UiO : Department of Physics
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FYS3150: Computational Physics I

Project 4

Studies of Phase Transitions in a Magnetic System, using the Ising model and the Metropolis Algorithm

Kristian Wold*

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Abstract

In this project we studied phase transitions exhibited by the square lattice Ising model for a ferromagnetic system. Using the Metropolis Algorithm, several finite lattices were simulated and the critical temperatures extracted. Finite scaling relations was then used to find the critical temperature in the thermodynamic limit, that is, for an infinitely large lattice. In this limit, the system completely loses its magnetization at the critical temperature T_c known as the Curie temperature. From Onsager work[1], this temperature is known to be $k_B T_c/J = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.269$. Our numerical approach yielded a estimate of $k_B T_c/J = 2.26767$, in good accordance with the analytical result.

*This project was embarked on as a collaborative effort between Lasse Braseth, Nicolai Haug, and Kristian Wold. Hence, our individual reports have a strong resemblance in both presentation and content. In particular, figures and tables with corresponding captions are nearly, or in some cases entirely, identical.

GitHub repository: https://github.com/KristianWold/Compphys/tree/master/P4

Contents

1 Introduction

The Ising Model is a model of magnetic, classical spins arranged in a lattice, where each spin is allowed to interact with its nearest neightbor. Although very simple, the model exhibits a second order transition. At a critical temperature, called the Curie temperature, the system loses its magnetization.

In this project, we study the manifestation of this phase transition in finite lattices with ferromagnetic ordering and use finite size scaling relations to approximate the Curie temperautre in the thermodynamical limit. This is done with help of the Metropolis Algorithm, which is a Markov chain Monte Carlo method.

Analytical results for the partition function, the mean energy, heat capacity and susceptibility have been derived in the 2×2 lattice case, and serves as a benchmark when testing the numerical precision of our implementation for various initial parameters, such as temperature and number of Monte Carlo cycles.

We study how fast the system reaches equilibrium, that is, the most likely state, for different temperatures and initial orderings. We also study the behaviour of the Metropolis Algorithm, looking at how the number of accepted states behaves as a function of cycles and temperature. Also the relative frequency of different energy states for different temperatures are explored, and the variance of this distribution is compared with the one derived from the heat capacity.

The mentioned expectation values are estimated for a range of temperatures for different sized lattice. From the susceptibility are the critical temperatures exctracted, which in turn are used to ultimatly approximate the Curie temperature.

In this project, we first introduce the Ising Model, a short review of statistical physics and the Metropolis Algorithm in Section 2. Then in Section 3, more on the specific implementation of the Ising Model, the Metropolis Algorithm and some challenges surrounding them are presented. In Section 4, the results of the simulations implementing the Ising Model and Metropolis Algorithm are presented, which is then discussed in Section 5 and 6. Finally, some comments on what work to be done next is presented in 7

2 Theory

2.1 The Ising Model and Phase Transitions

The Ising Model is a very simple way of modeling a 2D LxL lattice of classical spin, where each spin is either up or down($s = \pm$). The total energy of the system is given by [2, p. 422]

$$E = -J \sum_{\langle kl \rangle} s_k s_l \tag{2.1}$$

where $\langle kl \rangle$ means that for each spin, we sum over its nearest neighbors. Having the coupling constant $J > 0$ will make the spins tend to align parallel, since the system wants to minimize its energy. This is known as ferromagnetic ordering.

Although simple, the model is capable of showing a second order phase transition. Phase transitions in thermodynamics are characterized by discontinuities in quantities describing the system. For example the evaporation of liquid water into steam is a phase transition, since at $T_c = 100°\text{C}$, the critical temperature, the energy of the system makes a sudden jump. This is called a first order phase transition, since the energy is related to the first derivative of the systems partition function with respect to $\beta = \frac{1}{k_B T}$.

A second order phase transition, which the Ising Model exhibits, is hence characterized by a discontinuity in quantities related to the second derivative, typically heat capacity C_V or susceptibility χ. Note that these quantities are only truly discontinuous in the thermodynamic limit, that is $L \to \infty$, infinitely large lattices. For finite lattices, the heat capacity and susceptibility are strictly continuous [2, p. 431]. However, finite systems of size LxL will show a maximum in the heat capacity and susceptibility for a given temperature $T_c(L)$, which we will call the critical temperature for the finite system. Using finite size scaling relations, we can relate the critical temperature in the finite cases to the infinite case [2, p. 432]

$$T_c(L) = aL^{-1} + T_c(L = \infty) \tag{2.2}$$

By doing simulations for different L, we can extract $T_c(L)$ by looking for maxima in the susceptibility and use linear regression to fit (2.2). As $1/L \to 0$, $L \to \infty$, meaning we can identify the constant in the linear regression as the value of $T_c(L = \infty)$. Analytically, this value is known to be [1]

$$T_c(L = \infty) = \frac{2}{\log(1 + \sqrt{2})} \approx 2.269 \tag{2.3}$$

Since we are interested in the behaviour of the system in the thermodynamical limit, we want to simulate systems as large as possible. Since computational power is limited, a shortcut is to use periodic boundary conditions, meaning the spins on the edges of the lattice wrap around and interact with the spins of the opposite side. This helps eliminate some of the effect introduced by the boundary, and makes the lattice seem infinite. [3, p. 26].

2.2 Partition Function and Expectation Values

In our model, we assume that our system of spins is in contact with a reservoir of temperature T, meaning it is free to exchange energy, but not particles or volume. The reservoir is assumed so big that it does not lose a noticeable amount of energy. Thus our system can be described using the canonical ensemble.

For a temperature T, the chance of finding our system in a state i with a related energy E_i is given by

$$P_i = \frac{e^{-\beta E_i}}{Z} \tag{2.4}$$

where $\beta = \frac{1}{k_B T}$ and Z is the partition function, which is the sum of all states' Boltzmann factor

$$Z = \sum_i e^{-\beta E_i} \tag{2.5}$$

The partition function normalizes the probability, so $\sum_i P_i = \frac{Z}{Z} = 1$.

Using the probability, we can work out any expectation value $\langle O \rangle$

$$\langle O \rangle = \sum_i P_i O_i = \frac{1}{Z} \sum_i O_i e^{-\beta E_i} \tag{2.6}$$

For the 2×2 case for our spin system, we can easily work out the energy and magnetization of all the accessible states, and thus the partition function. Using (energy of system) with periodic boundaries, and $J/k_B = 1$, we get the following result:

Spins up	Degeneracy	E	M
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

Using (2.5), we can calculate the partition function

$$Z = \sum_i e^{-E_i/T} = 2e^{-(-8)/T} + 2e^{-(8)/T} + 12e^{-(0)/T} = 4\cosh(8/T) + 12 \tag{2.7}$$

using $\cosh(x) = \frac{e^x + e^{-x}}{2}$.

