FYS3150: Project 4: Studies of phase transitions in magnetic systems

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November 19, 2019

Abstract

The scope of this report is aimed at studying phase transitions in magnetic systems by using the well known Ising model to simulate a two dimensional lattice. By varying lattice size, temperature and the number of Monte-Carlo cycles the values of interest, mean energy, mean magnetization, susceptibility and specific heat, were calculated and their evolution in respect to number of Monte-Carlo cycles, was studied. Periodic boundary conditions was utilized.

Looking at phase transition of lattices of different sizes we found that the critical temperature in the thermodynamical limit was found to be $T_c = 2.262$

By parallelizing the code a near perfect speed up was achived.

1 Introduction

To continously innovate and improve technology and materials it is important to understand how external parameters such as temperature and magnetic fields affect the materials abilities and performance. By employing a simple and well known model, The Ising model, to simulate small magnetic systems, which have analytical solutions, we can simulate larger systems by adding layers of complexity to the model and evaluate our results in comparison with thermodynamical theory. The object is to better understand the phenomenon of phase transitions, and if their occurrence can be predicted.

To simulate how a larger magnetic system is affected by external parameters we start by looking at the simplest case of the Ising model, a two dimensional lattice of spins with no external magnetic field applied to it for which we have a simple expression for the energy of the system. Given an expression for the systems energy we can compute the other quantities of interest. In order to tell if our model sufficient to tackle larger systems the amount of Monte-Carlo cycles needed for the computed values are in good

agreement with the analytical ones. After the system reached a steady state we counted the most probable states.

In our study of phase transitions we wish to analyse the behaviour of the two dimensional Ising model near the critical temperature, at which phase transitions occur, for different sized lattices. In order to do this as efficiently as possible the code was parallelized. The main objective is to estimate the critical temperature using the data from our model.

2 Method

2.1 The Ising Model

To model a magnetic system in two dimensions of size L we use the Ising model to simulate the system. The system, containing N spins in a lattice configuration, can have a variety of different microstates based on the configurations of each individual spin. Each spin, s_k, is either ± 1. For such a system the energy, E, can simply be written as:

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

where the term $< kl >$ indicates that the first sum is summing over all the closest neighbours, s_l, of a spin s_k. J is a constant which describes the interaction between neighboring spins, while B is a magnetic field externally applied to the system. The N spins will set up a magnetic moment which the magnetic field will interact with. For low temperatures, which implies $J > 0$, a phenomenon called spontaneous magnetization occurs. What happens is that the system seeks the lowest energy configuration, in this case that is when all neighbouring spins, s_l, is aligned. When a magnetic field, B, is applied it will interact with the magnetic moment of the spins and possibly change the alignment of spins which are separated from a spin s_k by a macroscopic distance. In our model the external magnetic field, B, is always zero so the expression for the energy becomes:

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

In our studies we want to calculate the mean energy, $\langle E \rangle$ and the mean magnetization, $\langle M \rangle$. To accomplish this we use a probability distribution, the Boltzmann distribution, to express the probability of the system being in a specific configurtion, i. The Boltzmann distribution, $P_i(\beta)$, is given as:

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \, , \tag{3}$$

where Z is the partition function which describes the statistical properties of a system which has reached a thermodynamic equilibrium. $\beta = 1$, where k is the Boltzmann constant and T is a given temperature. The partition function is expressed by the following sum over all M microstates:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \ . \tag{4}$$

Because we use the Metropolis algorithm to compute the probability of finding the system in a state i we do not need to compute the partition function at all as long as the method used, when equilibrium is reached, to select spin configurations results in the Boltzmann distribution. The algorithm also has to be ergodic and satisfies the principle of detailed balance. The principle of detailed balance for Boltzmann distribution says that:

$$\frac{w_i}{w_j} = exp(-\beta(E_i - E_j)) \ , \tag{5}$$

where w_i is the probability of finding the system in a state i, and w_j is the probability of finding the system in a state j. E_i and E_j are the energies for the respective states i and j. Thermal equilibrium is assumed.

When using the Ising model it is important to utilise the right boundary conditions for a two dimensional system. Meaning that the number of closest spin neighbours, s_l differs with with the dimensionality of the system. In two dimensions a spin s_k has four closest neighbours, s_l. The number of possible microstates, M, is given by 2^N for a given $N = L \times L$ latteice in two dimensions. When simulation a two dimensional system periodic boundary conditions are used. This sets the spin s_l, which is to the right of spin s_N, to have value s_1(the value of the first spin in the lattice). It also sets the value of the spin to the left of s_N to have the same value as spin s_N. As an example take the simple case of $N = 2$:

$$E = -J \sum_{j=1}^{N-1} s_j s_{j+1} = -J(s_1 s_2 + s_2 s_1) \ , \tag{6}$$

and we get $2^N = 4$ different spin configuration with the energies $-2J, 2J, 2J$, and $-2J$.

