shows critical temperatures for different phase transitions, which were reached at temperature stepsize $\Delta T = 0.33$ as a function of L

5 Discussion

5.1 2×2 Lattice

In figure 4 we have multiple plots of different numerical values as a function of the temperature. We choose the range of the temperature to be $[0.5, 4.5]J/k_b$. When $T = 1\ J/k_b$ And we compare the value of $T = 1J/k_b$ to that of the analytical results. We notice that the more Monte Carlo cycles we take the closer the numerical results resemble that of the analytical results. The consequences of this is that the more cycle we take the more computational processing time is needed. However, this also leads to a more accurate result of the numerical calculations, which is also well portrayed in table. 3 and 4. We discover that the number of Monte Carlo cycles we need to get a good agreement with the analytical results begins around 10^5, but this also becomes better at 10^6 and best at 10^7.

5.2 20×20 Lattice

In figure 5. we compare the mean energy per spin against the number of Monte Carlo cycles. The transformation of both an ordered and unordered system is shown in each plot. In figure (5a) and (5c) the cycles are for a set temperature $T = 1.0\ J/k_b$, in figure (5b) and (5d) the same cycles were run, but for a higher temperature $T = 2.4\ J/k_b$. In the plots we are able to see that the mean energy for for both temperature starts at a peek and gradually drops before it starts stabilizing around $5.0 \cdot 10^5$ Monte Carlo cycles. However, the more cycles we perform the closer our systems reaches equilibrium. So, the more Monte Carlo cycles, the better the values for our physical quantities will be in exchange for computational processing time. It reaches equilibrium because for each spin we get a change in the mean energy and the system is trying to rearrange it self in a way that allows all the spins to point the same direction. For a temperature $T = 2.4\ J/k_b$ the vibrations of the particles becomes rigorous as a consequence of higher temperature, this ultimately leads to the time duration of which we reach equilibrium becomes a little longer than at a lower temperature.

In figure 6 we plot the mean magnetization against the number of Monte Carlo

cycles performed. We perform the same process for the mean magnetization as for the mean energy per spin. Calculating for both an ordered and unordered spin orientation, and for a temperature $T = 1.0\ J/k_b$ in figure (6a) and (6c), as well as for a temperature $T = 2.4\ J/k_b$ in figure (6b) and (6d). Compared to the mean energy per spin, we encounter the same trends, the only difference being that the magnetism drops as we reach higher temperatures. The reason for this being that a magnet is most optimal when all of the spins are pointing upwards.

5.3 Probability distribution

In figure(7) we create plots of the probability distribution as a function of the energy. In figures (7a) we see that there is a peak at $-1.9995J$. This occurs because the probability of finding a spin in that state is high. A consequence of this is low variance. The reason for it's low variance being that the temperature is at $T = 1.0\ J/k_b$. In figure (7b) we change the temperature to $T = 2.4\ J/k_b$ for this temperature we see that the peaks change and the probability is spread out. This is due to the temperature is now higher, which leads to a overall more vibration between the particles and higher variances in the overall system. In our plot we notice that our probability distribution is somewhat off, due to some numerical calculation errors the results are not as expected. The general idea of variance still applies as the change of temperature has an effect on the energy in the system.

5.4 Phase Transition

In figure 9 we take a look at the heat capacity and the susceptibility as a function of temperature, this is seen in figure (9c) and (9d). Now taking to account the phase transition for 4 different lattice sizes, we observe the trend following the plots in L = 40×40, 60×60, 80×80 and 100×100 size lattices. We can see that once we reach a peek in figure (9d) the susceptibility then starts to decrease. This shows a phase transition as the magnet goes from a ferromagnetic state to a paramagnetic state, this is due to the presence of unpaired spins. The same goes for the heat capacity, in the plot it reaches a peak and then starts to decrease. We notice that the larger the lattice the faster it reaches a peak and that also leads to rapid decreasing of the heat capacity and the susceptibility. The values of the critical temperature for each lattice size is written in table 5.

5.5 Issues

Due to being unable to fully utilize OpenMPI to parallelize our code, we ran all the different lattice sizes in series but on 4 different computers, and held ourselves to using 500000 Monte Carlo cycles over 10 steps for temperature. However, we compensated by running a second scan where the graphs changed rapidly with 10 steps in temperature.