Using (2.6), rewriting the equation for $O = E$, the expectation value of the energy and mean absolute value magnetization is

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = -\frac{\partial \ln(Z)}{\partial \beta} = \frac{-8\sinh(8/T)}{\cosh(8/T) + 3} \tag{2.8}$$

$$\begin{aligned} \langle |M| \rangle &= \frac{2 \cdot 4e^{8/T} + 4 \cdot 2e^{-0/T} + 4 \cdot 2e^{-0/T}}{4\cosh(8/T) + 12} \\ &= \frac{e^{8/T} + 2}{\cosh(8/T) + 3} \end{aligned} \tag{2.9}$$

Using $Cv = \frac{\partial \langle E \rangle}{\partial T}$, we get

$$\begin{aligned} Cv &= -\frac{1}{T^2} \frac{-256\cosh(8/T)(4\cosh(8/T) + 12) + 1024\sinh^2(8/T)}{(4\cosh(8/T) + 12)^2} \\ &= \frac{1}{T^2} \frac{64(3\cosh(8/T) + 1)}{(\cosh(8/T) + 3)^2} \end{aligned} \tag{2.10}$$

To get a suitable expression for evaluating the heat capacity numerically later, we express it in terms of the variance of the energy

$$Cv = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial \beta}{\partial T} \frac{\partial \langle E \rangle}{\partial \beta} = \frac{1}{k_B T^2} \frac{\partial^2 \ln(Z)}{\partial \beta^2}$$

$$\frac{1}{T^2}\frac{\partial}{\partial\beta}[\frac{1}{Z}\frac{\partial Z}{\partial\beta}] = \frac{1}{T^2}[\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2} - (\frac{1}{Z}\frac{\partial Z}{\partial\beta})^2] = \frac{1}{T^2}[\langle E^2\rangle - \langle E\rangle^2]$$

Likewise, you can derive the susceptibility by the variance of the magnetization

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

By inserting the expression for $\langle M^2\rangle$ and $\langle |M|\rangle$ given by

$$\left\langle M^2\right\rangle = \frac{1}{Z}\sum_i M_i^2 e^{-\beta E_i} = \frac{8e^{8J\beta}+8}{\cosh(8J\beta)+3}$$

we get

$$\chi = \frac{1}{k_B T}\left[\frac{8e^{8J\beta}+8}{cosh(8J\beta)+3} - \left(\frac{4+2e^{8J\beta}}{cosh(8J\beta)+3}\right)^2\right] \tag{2.11}$$

By dividing all the analytical expressions by 4, we obtain the quantities per spin, which we will use when comparing to our numerical results.

2.3 Metropolis Algorithm and Ergodicity

When studying systems that can assume different states by certain probabilities, the Metropolis Algorithm is a powerful tool. To find the most likely configuration of spins for a certain temperature, that is, equilibrium, we would like to let the system evolve in a random fashion, flipping spins until we achieve the most likely state. This is reminiscent of a random walker, with some differences. Firstly, we are not walking randomly through real space, but rather through the space of possible states the system can assume. Secondly, the walk is not uniformly random, but biased in a way that favors states that are more likely to arise according to the thermodynamical laws, viz. (2.4). The reason we cannot use (2.4) directly is because the partition function becomes unfeasible to compute for moderatly large systems. Instead, the metropolis algorithm relies on the ratio of two probabilities for two different stats. Given we are in a state i, we flip a spin at random to attain state j. The ratio reads

$$\frac{P_j}{P_i} = \frac{\frac{e^{-\beta E_j}}{Z}}{\frac{e^{-\beta E_i}}{Z}} = e^{-\beta(E_j - E_i)} = e^{-\beta\Delta E} \tag{2.12}$$

Note how the partition functions cancel, to our great relief. The resulting exponential is often referred to as the accpetance amplitude. The metropolis algorithm for Ising model can be summerized as follows:

1. Initialize with some microstate i of energy E_i.
2. Flip one spin at random to create the new state j.
3. If $\Delta E = E_j - E_i <= 0$, accept the new state.
4. Otherwise, accept the new state only if $e^{-\beta\Delta E} > r$, where r is some uniformly distributed random number between 0 and 1.

This methodology conserves two important properties of the system: It creates the well known tendency for systems to minimize its energy, in the sense that we all ways accept a new state if the energy is lower. However, the system does not assume the lowest possible energy and stay there: It fluctuates. We must allow it to sometimes go up in energy as well. This concept is called ergodicity, which means that the system is able to assume all possible states given enough time, although some of the states are extremely unlikely. Had our system not been able to make fluctuations from time to time, it would result in faulty physics, because it would cause artificially low variance in e.i. the energy.

2.4 Correlation and weaknesses of the Metropolis Algorithm

As described in the previous section, the Metropolis Algorithm is a type of importance sampling. Rather than summing the contribution of all possible configurations, since many of these are highly unlikely to occur anyway, the Metropolis Algorithm picks out a string of more likely states. Although this saves a lot of computational time, it also introduces problems. Since the Metropolis Algorithm makes small changes to the lattice for each sweep, the consecutive energy states will likely be very close lying, i.e. correlated [3, p. 258]. Correlation introduces errors in the statistics produces by the simulation.

3 Method

3.1 Metropolis Algorithm on The Ising Model

Using the Metropolis algorithm as in section 2.3, we have a way to evolve our spin-matrix given a initial state. For a $N \times N$ matrix, we apply Metropolis N^2 times. This is known as sweeping over the matrix, allthough we really choose a random spin each time. One sweep of the matrix makes one Monte-Carlo cycle. For each cycle, we sample the energy and magnetization and writes them to file. From these values we compute all the our expectation values as described in section 2.2. However, some care should be taken, as we must wait until the system has reached equilibrium before calculating expectation values. An easy way to identify when equilibrium is reach is simply by plotting the total energy as a function of cycles and see when it flattens out. For the 20×20 lattice we studied, the number of cycles before equilbrium were quite low, around 50. For larger lattices and the temperatures however, the time was somewhat longer. Therefore, for good measure, a cutoff of 1000 cycles for all simulations have been used in this project to ensure good expectation values.

3.2 Benchmarking The Simulation Against Analytical Solutions in 2×2 case

When checking our numerical solutions against the analytical, the simulation based on section 3.1 was run several times for a 2×2 lattice. First, the simulation was run for every magnitude of order 10^3 through 10^7 for temperature $T = 2$. All the relevant quantities mentioned in section 2.2 was compared with the analytical values. This was done to observe the convergernce of the numerical solution towards the analytical for increasing temperatures.

We chose to do this for $T = 2$ rather than $T = 1$ to better see the improved precision of using more cycles, since the system tends to fluctuate more.

We then did the same analysis, but for a range of temperatures $T = [1, 3]$ for different number of cycles. This was to see if the trend of convergence held for a more general range of temperatures.

3.3 Investigating Time to Reach Equilibrium

When investigating the time the system used to reach equilibrium, we plotted the evolution of the total energy and magnetization of the system as a function of number of cycles. This was done rather than looking at the expectation value as a function of cycles, as expectation values might still be very skewed long after the system have equibriated. This is due to the first samples acquired when the system still was approaching equilibrium.