2.2 Analytical Solution for L = 2

For the two dimensional system of four spins in a two by two square we can find analytical values for the mean energy, mean absolute value of the magnetization, specific heat capacity and the magnetic susceptibility. This

is done by looking at the canonical ensemble. Here we can find a partition function

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}. \tag{7}$$

Here the partition function is a sum of all the M microstates of the system. For our two dimensional lattice with L = 2 we get that $M = 16$ so then the partition function becomes

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

So now we can use this partition function to calculate the values we want to know. First we can find the mean energy which is given by

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{16} E_i e^{-\beta E_i} = \frac{J}{Z} \left(16e^{-8J\beta} - 16e^{8J\beta} \right) \tag{9}$$

The expression for the mean squared energy is very similar where the only difference is that the energy, E_i, in the sum is squared. So with this we can find the specific heat capacity of the system using the variance of the energy. This gives

$$C_v = \frac{1}{k_b T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{10}$$

Using the same method as for the energy we can find the mean absolute value of the magnetization with

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{1} 6|M_i| e^{-\beta E_i} = \frac{1}{Z} \left(8e^8 + 16 \right) \tag{11}$$

Furthermore we can find the susceptibility with the same method we did for finding the heat capacity. Then it is given by

$$\chi = \frac{1}{k_b T} \left(\langle M^2 \rangle - \langle |m| \rangle^2 \right) \tag{12}$$

2.3 The Metropolis Algorithm

The Ising model requires a probability distribution function. In our case this is the Bolzmann distribuiton function. By using the Metropolis algorithm we can end up with the right distribution without using a partition function. This is done by utilising two probabilities. A probability for proposing a move from a state i to a state j, $T_{i \to j}$, and a probability for

accepting a move from a state i to a state j, $A_{i\to j}$. The acceptance probability is here:

$$A_{i\to j} = e^{-\beta(E_i - E_j)} \ , \tag{13}$$

with $E_i - E_j = \Delta E$ as the energy difference between the states i and j. For every Monte-Carlo iteration over the lattice ΔE is computed so we can find $A_{i\to j}$ for flipping a spin. When flipping an arbitrary spin in the lattice we must compute the energy difference, ΔE, between the new state, j, and the old state i in order to check if the move to the new state should be accepted:

$$E_i - E_j = -J \sum_{<kl>}^{N} s_k^i s_l^i + J \sum_{<kj>}^{N} s_k^j s_l^j = J \sum_{<kl>}^{N} s_k^j (s_l^j - s_l^i) \ . \tag{14}$$

If $s_l^i = 1$ then $s_l^j = -1$, and if $s_l^i = -1$ then $s_l^j = 1$, thus $s_l^j - s_l^i = 2$. Regardless of s_l^i avlue before the flip the closest neighbours, s_k, keep their values so $s_k^i = s_k^j = s_k$. This gives us a simple expression:

$$\Delta E = 2J s_l^i \sum_{<k>}^{N} s_k \ , \tag{15}$$

which entails that the sum runs over the closest neighbours, k, of an arbitrary spin ,s_l^i, in the lattice. What remains is to evaluate the acceptance probability in relation to a randomly generated number, α, so if the following is true the move from state i to j is accepted:

$$A_{i\to j} \geq \alpha \ , \tag{16}$$

and the lattice is updated and the thermodynamic quantities of interest are computed for this new configuration of the system. The algorithm can be summarized as follows:
1: Choose an arbitrary spin in the lattice at a given configuration/state, i.

2: Flip the spin and compute the energy of the new state, E_j, and compare it to the energy of the intioal state E_i.

3: Accept the move to state j if $\Delta E \leq 0$, this is to ensure that we move towards the systems minimal energy at a given temperature. If the condition is met; proceed to step 6.

4: Calculate the acceptance probability $A_{i\to j} = e^{(} - \beta \Delta E)$.

5: Generate a random number α. If $A_{i\to j} \geq \alpha$ the move to the new state is accpted. If not, then the initial configuration is kept.

6: Compute the thermodynamic quantities of interest, the expectation values, and update them.

7: Repeat steps 2-6 to ensure a good representation of states.

8: Divide the computed expectation values by the number of Monte-Carlo cycles(sweeps of the lattice) used. To find the quantities per spin just divide by the number of spins.

2.4 Parallelization

We also wanted to parallize the code so that we could achieve a significant speed up by using several processors on the computer for different tasks. This was achieved with openMPI. Here we could then choose the amount of cores we wanted to use and thereby how much speedup we could get. For the parallelization of our code we wanted to divide the montecarlo cycles between the different cores. The computer which ran the parallelized code had two cores capable of running at 2.3GHz. Each core perfomed $L/2$ computations which where then summed and taken the average of to find the thermodynamic values of interest.

2.5 Linear regression to approximate critical temperature when $L \to \infty$

To approximate the critical, T_c at the thermodynamic limit $L \to \infty$ linear regression is utilized. The critical temperature is defined as the temperature at which phase transitions occur in a medium. By regarding a plot of specific heat, C_v versus Temperature, T, we find the highest values for specific heat, $C_{v_{max}}^L$, for different lattice sizes, L. By plotting the respective max values(y-axis) against the max values divided by L(x-axis) and using a linear regression we get a straight line. The y value at which the line intersects with $x = 0$ is the approximate critical temperature, T_c. The larger L is the closer we get to the right critical temperature, which is why the linear regression is only an approximation as we only run the computations for a few selected L values.

3 Results

We used the analytical results for the $L = 2$ case and compared it with our results using $T = 1, k_b = 1$ and $J = 1$. We also looked at the results per spin so every result was divided by $L^2 = 4$. This gave us the results in table 1.

Below, in figures 1 and **??** we see the acceptance rate as a function of the number of Monte Carlo cycles. In the ordered case all the initial spins are set to -1.