If we were to have more time we would run our code for higher number of Monte Carlo cycles and with more steps, to get a numerical value closer to the analytical values of Lars Onsager. This is something we will take with us.

6 Conclusion

What we are able to accumulate from this is an understanding of all the little pieces that ad up to a final goal, we are now able to utilize the Markov chain Monte Carlo method to simulate a random system that otherwise would be difficult to sample. We are also able to employ the Ising model to simulate a phase transition of magnetic elements as well as discover the physical values and visualize the way spins act upon neighbouring spins in a lattice of a given size N.

This has given us a good basic knowledge of when and how both mean energy and mean magnetism behave when they reach an equilibrium, as well as how the heat capacity and susceptibility changes and affects those elements depending on the temperature they are exposed to. We can conclude with that we have shown how we are able to get the values for $\langle E \rangle$, $\langle M \rangle$, C_v and χ.

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A Appendix

A.1 Source code

All the source code is located in this GitHub Repository

A.2 Sum of quantities for all possible states of a 2×2 system:

Spin state +1	Total E	Total M	Degeneracy
0	-8J	-4	1
1	0	-2	4
2	0	0	4
2	8J	0	2
3	0	2	4
4	-8J	4	1

Table 6: A table showing the sum of all possible states and important quantities for a 2×2 lattice with periodic boundary conditions

A.3 Defining the Partition Function Z for a 2×2 system:

$$Z = \sum_{i=0}^{16} e^{-\beta E(\vec{s}_i)} \tag{6}$$

Based on Table 6, this gives us

$$Z = e^{-\beta 0J} \cdot 4 \cdot 3 + 2 \cdot e^{8\beta J} + e^{-8\beta J} \tag{7}$$

$$Z = 12 + 2 \cdot e^{8\beta J} + 2e^{-8\beta J} \tag{8}$$

where the two exponential terms can be simplified into one cosh hyperbolic function.

$$Z = 12 + 4cosh(8\beta J) \tag{9}$$

$$Z = 4(3 + cosh(8\beta J) \tag{10}$$

A.4 Defining the probability for a system state $\vec{s}$ for a 2×2 system:

$$p(\vec{s}) = \frac{1}{Z}e^{-\beta E(\vec{s})} \tag{11}$$

Inserting in Z from the previous definition, we get

$$p(\vec{s}) = \frac{e^{-\beta E(\vec{s})}}{4(3 + cosh(8\beta J)} \tag{12}$$

A.5 Calculating the expected value of the energy per spin $\langle\varepsilon\rangle$ for a 2×2 system:

Per definition, the expected value is the generalization of the weighted average of a data set. Thus by deriving the general formula for the expected value of energy per spin for a 2×2 system,

$$\langle\varepsilon\rangle = \frac{1}{N}\sum_{i=0}^{2^N} E(\vec{s})p(\vec{s}) \tag{13}$$

we get

$$\langle\varepsilon\rangle = \frac{1}{ZN}\sum_{i=0}^{16} E(\vec{s_i})e^{(-\beta E(\vec{s}_i))}. \tag{14}$$

Using Table 6 to calculate for all possible micro-state, we are left with

$$\langle\varepsilon\rangle = \frac{1}{NZ}(-8J \cdot 2e^{8\beta J} + 8J \cdot 2e^{-8\beta J}), \tag{15}$$

which can further be derived to

$$\langle\varepsilon\rangle = \frac{-8J}{ZN}(2e^{8\beta J} - 2e^{-8\beta J}) = \frac{-8J}{NZ}(4sinh(8\beta J)) \tag{16}$$

and

$$\langle\varepsilon\rangle = \frac{-32J \cdot sinh(8\beta J)}{4(12 + 4 \cdot cosh(8\beta J))}, \tag{17}$$

thus giving us the final analytical definition for the expected value $< \epsilon >$ for a 2×2 system

$$\langle\varepsilon\rangle = \frac{-2J \cdot sinh(8\beta J)}{3 + cosh(8\beta J)}. \tag{18}$$

A.6 Calculating expected value of the energy per spin squared $\langle \varepsilon^2 \rangle$ for a 2×2 system:

Similar to the derivations above, we start with the general formula for the expected value, except this time we calculate the energy per spin squared. Thus giving us

$$\langle \varepsilon^2 \rangle = \frac{1}{N^2} \sum_{i=0}^{2^N} E^2(\vec{s}) p(\vec{s}). \tag{19}$$

Utilizing Table6, we arrive to

$$\langle \varepsilon^2 \rangle = \frac{1}{N^2 Z} (64J^2 \cdot 2e^{8\beta J} + 64J^2 \cdot 2e^{-8\beta J}) \tag{20}$$

and

$$\langle \varepsilon^2 \rangle = \frac{64J^2 \cdot 4cosh(8\beta J)}{16(4(3 + cosh(8\beta J)))}, \tag{21}$$

or simply

$$\langle \varepsilon^2 \rangle = \frac{4J^2 cosh(8\beta J)}{3 + cosh(8\beta J)}. \tag{22}$$

A.7 Calculating expected value of the absolute value of the magnetization per spin $\langle |m| \rangle$ for a 2×2 system:

$$\langle |m| \rangle = \frac{1}{N} \sum_{i=0}^{2^N} |M(\vec{s_i})| p(\vec{s_i}) \tag{23}$$

$$\langle |m| \rangle = \frac{1}{NZ} \sum_{i=0}^{2^N} |\vec{s_i}| e^{-\beta E(\vec{s}_i)} \tag{24}$$

Inserting our values:

$$\langle |m| \rangle = \frac{1}{NZ} \Big(8e^{\beta 8J} + 16 \Big) = \frac{8(e^{\beta 8J} + 2)}{4(4(3 + cosh(8\beta J)))} \tag{25}$$

which ultimately leads to

$$\langle |m| \rangle = \frac{e^{8\beta J} + 2}{2(3 + cosh(8\beta J))} \tag{26}$$

A.8 Calculating expected value of the magnetization per spin squared $\langle m^2 \rangle$ for a 2×2 system:

$$\langle m^2 \rangle = \frac{1}{N^2} \sum_{i=0}^{2^N} M^2(\vec{s}) p(\vec{s}) \tag{27}$$

$$\langle m^2 \rangle = \frac{1}{N^2 Z} \sum_{i=0}^{2^N} \vec{s_i}^2 e^{-\beta E(\vec{s}_i)} \tag{28}$$

$$\langle m^2 \rangle = \frac{1}{N^2 Z}(16 \cdot e^{8\beta J} + 16 \cdot e^{8\beta J} + 4 \cdot e^0 \cdot 4 + 4 \cdot e^0 \cdot 4) \tag{29}$$

$$\langle m^2 \rangle = \frac{1}{N^2 Z}(32e^{8\beta J} + 32) = \frac{32(e^{8\beta J} + 1)}{16(4(3 + cosh(8\beta J)))} \tag{30}$$

which ultimately leads to

$$\langle m^2 \rangle = \frac{e^{8\beta J} + 1}{2(3 + cosh(8\beta J))} \tag{31}$$

A.9 Defining the Specific Heat Capacity of a 2×2 System:

$$C_v = \frac{1}{k_B T^2}(\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2) \tag{32}$$

$$C_v = \frac{1}{k_B T^2}(\frac{4J^2 cosh(8\beta J)}{3 + cosh(8\beta J)} - (\frac{-2J \cdot sinh(8\beta J)}{3 + cosh(8\beta J)})^2) \tag{33}$$