The evolution of the quantities was investigated for $T = 1$ and $T = 2.4$, and for a lattice that started both in a ordered and disordered state.

3.4 Counting of Accepted States

The number of accepted cased produced by the Metropolis Algorithm was counted and plotted for both for different number of cycles, and different temperatures.

3.5 Probability Distribution of Different Energy States

For a single simulation of a 20×20 crystal for a specific temperature, the evolution of total energy for each cycle was examined and the relative frequency of each unique energy state was extracted, thus yielding a probability distribution. This was then plotted.

3.6 Critical Temperature in the Thermodynamic Limit

In determining the critical temperature of the Ising model in the thermodynamic limit, the critical temperature of finite crystals with $L = [40, 60, 100, 160]$ was extracted. This was done by performing the simulation with 10^6 cycles and 1000 precycles for each crystal for a range of temperatures. This range was chosen to be $T = [2.2, 2.4]$ with a step of $\Delta T = 0.01$. The critical temperature was extracted by finding the temperature in which the numerically calculated susceptibility had its maximum. The sampled critical temperatures was then linearly fitted to equation (2.2), and the resulting constant in the expression was identified as the critical temperature in the thermodynamic limit.

3.7 Parallelization Using MPI

The simulations using Monte Carlo have all been parallelized using MPI. The parallelization was done in a very straight forward way, simply running a unique MC simulation on each core, seeded differently, then collecting all the sampled values at the end.

4 Results

4.1 The Metropilis Algorithm

The program containing the implementation of the Metropolis method and accompanying programs that produces all the results presented in this project can be found at the GitHub repository

https://github.com/KristianWold/Compphys/tree/master/P4

4.2 Comparing Numerical and Analytical Results for 2×2 Lattice

In Table 4.1 is a comparison of the numerical and analytical solutions for the 2×2 Ising model. The numerical calculations is generated for various Monte Carlo cycles N with temperature T=2. The analytical values are from section 2.2

Table 4.1: *This table shows the mean energy, absolute value of mean magnetization, heat capacity and susceptibility for several monte carlo cycles N, $T = 2$ and 1000 precylces. The table also shows the comparison of these values compared to the analytical expression.*

$\boldsymbol{N}$	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	C_v	χ
10^3	-1.778	0.928	0.40272	0.095632
10^4	-1.791	0.93095	0.37672	0.093414
10^5	-1.80125	0.9341	0.35812	0.090544
10^6	-1.80119	0.93393	0.36073	0.090415
10^7	-1.80072	0.93366	0.36129	0.090893
Analytical	-1.8008	0.93371	0.36110	0.090798

In figure 4.1, 4.2 and 4.3 are plots of the energy, mean magnetization, heat capacity and susceptibility, all per spin, as a function of temperature. The plots have been generated using cycles $N = 10^3$, 10^4 and 10^6, respectively. In addition to the numerical results, also the analytically values from 2.2 have been been plotted.

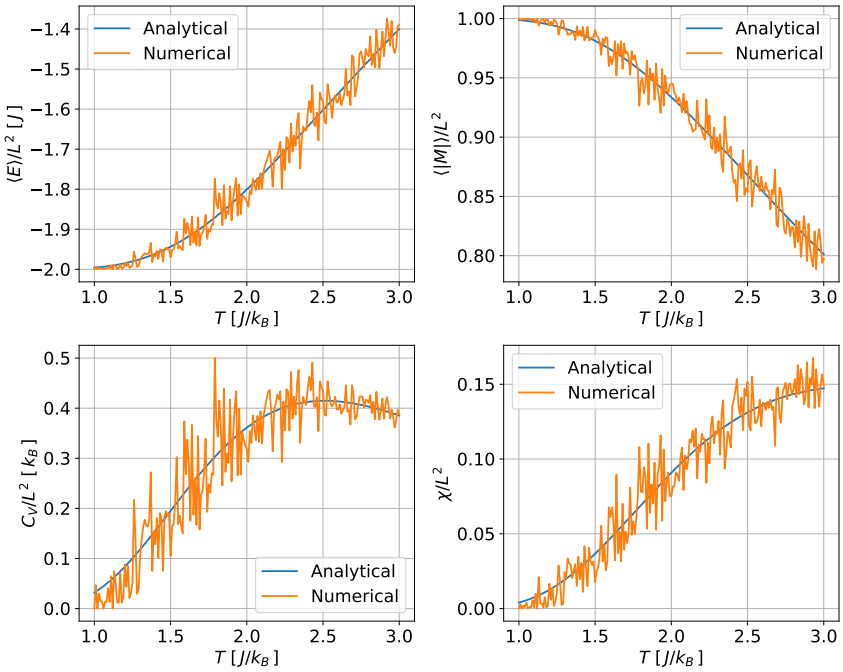


Figure 4.1: *Plots of various numerically calculated quantities for a 2×2 lattice. The values have been calculated using a Monte Carlo approach, utilizing the Metropolis Algorithm on the Ising Model. The step in temperature is $\Delta T = 0.01$, and number of cycles is $N = 10^3$*

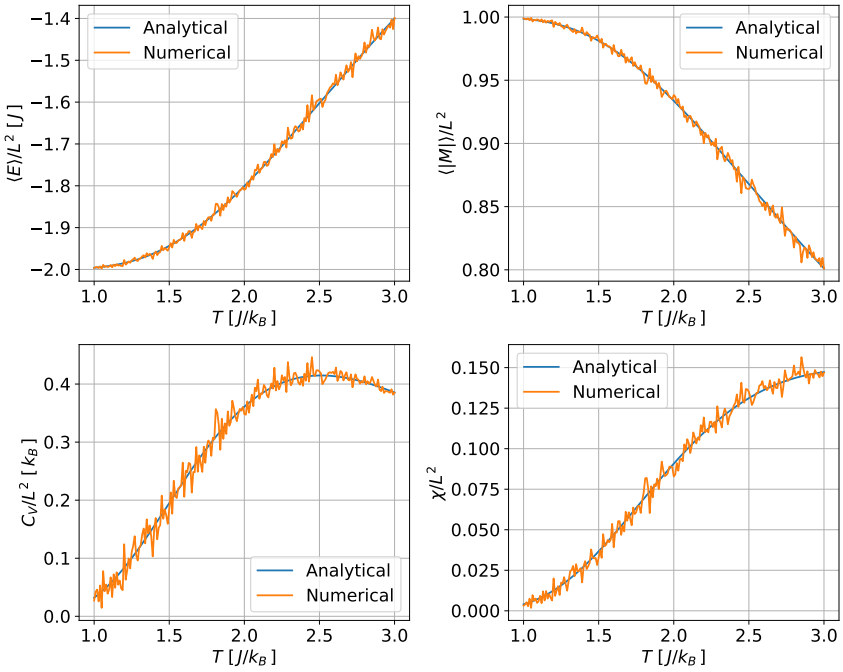


Figure 4.2: *Plots of various numerically calculated quantities for a 2×2 lattice. The values have been calculated using a Monte Carlo approach, utilizing the Metropolis Algorithm on the Ising Model. The step in temperature is $\Delta T = 0.01$, and number of cycles is $N = 10^4$*