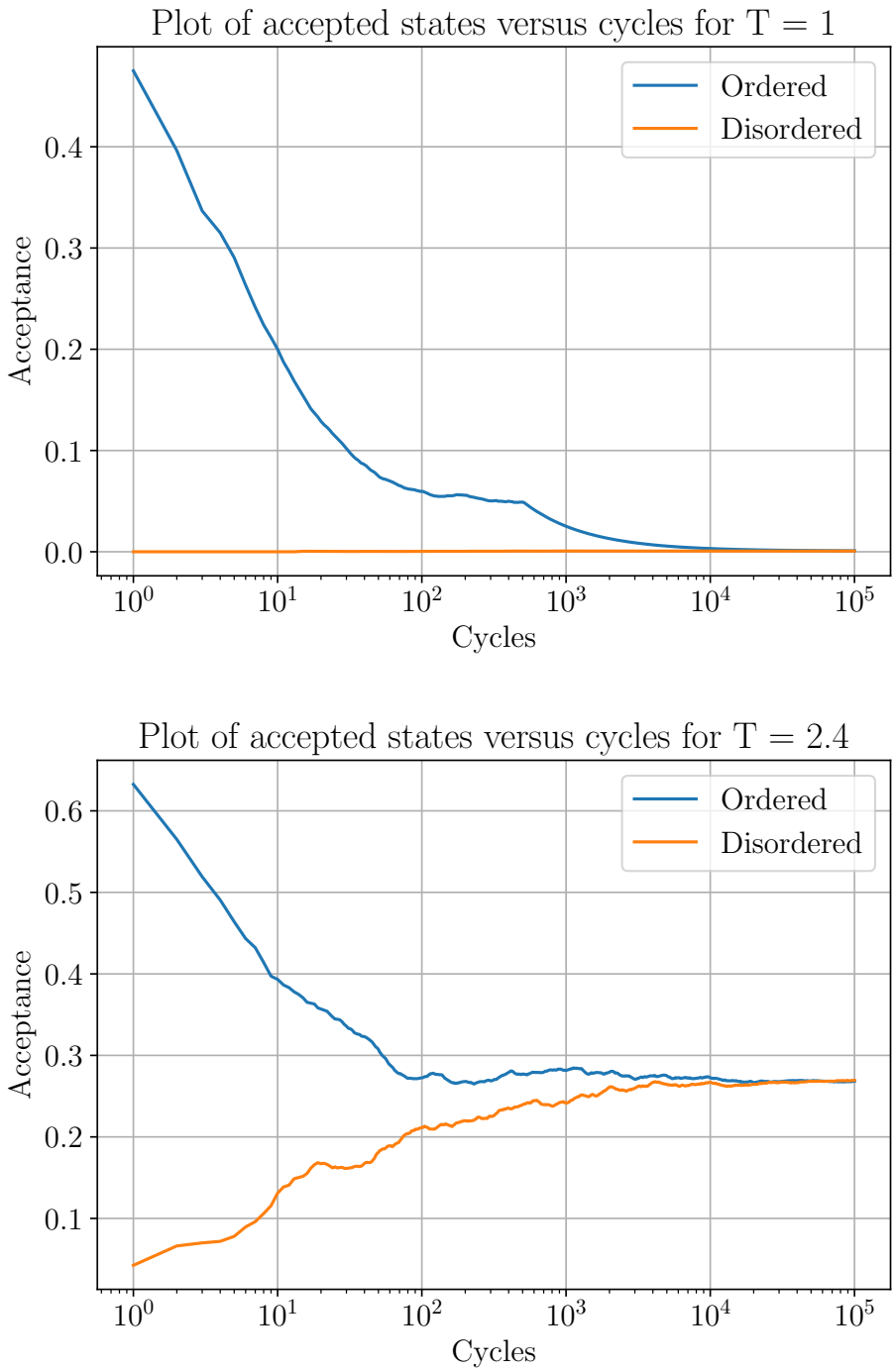

Figure 1: Average number of accepted configurations as functions of cycles for temperature

Table 1: Analytical vs numercal values for the $L = 2$ case

	Analytical	Numerical	Error
$\langle E \rangle$	-1.99598	-1.99564	0.00034
C_v	0.03183	0.03480	0.00297
$\langle \lvert M \rvert \rangle$	0.99866	0.99862	0.00004
χ	0.00409	0.00394	0.00015

Figure 3: Analytical and numerical results for L=2. The numerical results were produced running the Metropolis algorithm for 10^6 cycles.

In figure 5 and **??** we see the energies as a function of time. In the $T = 1$ case the ordered lattice starts out in its equilibrium position. For $T = 2.4$ they both reach equilibrium at about 10^4 cycles. This is consistent with figure 1 where we see that the number of accepted states stops changing slightly after 10^4 for $T = 2.4$ and approximately at 10^4 for $T = 1$.

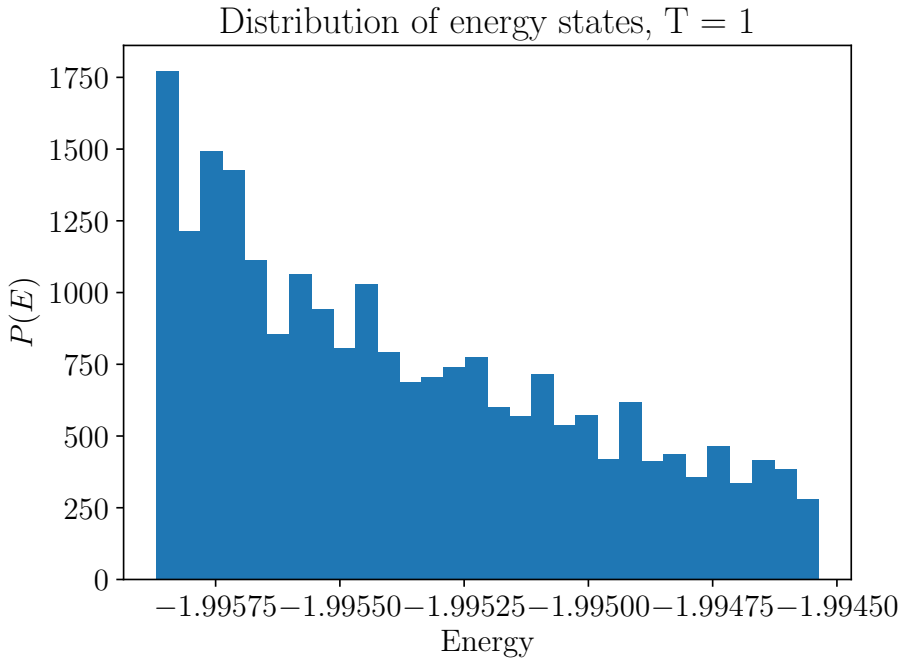

Figure 2: Histogram showing the distribution of energy states for $T = 1$ after equilibrium has been reached. The variance was $\sigma^2 = 1.36 \times 10^{-7}$.