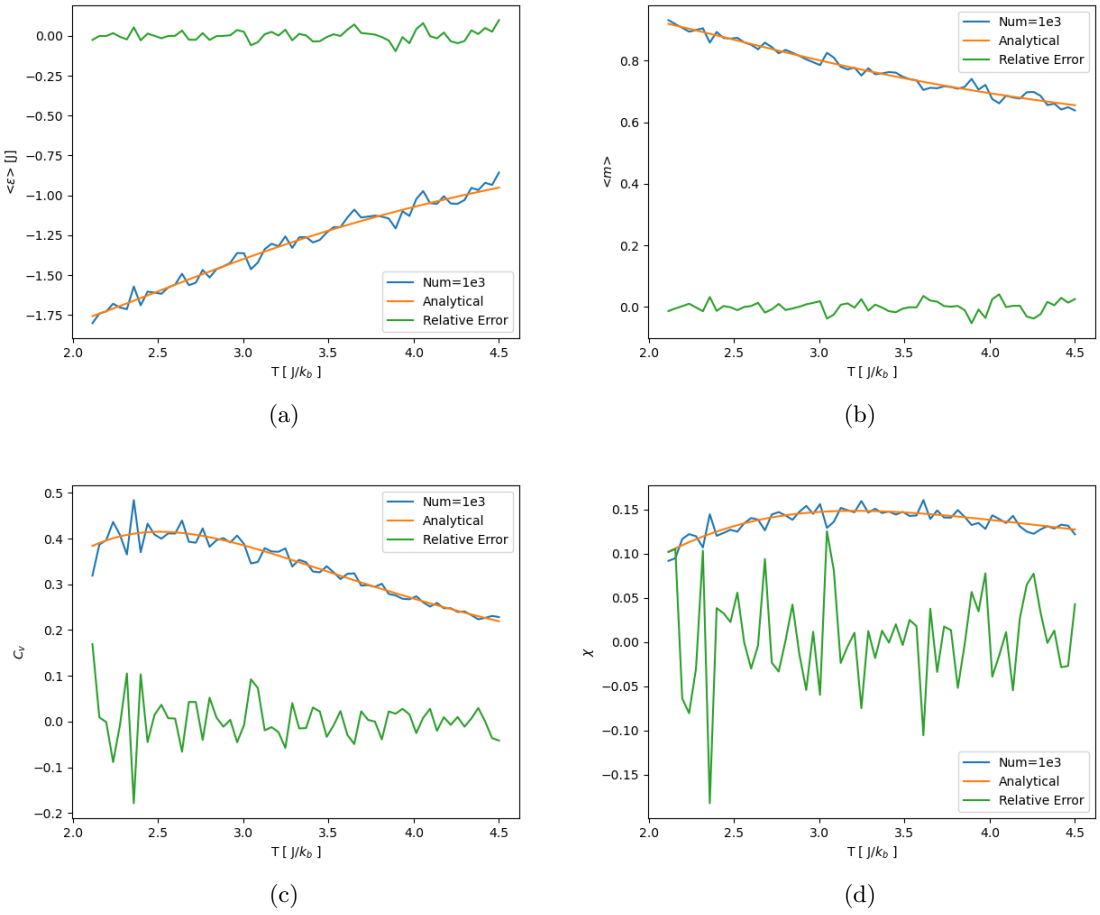
A.10 Defining the Magnetic susceptibility of a 2×2 System:

$$\chi = \frac{1}{k_B T}(\langle m^2 \rangle - \langle m \rangle^2) \tag{34}$$

$$\chi = \beta(\frac{e^{8\beta J} + 1}{2(3 + cosh(8\beta J))} - (\frac{e^{8\beta J} + 2}{2(3 + cosh(8\beta J))})^2) \tag{35}$$

A.11 Relative Error

A.11.1 Monte Carlo cycles 10^3



(a) (b)

(c) (d)