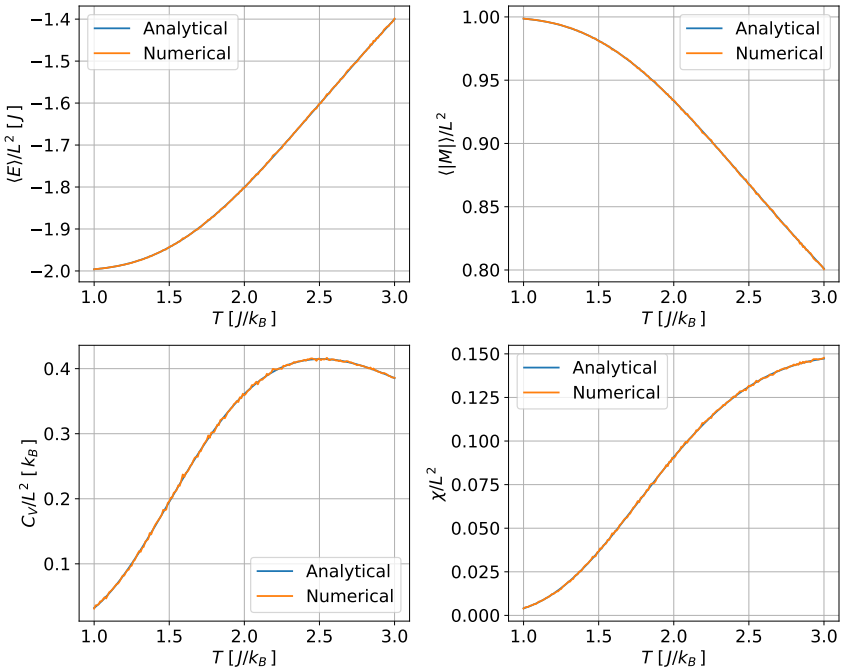
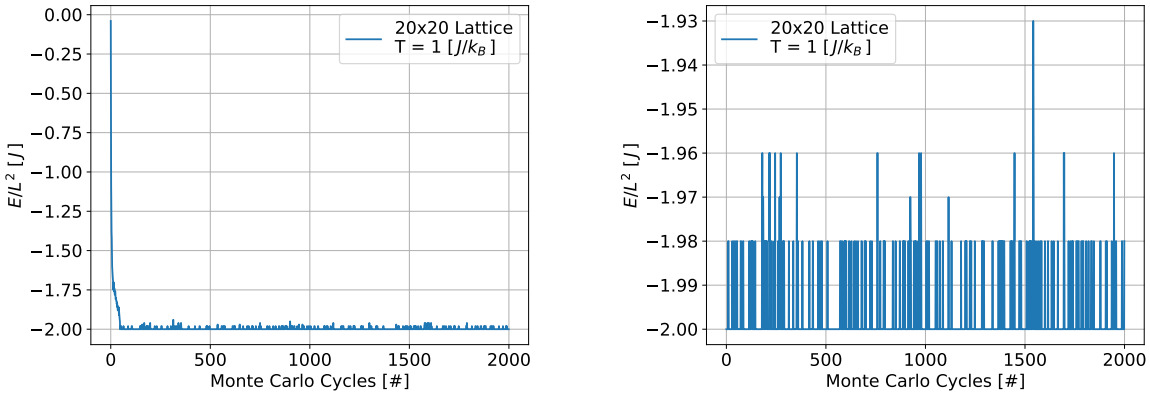


Figure 4.3: *Plots of various numerically calculated quantities for a* 2×2 *lattice. The values have been calculated using a Monte Carlo approach, utilizing the Metropolis Algorithm on the Ising Model. The step in temperature is* $\Delta T = 0.01$*, and number of cycles is* $N = 10^6$

4.3 Equilibrium for Ordered and Disordered Initial State

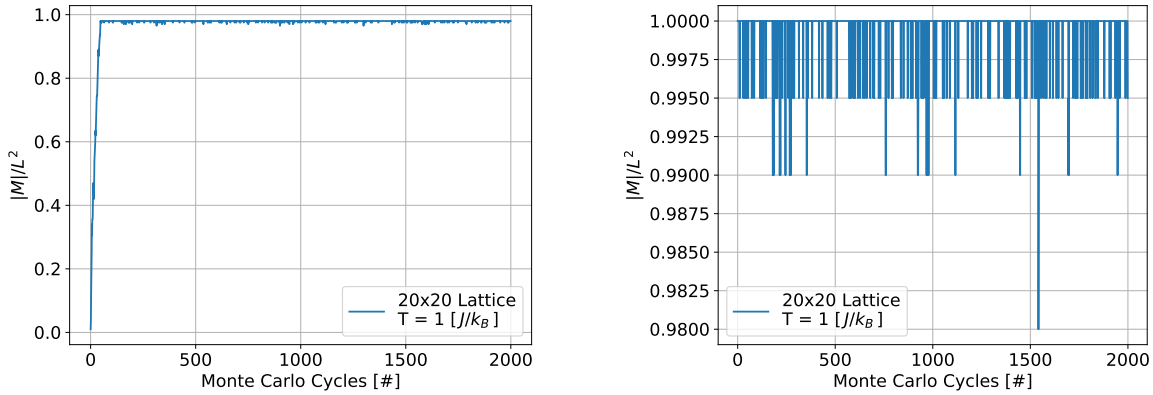
Figure 4.4 shows the evolution of the total energy for an ordered and disordered 20×20 lattice for temperature $T = 1$. The number of Monte Carlo cycles is 2000.



(a) **(b)**

Figure 4.4: *Evolution of the total energy for a ordered and disordered* 20×20 *lattice for temperature* $T = 1$*. The number of Monte Carlo cycles is 2000.*

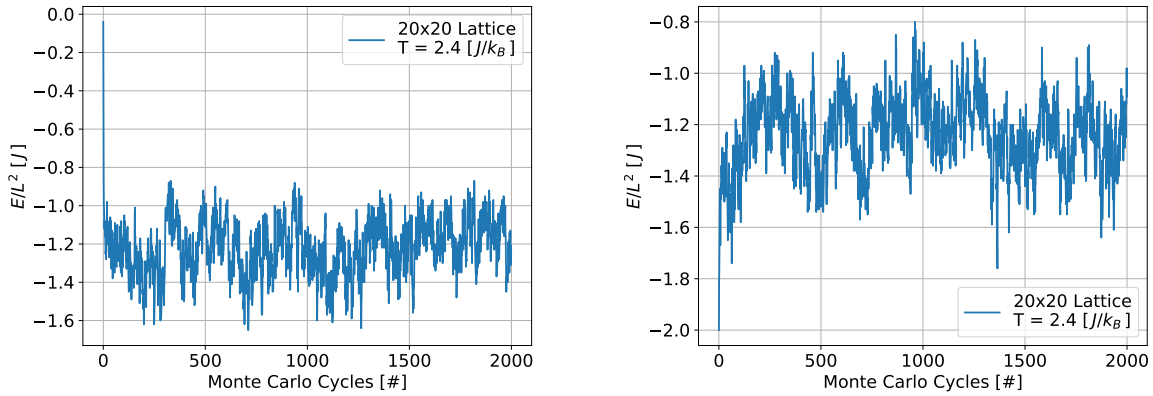
Figure 4.5 shows the evolution of the total magnetization for an ordered and 20×20 lattice for temperature $T = 1$. The number of Monte Carlo cycles is 2000.