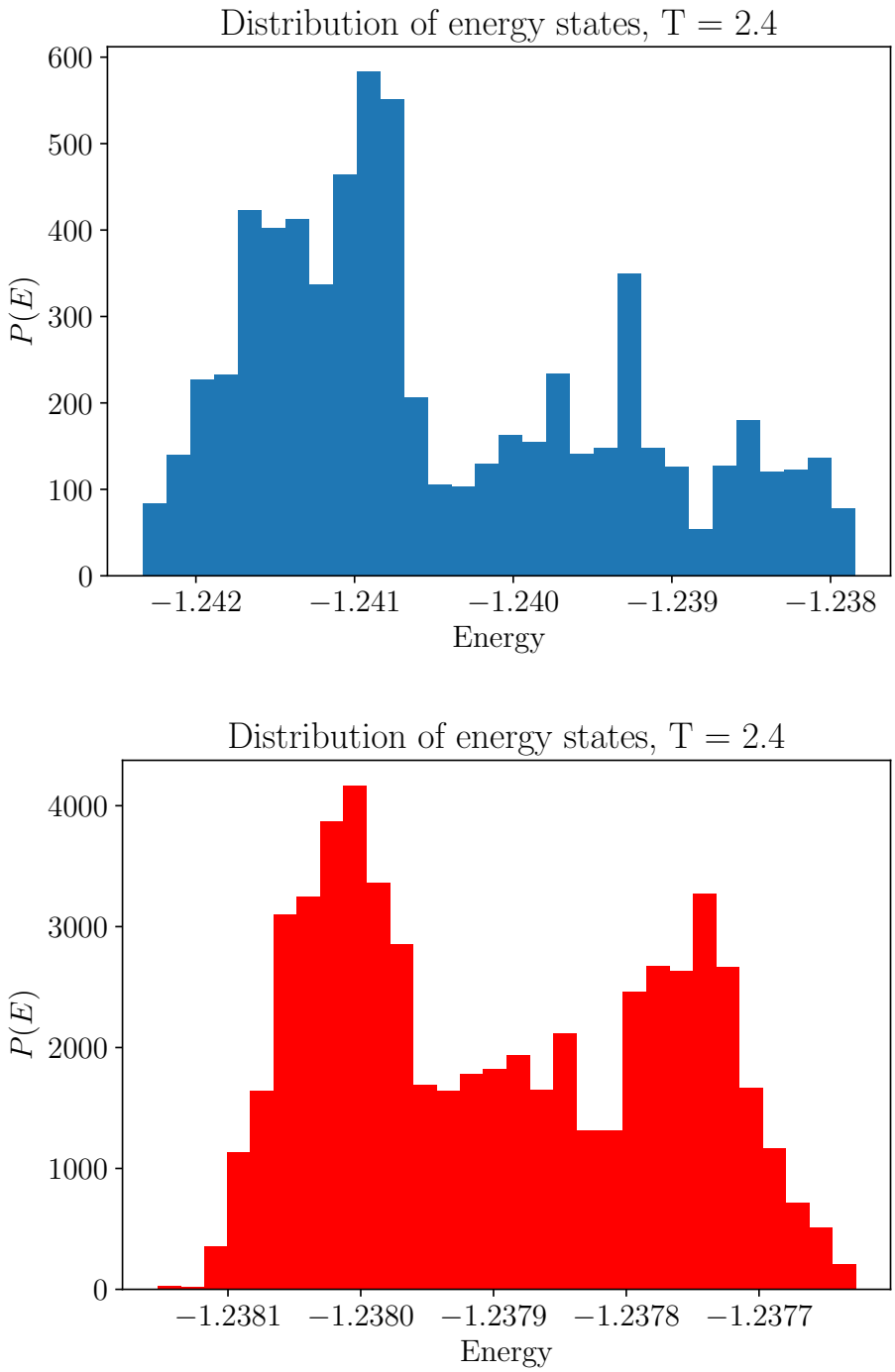

Figure 4: Histograms showing the distribution of energy states for $T = 2.4$ after equilibrium has been reached. For the red histogram the variance was $\sigma^2 = 1.59 \times 10^{-8}$.