Figure 10: Relative Error for 10^3 MC cycles as a function of Temperature T

A.11.2 Monte Carlo cycles 10^4

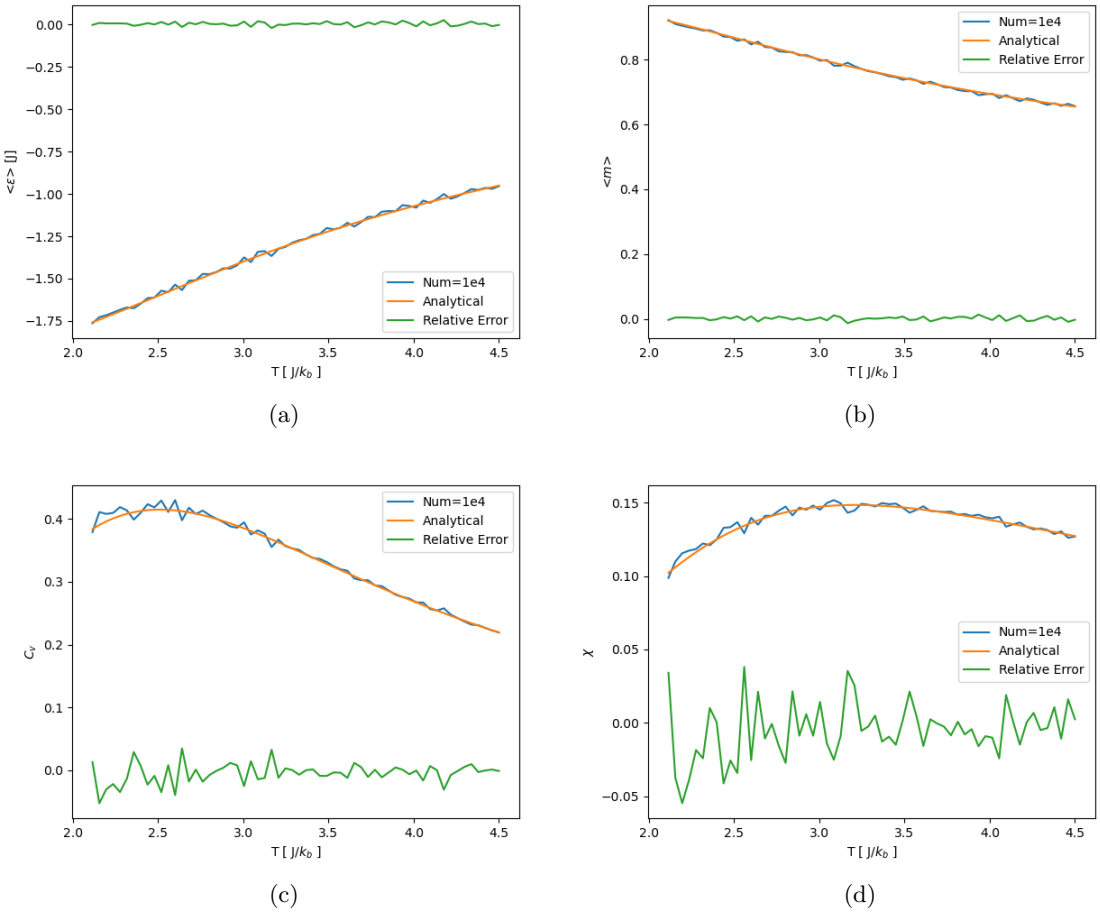
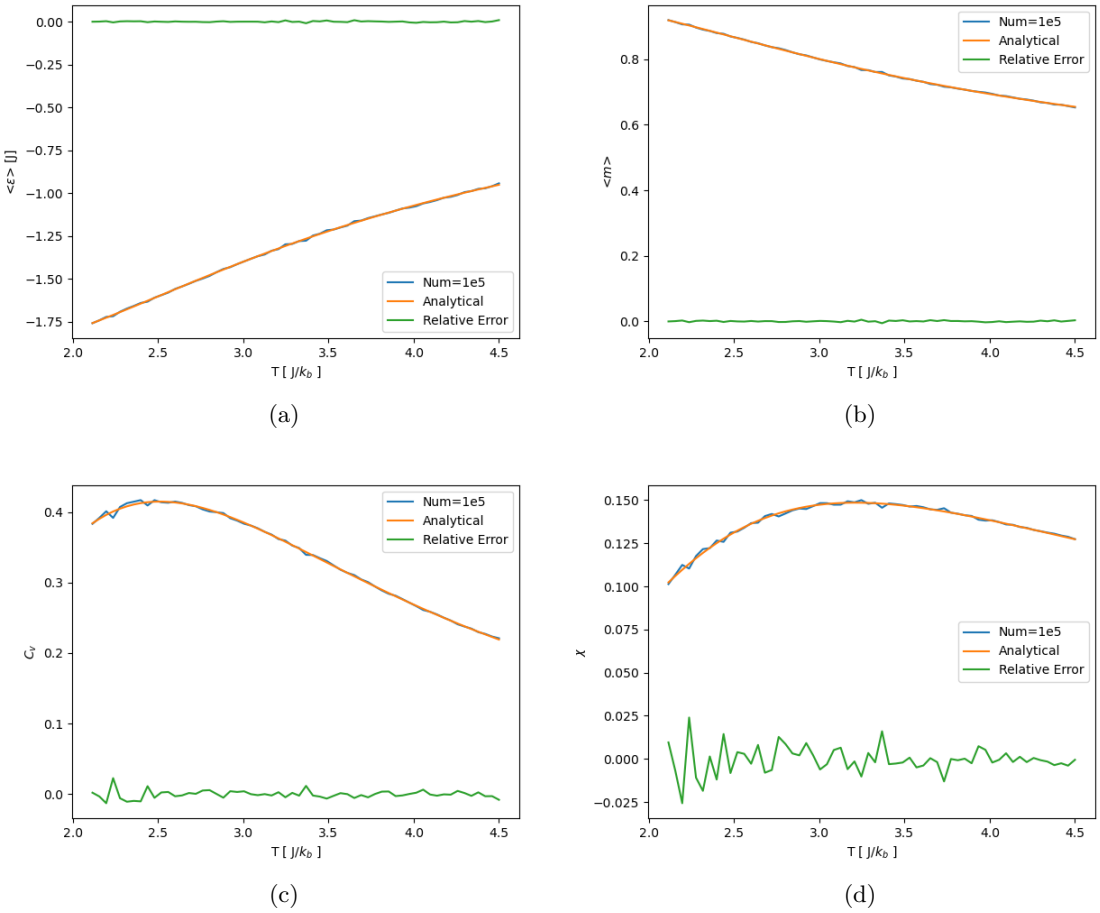