(a) **(b)**

Figure 4.5: *Evolution of the total magnetization for a ordered and disordered* 20×20 *lattice for temperature* $T = 1$*. The number of Monte Carlo cycles is 2000.*

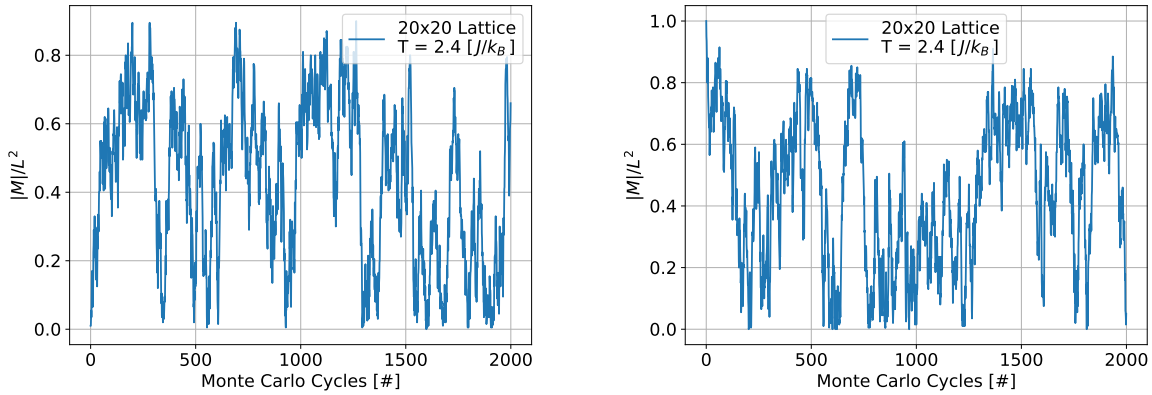
Figure 4.5 shows the evolution of the total energy for an ordered and 20×20 lattice for temperature $T = 2.4$. The number of Monte Carlo cycles is 2000.



(a) **(b)**

Figure 4.6: *Evolution of the total energy for a ordered and disordered* 20×20 *lattice for temperature* $T = 2.4$*. The number of Monte Carlo cycles is 2000.*

Figure 4.5 shows the evolution of the total magnetization for an ordered and 20×20 lattice for temperature $T = 2.4$. The number of Monte Carlo cycles is 2000.



(a) (b)

Figure 4.7: *Evolution of the total magnetization for a ordered and disordered* 20×20 *lattice for temperature* $T = 2.4$*. The number of Monte Carlo cycles is 2000.*

4.4 Number of Accepted States

Figure 4.8 shows the number of accepted states as a function of Monte Carlo cycles. The plot was generated by simulating with L=20 and with a temperature, T=2.

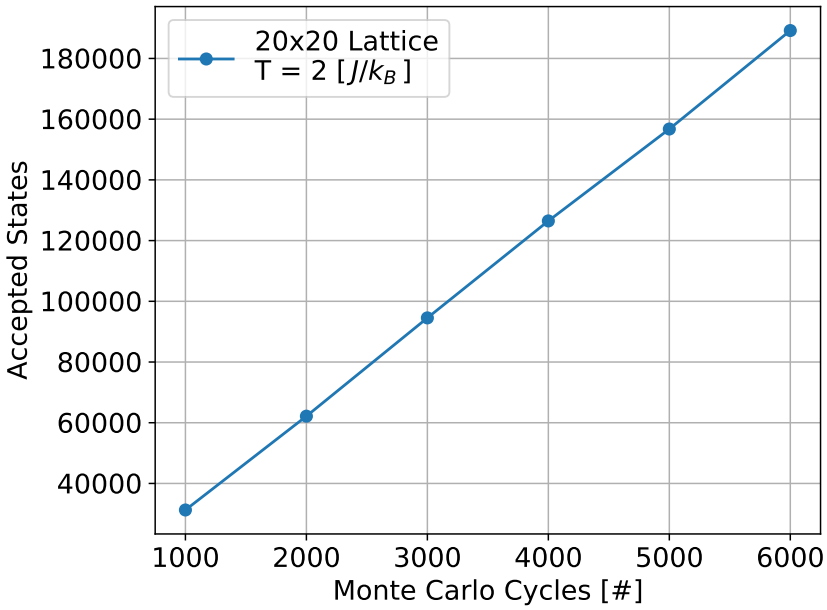


Figure 4.8: *This is a plot of the number of accepted states per sweep of the lattice as a function of the number of Monte Carlo cycles. This plot was generated for a* 20×20*-Lattice with a temperature, T=2.*

Figure 4.9 shows the number of accepted states per sweep as a function of temperature. The plot was generated by simulating with $L = 20$ and for $N = 10^4$ Monte Carlo cycles.