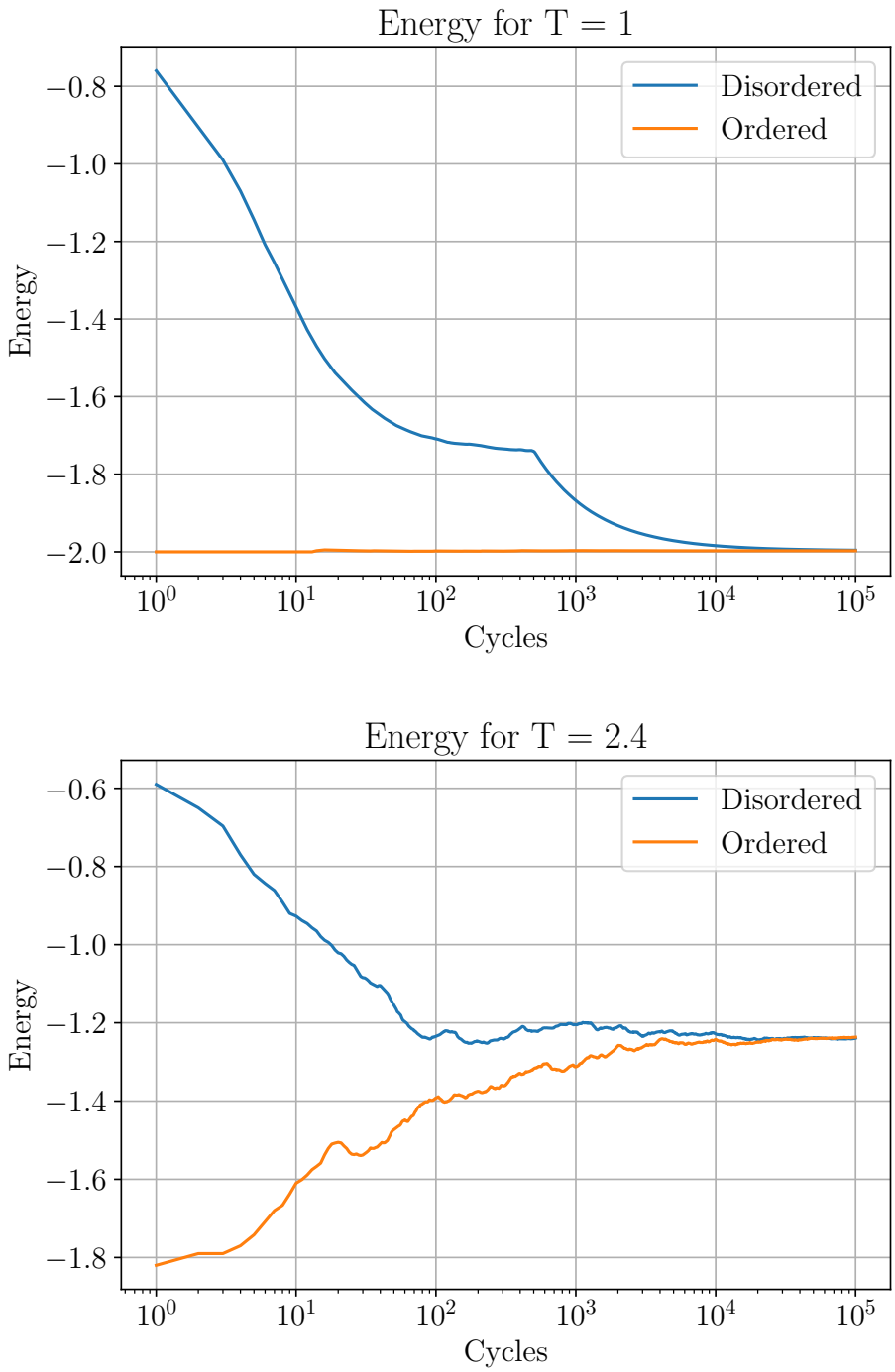

Figure 5: Mean energy as a function of cycles for both an ordered and a disordered lattice.