Figure 11: Relative Error for 10^4 MC cycles as a function of Temperature T

A.11.3 Monte Carlo cycles 10^5

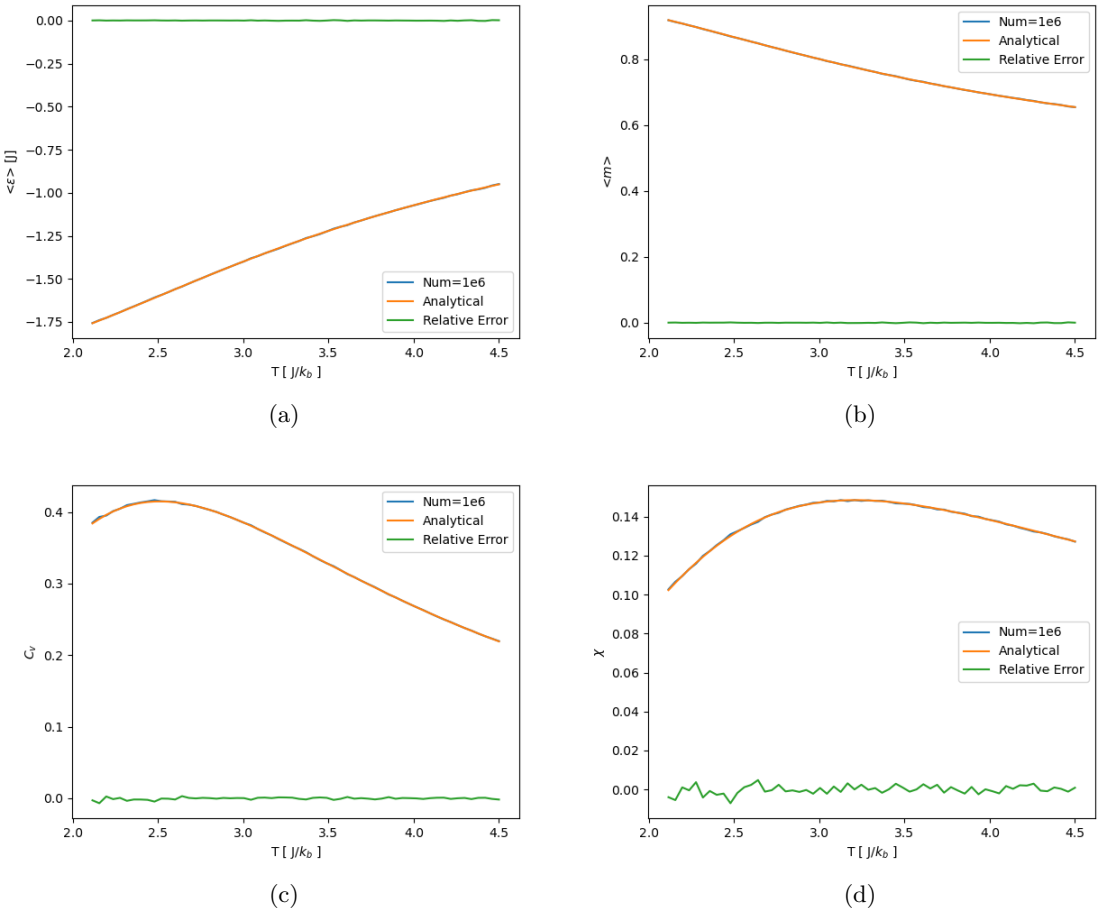


(a) (b)