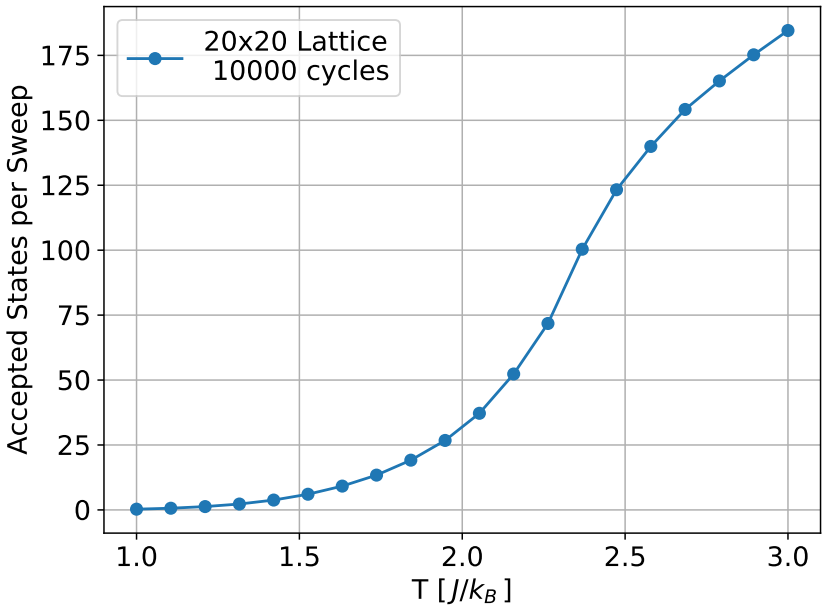
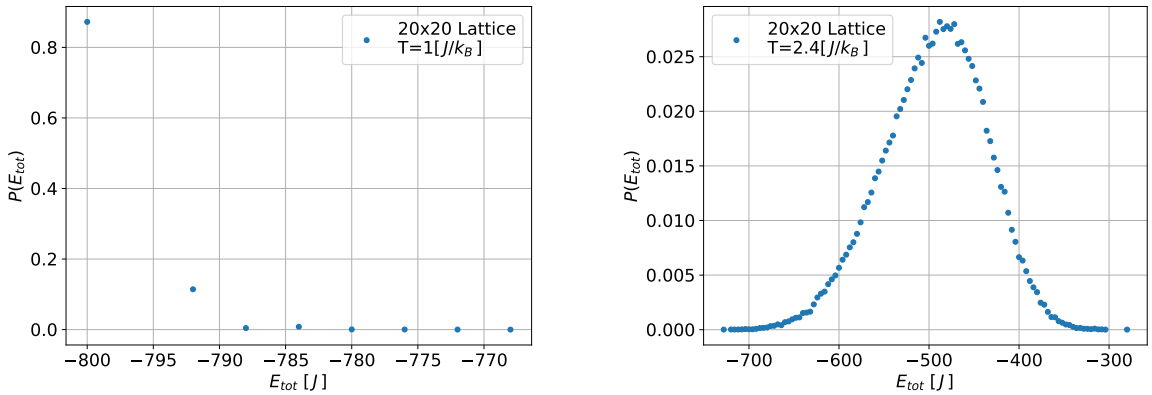


Figure 4.9: *This plot of the number of accepted states per sweep as a function of the temperature. The plot was generated for a* 20×20*-Lattice with* $N = 10^4$ *Monte Carlo cycles.*

4.5 Probability Distribution

Figure 4.10 is a plot showing the relative frequency of unique energy states for a 20×20 lattice, for temperatures $T = 1$ and $T = 2.4$. The simulation was ran using $N = 10000$ Monte Carlo cycles and 1000 precycles.



(a) **(b)**

Figure 4.10: *Relative frequency of unique energy levels for a* 20×20 *lattice, for temperatures* $T = 1$ *and* $T = 2.4$*. The simulation was ran using* $N = 10000$ *Monte Carlo cycles and* 1000 *pre-cycles.*

The variance of the energy σ_E^2, calculated from the heat capacity 2.10, for $T = 1$ and 2.4 is 9.216 and 3258, respectively.

4.6 Studies of Phase Transitions

In Figure 4.11 a plot of the mean energy per spin as a function of temperature is presented. The chosen interval of the temperature is $T \in [2.2, 2.4]$ with a stepsize of $\Delta T = 0.01$, and the result is plotted for several lattice sizes.

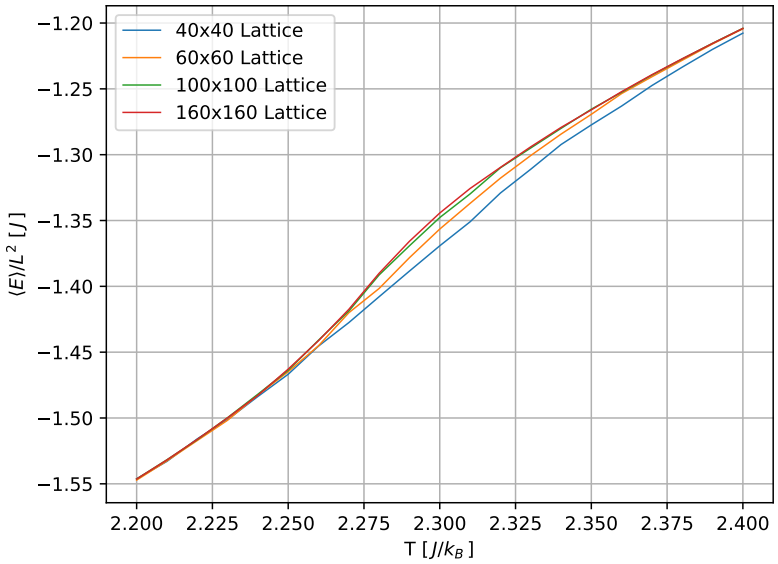


Figure 4.11: *This plot shows the mean energy per spin as a function of temperature. The simulation was chosen to run in a interval $T \in [2.2, 2.4]$ with a stepsize $\Delta T = 0.01$. The simulation is generated with $N = 10^6$ Monte Carlo cycles, and is done for several lattice sizes L= 40, 60, 100, 160.*

In Figure 4.12 a plot of the mean absolute magnetization per spin as a function of temperature is presented. The chosen temperature interval is $T \in [2.2, 2.4]$ with a stepsize of $\Delta T = 0.01$. The simulation was performed with $N = 10^6$ Monte Carlo cycles, and is presented for several lattice sizes.

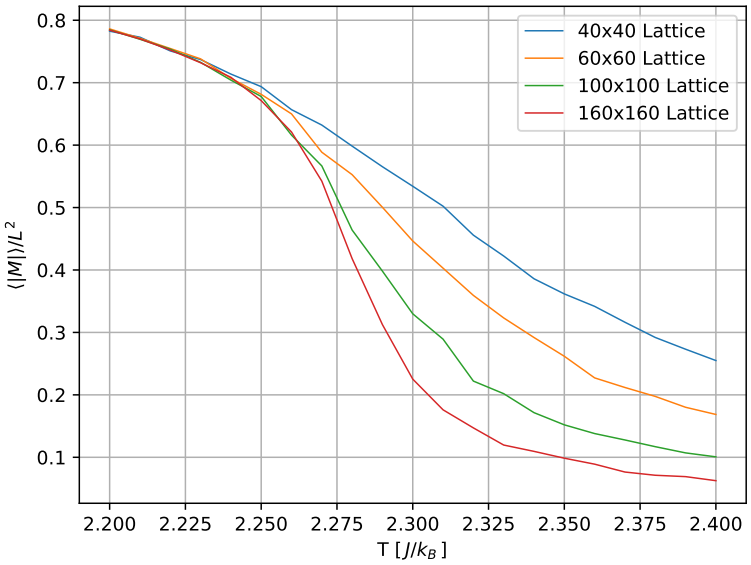


Figure 4.12: *This plot shows the absolute value of the mean magnetization per spin as a function of the temperature. The simulation was chosen to run in a interval* $T \in [2.2, 2.4]$ *with a stepsize of* $\Delta T = 0.01$*. The simulation is generated with* $N = 10^6$ *Monte Carlo cycles, and is done for several lattice sizes L= 40, 60, 100, 160.*

Figure 4.13 shows the heat capacity per spin as a function of temperature. The chosen temperature interval is $T \in [2.2, 2.4]$ with a stepsize of $dT = 0.05$. The simulation was performed with $N = 10^6$ Monte Carlo cycles, and is presented for several lattice sizes.

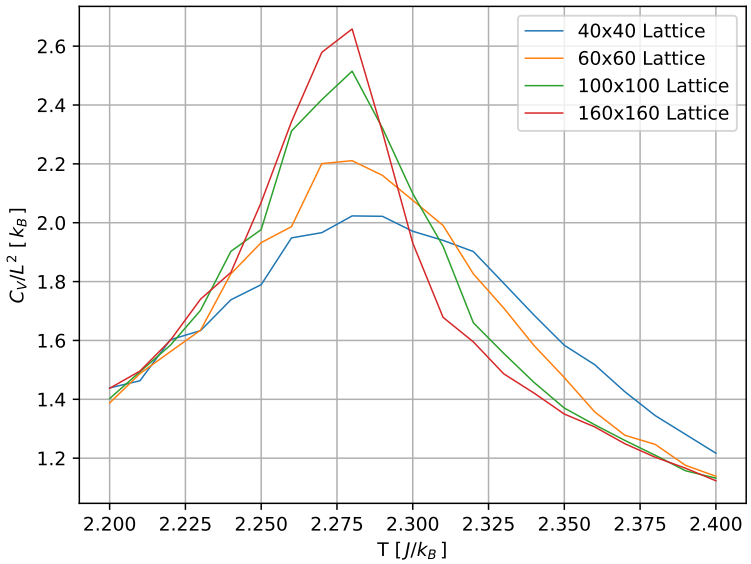


Figure 4.13

Figure 4.14 shows a plot of the susceptibility per spin as a function of temperature. The chosen temperature interval is $T \in [2.2, 2.4]$ with a stepsize of $\Delta T = 0.01$. The simula-

tion was performed with $N = 10^6$ Monte Carlo cycles, and for several lattice sizes using L=40,60,100,160.

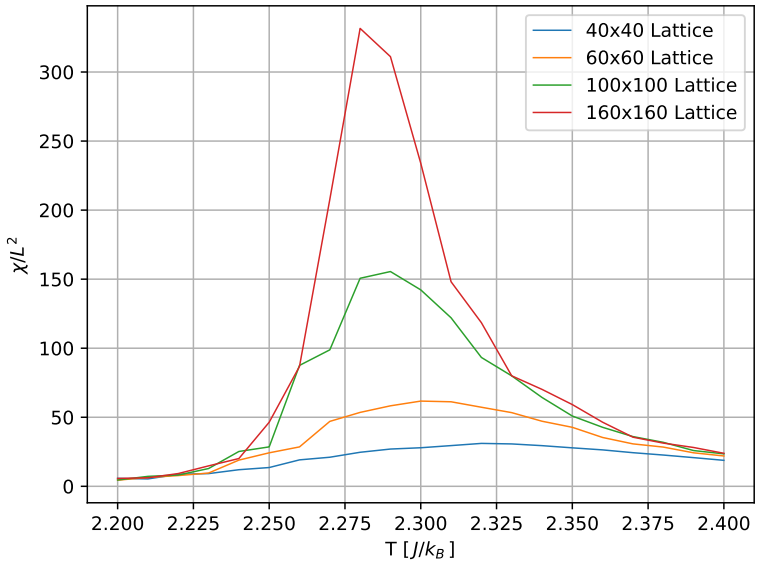


Figure 4.14: *This plot shows the susceptibility per spin as a function of temperature, where $T \in [2.2, 2.4]$ with $\Delta T = 0.01$. This was done for $N = 10^6$ Monte Carlo cycles, and for L= 40, 60, 100, 160.*

4.7 Parallelization Speed Up

In Table 4.2 and Table 4.3 a comparison of the CPU-time with and without parallelization is presented. The parallelization is done on eight threads vs one thread without parallelization. The table also shows the ratio of the two, which will show the relative speed up.

N	With MPI[s]	Without MPI[s]	Ratio
10^5	0.48	2.65	5.56

Table 4.2: *This figure shows the comparison of CPU-time with and without parallelization for number of monte carlo cycles $N = 10^5$ and zero pre-cylces. The ratio of these numbers is also given in the last column, which gives the relative speed up.*

N	With MPI[s]	Without MPI[s]	Ratio
10^5	0.56	2.79	4.98

Table 4.3: *This figure shows the comparison of CPU-time with and without parallelization for number of monte carlo cycles $N = 10^5$ and 1000 pre-cylces. The ratio of these numbers is also given in the last column, which gives the relative speed up.*

4.8 Extracting the Critical Temperature

In Figure 4.15 a plot of the critical temperature as a function of $1/L$ is presented. The plot is generated by extracting the critical temperature from Figure 4.14, and these values are linearly fitted in order to find the true critical temperature. The simulation is performed with $N = 10^6$ Monte Carlo cycles, and is done for L= 40, 60, 100, 160.

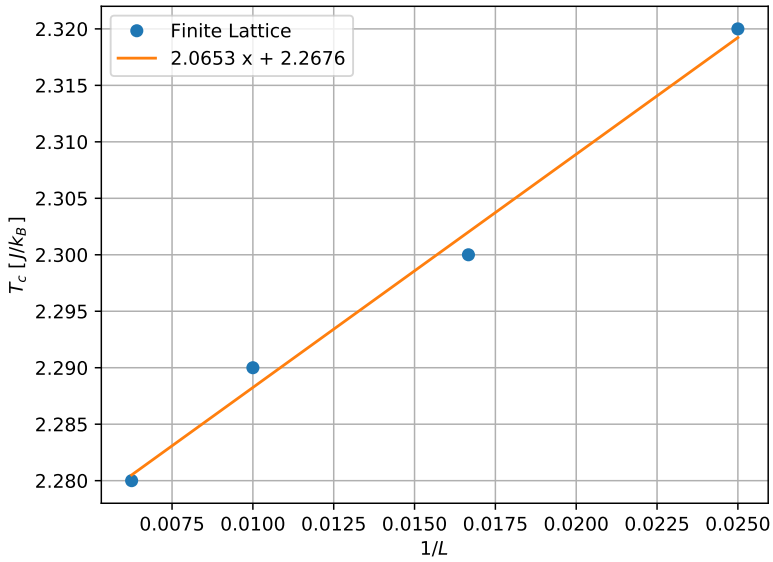


Figure 4.15: *This plot shows the critical temperature as a function of $1/L$. The points corresponds to simulations with finite lattices $L = 40, 60, 100, 160$ and these are linearly fitted in order to find the true critical temperature. The critical temperature is read of from the linear function as the constant term.*

5 Discussion

5.1 Comparing Numerical and Analytical Results for 2×2 Lattice

From table 4.1 we see trend of increasing numerical precision for higher number of Monte Carlo cycles, ending in a relative error of 4×10^{-5}, 5×10^{-5}, 5×10^{-4} and 1×10^{-3} for respectivly the mean energy, mean magnetization, heat capacity and susceptibility for $N = 10^7$. The simulation produces thus results of good numerical results for $T = 2$.

The figures 4.1, 4.2, 4.3 confirms that the numerical results also are accurate for a wider range of temperatures, as can be seen from the convergence of the numerical solution towards the analytical for increasing number of cycles.

This benchmark gives confidence that the model will yield reliable results also for larger lattices.

5.2 Equilibrium for Ordered and Disordered Initial State

Figure 4.4 (a) showns the energy starting near 0. This is expected, since the lattice is initiated randomly and anti parallel spins contribute positive energy. As the equilibrium energy for $T = 1$ is presumably much lower, the Metropolis Algorithm will favor lowering of the energy, resulting in a steep drop. Altough a litte hard too see, the energy seems to reach a equilibrium and flatten out after a mere 50 cycles.

The ordered chase 4.4 (b) for $T = 1$ appears to be already at equilibrium, as the change is energy seems uniform from the start. This is reasonable, as the ordered initial state is the lowest energy level. The equilibrium energy at $T = 1$ is marginally higher, effectively resulting in the system starting at equilibrium.

4.5 (a) and (b) shows the same trend for the magnetization as the energy.

For a higher temperature $T = 2.4$, 4.6 (a) shows that the disordered system equilibriates even faster, as the system doesn't have to fall all the way down to almost the minimum energy, but settles some time before it. The time to reach equilibrium for the ordered system (b) is now slightly longer for $T = 2.4$, since it needs to rise somewhat in energy. The number of cycles is however hard to count, but most certainly a small number.

Figure 4.7 (a) and (b) are hard to interpret, as the plots exhibit large amount of noise and fluctuations. This is however not surprising, as $T = 2.4$ is likely above the critical temperature of the finite crystal, causing the demagnetization of the crystal. The noise is thus presumably thermal noise.

Accurate number of cycles needed to reach equilibrium is hard to determine, as the number is often very small and the quantities are polluted with noise and fluctuations. Studying a larger lattice, e.i. 100×100, would be more insightful, as the time to equilibriate is longer and the relative amount of fluctuation is smaller.

5.3 Number of Accepted States

Figure 4.8 shows a linear relation between the number of stated accepted by the Metropolis algorithm as a function of number of cycles. This means a doubling of the cycles will roughly result in a doubling of accepted states. As the system reached equilibrium, as it was seen it does rather quickly, it tends to fluctuate around this energy. The average number of accepted states will thus be constant in time.

Figure 4.9 is a bit more interesting. It shows that the number of accepted states per sweep increases with temperature. As T grows, the acceptance amplitude moves towards unity, meaning states with relative higher energies become more easily accepted. This results in a more mobile system that more easily moves between different states, hence fluctuates more.

5.4 Probability Distribution

Figure 4.10 (a) is heavly skewed towards left, meaning for $T = 1$ the by far most likely state is the lowest energy state, $E = -800$. For higher temperatures, intuition tells us the most

probable energy should move to the right towards higher energies. Figure 4.10 (b) shows just this, a more or less normal normal distribution around approximatly $E = -480$.

A variance $\sigma_E^2 = 3258$ for $T = 2.4$ yields a standard deviation $\sigma_E = 57.08$. From 4.10 (b) this seems fair at a glance. Of course the calculated standard deviation of the distribution is identical, because they originate from the exact same data.

5.5 Studies of Phase Transitions

Figure 4.11 gives little insight beyond what has already been discussed, that the mean energy tends to increase for higher temperatures. This is a fact for several different lattice sizes.

Figure 4.12 is more interesting however. We know that for lattices approaching infinite size, we expect to observe a critical temperature T_c for which the system loses its magnetization. From the figure, we see that for incrementally larger lattices, the magnetization drops more and more sharply in the approximate range $T = [2.25, 2.30]$. This is hinting at a critical temperature for which the system rapidly loses it magnetization.

Figure 4.13 and 4.14 clearly shows maxima in the heat capacity and susceptibility for temperatures around the same range of temperature. These maxima are also increasing in size for larger lattices, pointing towards the divergencies we expect the system to exhibit in the thermodynamic limit. It is evident that the finite systems experience a approximate phase transition around the peaks of the heat capacity and susceptibility. Because of the more evenly spaced points, we have chosen the temperatures at which the maxima of the susceptibiltiy occur to be the critical temperature of the finite system.

Doing the finite scaling according to (2.2), we get the linear regression 4.15. Identifying the constant terms as the critical temperature in the thermodynamic limit $T_c(L = \infty)$, it is evaluated as $T = 2.2676$ against the analytical 2.2692, thus yielding a relative error of 6×10^{-4}. The approximation is correct to 3 digits, which is very good in that the resolution of the temperature in figure 4.14 was 0.01. Overall good correspondence.

5.6 Parallelization Speed Up

When moving from 1 to 8 threads, we got a speedup of about 5.56. For isolated processes that don't communicate much, one could expect a speedup closer to 8. However, at the end of the simulation, each node communicates $2 \times N$ long array at the end to the master node. This introduces a slowdown that scales with N. If the we had calculated all values in c++ rather than python, we could instead communicate just the expectation values at the end, resulting in a constant slowdown. MPI does not implement a perfect paralellization, so a speedup of 8 is not attainable.

When using 1000 pre-cycles, the speedup was even poorer. This is because each node must perform the pre-cycles to thermalize, meaning the more nodes you use, the more time you spend just thermalizing the system. This could have been mostly avoided using some clever tricks, such as using the last configuration as the initial configuration when simulation consecutive temperatures.

6 Conclusion

To summarize, our implementation showed good precision when benchmarked against analytical results in the 2×2 lattice case, peaking with a $10^{-5} - 10^{-4}$ relative error for $N = 10^7$ cycles. The numerical precision was also conserved for temperatures in the range $T = 1$ to $T = 3$.

The simulation of finite lattices showed clear tendencies of a second order phase transition. Especially the numerically estimated susceptibility showed clear maxima for given temperatures, i.e. critical temperatures the for finite systems. These peaks also got larger for larger lattice, hinting at divergencies in the susceptibility in the thermodynamical limit. The critical temperatures of the finite systems where distinct enough to yield a very accurate estimate of the Curie temperature in the thermodynamical limit of $T_c = 2.2676$, as opposed to the analytical value of $T_c \approx 2.2692$

7 Future Work

For future work, the implementation can be somewhat optimized. Most importantly would be to add a smarter way of initializing the system to ensure the shortest time to reach equilibrium. As discussed in 5.6, using the final configuration of last simulation as the initial for the next when simulation consecutive temperatures, as the equilibrium states ought to be very similar.

Further, the class Ising can easily be changed to explore different physical system, without changing the Metropolis class. E.g. an external magnetic field could be added to study phenomenons such as magnetic hysteresis. The Ising class could also be extended to model a 3D lattice.

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