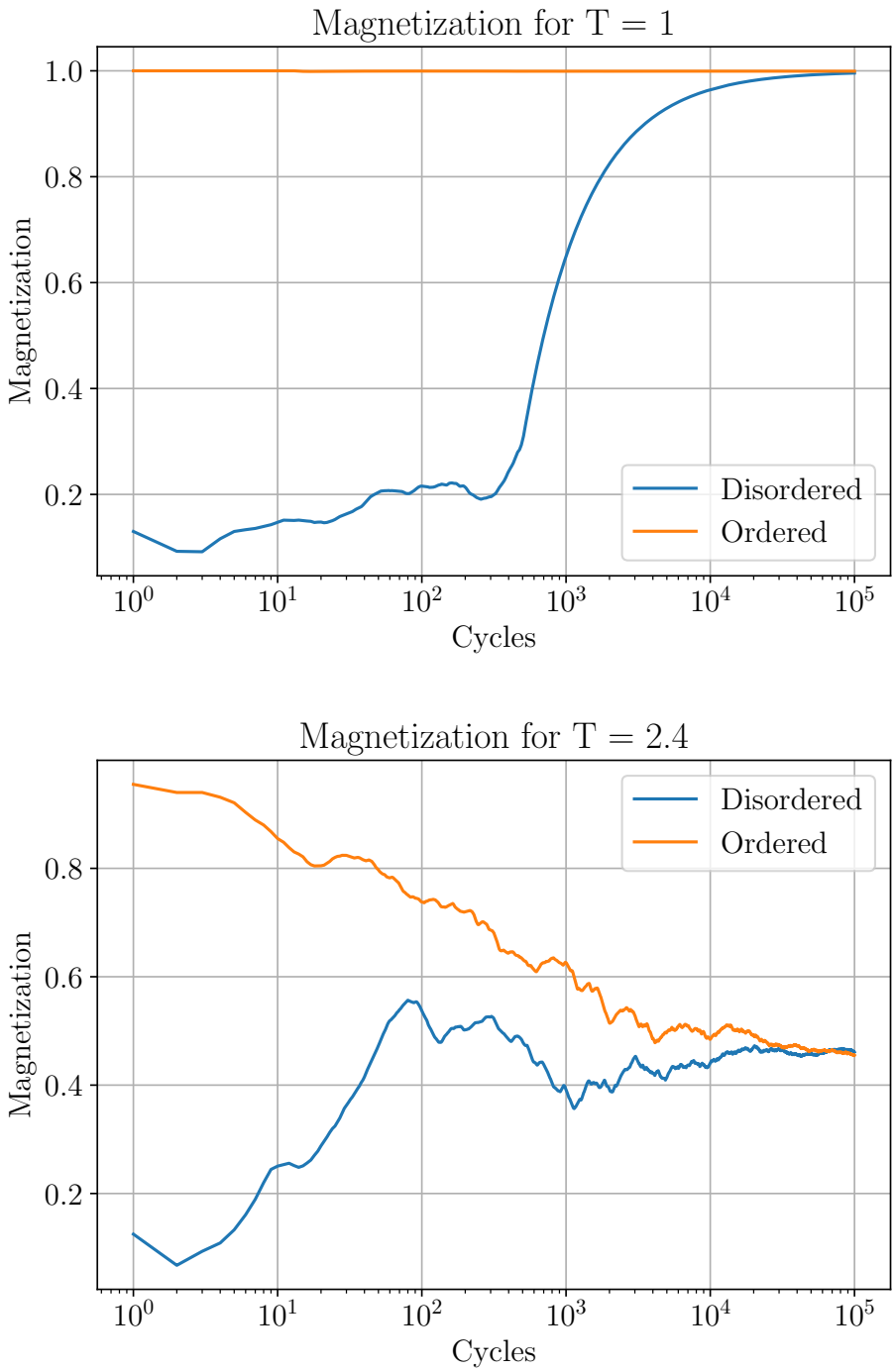

Figure 6: Mean absolute magnetization as a function of cycles for both an ordered and an disordered lattice.

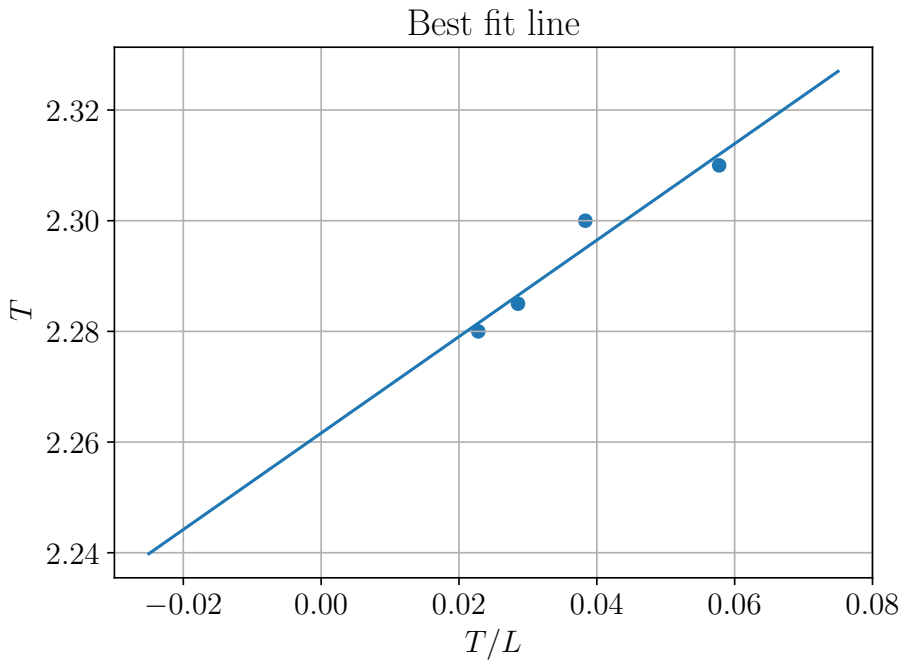

Figure 7: Plot of the best fit line for T as a function of $\frac{T}{L}$. The intercept is at $T = 2.262$, which gives us an estimate for the critical temperature T_C in the limit $L \to \infty$.

In figure 2 and 4 we see the distribution of energy states after the crystal has reached equilibrium. The energies in the blue colored histograms were computed with a disordered initial state with the simulations running for a total of 10^5 cycles. The plots were made with energy values for the last 5×10^4 cycles. The red colored histogram was found by computing the energy for 10^6 cycles four times and taking their average. We then plotted the frequency of the energies after 5×10^5 cycles.