(c) (d)

Figure 12: Relative Error for 10^5 MC cycles as a function of Temperature T

A.11.4 Monte Carlo cycles 10^6

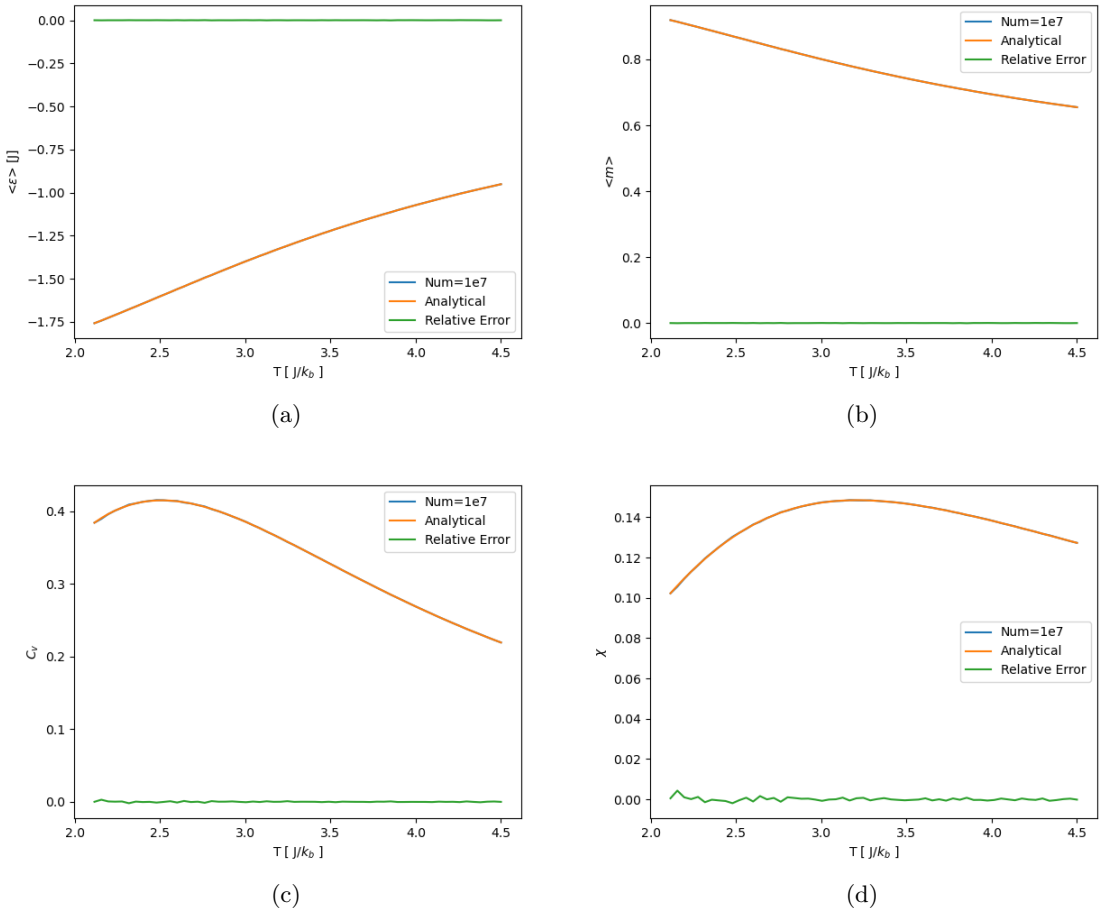


(a) (b)

(c) (d)

Figure 13: Relative Error for 10^6 MC cycles as a function of Temperature T

A.11.5 Monte Carlo cycles 10^7



(a) (b)

(c) (d)

Figure 14: Relative Error for 10^7 MC cycles as a function of Temperature T