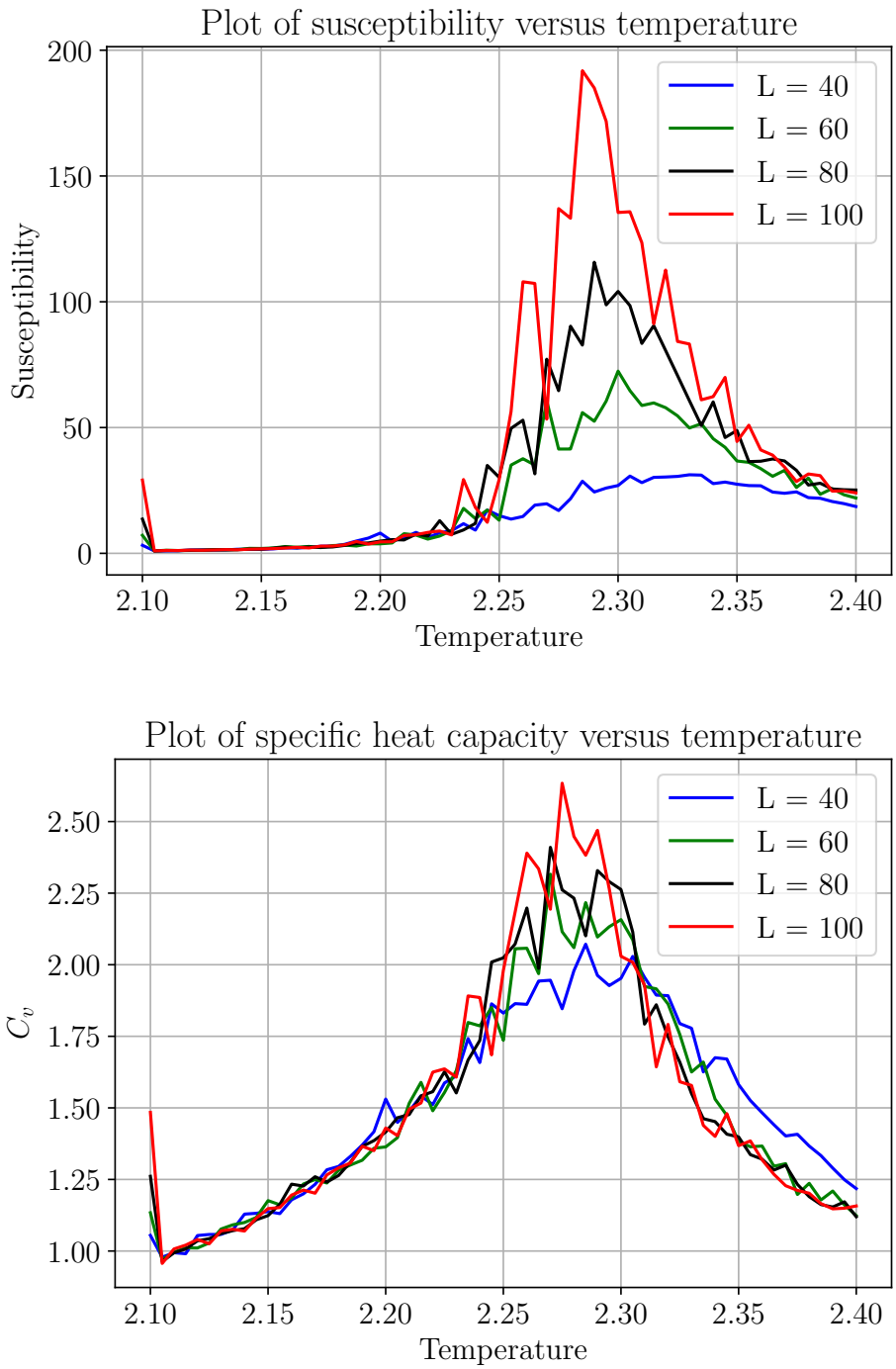

Figure 8: Average magnetic susceptibility and average specific heat plotted as a function of temperature for various lattice sizes.

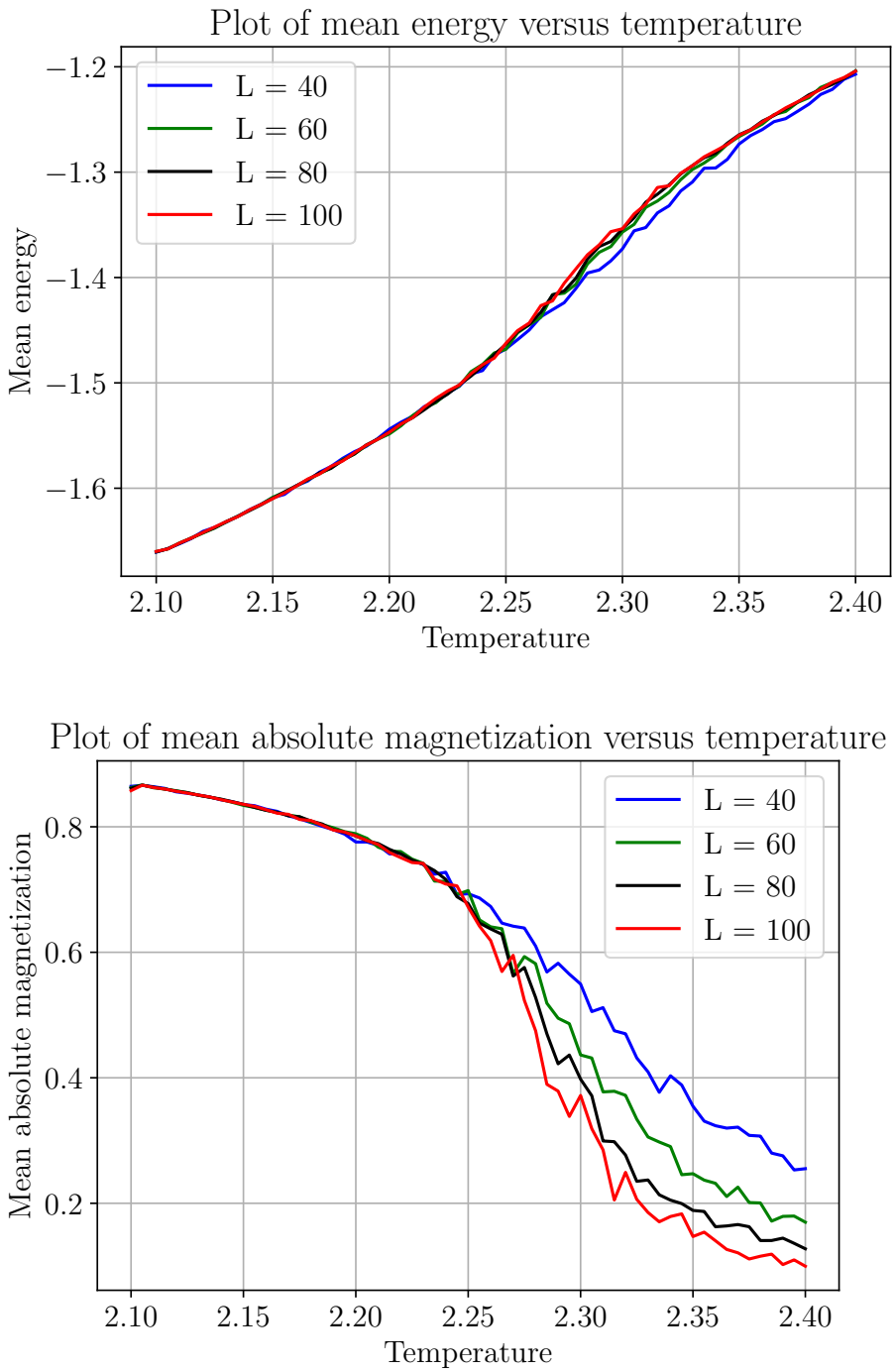

Figure 9: Average energy and average absolute magnetization as functions of temperature for various lattice sizes.

The speed up between parallized and regular code was also tested for a few selected runs with $L = 20$ and $L = 30$. For these runs we saw a significant speed up for two cores with their times presented in table 2

Table 2: The time spent for the parallized and regular code for different lattice sizes

L	Parallized(s)	Regular(s)	speed-up
20	354	663	1.87x
30	661	1215	1.84x

4 Discussion

4.1 Cycles Required to Reach Steady State

When we want to check our numerical results we do this by comparing our computations versus the analytical values we get for the $L = 2$ case. Here we run our simulations for 1 million montecarlo cycles. From table 1 we can see that for most of the values we have a really good comparison like for the mean energy and mean absolute magnetization with the worst being a 10% error in the heat capacity. The analytical solution should agree with the numerical solution when the system reaches equilibrium.
We see from figures 5, 6 and 1 that the time for the systems to reach equilibrium seems to be slightly more than 10^4 cycles. The exception for this is the ordered lattice in the case $T = 1$, which seems to start out in the equilibrium state. This likely means that all the spins pointing in one direction is the lowest energy state for the lattice. Other than for the special case of an ordered lattice at $T = 1$, the time is takes to reach the equilibrium state does not seem to vary much between $T = 1$ and $T = 2.4$.

4.2 Distribution of Energy States

In figure 2 we see the distribution of energy states after the system reaches equilibrium for $T = 1$. As we can see the lowest allowed energy state of the system is also the most common. This makes sense as $T = 1$ is the lowest temperature we can have, so the equilibrium state of the system should be the lowest energy state. We see that the system also sometimes enters higher energy states, but these are less likely than the lowest energy state and the higher the energy the less likely it is that the system will enter the state. This is consistent with what we expect.
In figure 4 we have the distributions of energy states for $T = 2.4$. As we can see the most likely energy state for this temperature is around -1.242. The distribution does seem to be biased towards lower energies, which is

unexpected. We should see that the plot is approximately normally distributed around some equilibrium energy value. This could just be that we haven't simulated the system for long enough, or that we included energies in our histograms from before the system reached equilibrium. To check that this wasn't the case we included the red colored histogram, which is the average of four histograms where we computed the energy for 10^6 cycles and plotted the energy distributions after 5×10^5. This is long after we have reached equilibrium and with far more states than the blue plot, yet the distribution is still not as Gaussian as we would like. Looking at the red histogram it is also no longer obvious that the distribution is as biased against lower energies. The variance for both the distributions we calculated it for was quite low. This suggests that the system does not tend to deviate far from the equilibrium state once it has reached it.

4.3 Critical Temperature for $L \to \infty$

To find the critical temperature of an infinitely big lattice we used linear regression. When we wanted to find the temperatures at which a phase change happened we simply read off the susceptibility plots in figure 8. This is not a very sophisticated or reliable way to measure the exact point at which the phase change occurs and as such our result should be taken with a grain of salt. We could have tried to approximate a smoother curve using pandas moving average method or using a similar method like finding a least squares fit with some polynomial, which would then have a more clear cut, less noisy maximum point. The reason we used the susceptibility data is that the specific heat data is so noisy that we were unable to tell where the maximum of the curve really was. If we had fitted a curve we would have had two ways of calculating the critical temperature for an infinitely large lattice, which would have allowed us to compare results. In spite of the unreliable method we did end up getting a surprisingly accurate result. As you can see in figure 7 we got a valueu of $T_C = 2.262$ whereas the exact result is approximately $T_C^{exact} = 2.269$.

4.4 Parallelization

By parallelization we can achieve a speed up that nearly halves the amount of time spent which we can see from the table 2. This means we can get a more precise value for the same amount of computation time or a similar value for half the computation time. This is especially valuable for Monte Carlo processes because their accuracy largely depends on the number of simulations. If had access to even more cores this time could be reduced further.

5 Conclusion

In conclusion we can see that we have a good comparison to the analytical case for $L = 2$ and thereby we can with good confidence say that our numerical calculations for the other systems will also give an answer that is close to the actual values of that system.

In the future we could, in order to achieve better results, run many simulations under the same conditions and take the average of the results. Further parallelization would be useful for achieving this in a reasonable amount of time. Curve fitting the average specific heat and the average magnetic susceptibility as functions of temperature would also help us find more accurate maximum points which would reduce the amount of eyeballing needed to find the critical temperature for $L \to \infty$ and increase the reliability of the estimate. Translation of the model to three dimensions could make for further interesting computational analysis.

6 References

[2]: Hjorth-Jensen, M.(Fall 2015), Lecture notes, Computational Physics FYS3150, Chapter 13. `https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf`