STUDIES OF PHASE TRANSITIONS IN MAGNETIC SYSTEMS

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Abstract

In this project we have performed different experiments using the Ising model in two dimensions, which is a well-known model for studying phase transitions. The binary system will in this project consist of spins pointing either up or down. During this project, the values to be evaluated are mainly the mean energy $\langle E \rangle$, mean magnetization $\langle M \rangle$, mean absolute magnetization $\langle |M| \rangle$, specific heat (C_V) and the susceptibility χ. The implemented algorithms were first tested against analytical solutions for a 2×2 lattice and temperature $T = 1.0$. Using an ordered spin configuration (with all spins up) yielded good agreement for a sufficiently large number of Monte-Carlo cycles (10^7). The system was then expanded to a 20×20 lattice, also including a disordered (spin randomly up or down) initial configuration and temperature $T = 2.4$. By plotting expectation values, the time of equilibrium was found to be $\sim 10^-5$ Monte-Carlo cycles (though, the low temperature reached steady state a little earlier). In addition, the use of either an ordered or disordered initial spin configuration, turned out to be insignificant for the equilibrium time. In line with expectations, the probability distribution of the energies, showed increased variance σ^2 for a higher temperature, and the distribution took a Gaussian form for $T = 2.4$. Finally, we investigated phase transitions of lattices with size 40×40, 60×60, 80×80, 100×100, where the CPU time presented some problems and code optimization became valid.

1 Introduction

The Ising model was originally used to describe the magnetic properties of solids, and is today a widely used model in statistical physics and can be used to simulate phase transitions in thermodynamical system. The statistical model is a binary system where the objects at each lattice site can only take two values. For a lattice of atomic spins, the values are up or down. This project will use both ordered and disordered initial states of the lattice.

We will investigate how multiple interesting thermodynamic quantities, such as the expectation values mean magnetization and mean energy, as well as heat capacity and magnetic susceptibility, behave over time in the Ising model. This will give us the means to study phase transitions, by observing these quantities vary as functions of the temperature.

The behaviour of the spins will be estimated using the Metropolis algorithm, which is a particular Markov Chains Monte Carlo method. We will implement periodic boundary conditions. We want to study the Ising model in two dimensions because there are analytical solutions for several expectation values, which can be used as benchmark calculations for further simulations. For this project we used the programming language `Python`. To reduce CPU time during simulations, `Numba` will be implemented in our code [8].

In this report we will first present the necessary theory needed, before a quick method section describing our implementation. At the end we present and discuss our results, before concluding our findings. All figures and Python code used for this project can be found on our GitHub page [1].

2 Theory

2.1 Thermodynamics

Consider a system of M identical possible microstates. The probability of the system to be in microstate i, for a given energy E_i and temperature of the system T, is given by the Boltzmann distribution

$$P_i = \frac{e^{-\beta E_i}}{Z} \tag{1}$$

where $\beta = 1/k_B T$ and Z is the normalization factor, also called the partition function

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{2}$$

We will need certain statistical quantities to investigate this system. First, the mean energy and the mean squared energy are computed like this

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{3}$$

$$\langle E^2 \rangle = \sum_{i=1}^{M} E_i^2 P_i = \frac{1}{Z} \sum_{i=1}^{M} E_i^2 e^{-\beta E_i}. \tag{4}$$

where Z and E_i is given by equation (2) and (9) respectively. The energy variance is important as it relates to the specific heat capacity C_V of the system, given by

$$C_V = \frac{Var[E]}{k_B T^2} = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{5}$$

The mean magnetization and the mean squared magnetization are similarly found by

$$\langle \mathcal{M} \rangle = \sum_{i=1}^{M} \mathcal{M}_i P_i = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{-\beta E_i} \tag{6}$$

$$\langle \mathcal{M}^2 \rangle = \sum_{i=1}^{M} \mathcal{M}_i^2 P_i = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i^2 e^{-\beta E_i}, \tag{7}$$

where $\mathcal{M}_i$ is given by equation (10) in section 2.2. The susceptibility can be found in a similar way as the specific heat capacity, as it is proportional to the variance of the magnetization.

$$\chi = \frac{Var[\mathcal{M}]}{k_B T} = \frac{1}{k_B T}(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2) \tag{8}$$

Section based on *Ising Model and Phase Transitions in Magnetic System* lecture notes by M. Hjorth-Jensen [2].

2.2 The Ising model in two dimensions

The Ising model is a widely used statistical model for simulating phase transitions in a magnetic system with spin-spin interactions between particles. With the Ising model, we can get an better view of how magnetic materials respond to thermal energy and an external magnetic field. In this project we will consider the model for a 2 dimensional lattice of discrete particles with only two possible states, spin-up and spin-down, or simply $s = \pm 1$ [6].

The Ising model can be used for all n-dimensional systems, but we will focus on the 2-dimensional case. With zero external magnetic field, this is the only system that have been solved analytically. The general form of the Ising model is defined as the total energy of the system (the Hamiltonian)

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l - \mathcal{B} \sum_{k}^{N} s_k$$

The second term represents the effects of an external magnetic field, and $\mathcal{B}$ is the constant representing the strength of the field. We will not consider this in this project, so we set $\mathcal{B} = 0$ The Ising model that we will study is then on the form

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l \tag{9}$$

where the spins are given by $s_k = \pm 1$. The notation for the summation index $\langle kl \rangle$ indicates that we sum over nearest neighbors only. J is a coupling constant representing the strength of the spin-spin interaction, or interaction between neighbour spins.

We assume this strength to be the same for all interactions. The total number of spins is N. In this report we assume that we have a ferromagnetic ordering, $J > 0$. This models the tendency of physical systems to be in the lowest possible energy state, as microstates where the spins align are preferred.

The magnetization of the system in state i is the sum of all the individual spins

$$\mathcal{M}_i = \sum_{k=1}^{N} s_k \tag{10}$$

Because the sum in (9) iterates over all neighbors, we need boundary conditions for the border of the lattice. We will employ periodic boundary condition, that is the neighbor of the particles along the border are the ones on the other side, left-right and up-down. Intuitively is can be visualized as folding the lattice into a torus.

2.2.1 Analytical solution for a 2×2 lattice

Consider a simple model with four particles, arranged in a square 2×2 lattice. We then have dimension L=2 and 2^4=16 possible spin configurations (microstates). We can uniquely characterize the microstate by counting the number of spin-up states. The energy and magnetization can be computed using (9) and (10) respectively. Each energy represents a macrostate. We can from there count how many microstates give any energy. This number is called the degeneracy. The degeneracy, energy and magnetization of all spin configurations are represented in table 1. All spin configurations and the degeneracy number is explained in Appendix A.

Table 1: Degeneracy (nr. of microstates), energy and magnetization of all configurations of spins in a 2×2 grid. The table is the same as table 13.4 in chapter 13.3.1 in the course LN [2].

Number of ↑	Degeneracy	Energy (E_i)	Magnetization ($\mathcal{M}_i$)
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

In order to simplify our computations we will make use of the definition of degeneracy. Since degeneracy is the number of spin-configurations (microstates) that correspond to each energy level (macrostate), instead of summing over each microstate, we can instead sum over each macrostate and refer to table 3.

The detailed derivations of the expectation values, C_V and χ can be found in Appendix B. The analytical partition function is

$$Z = 2e^{8\beta J} + 2e^{-8\beta J} + 12 \tag{11}$$

The energy expectation values are

$$\langle E \rangle = \frac{16J}{Z}\left[e^{-\beta 8J} - e^{\beta 8J}\right] \tag{12}$$

$$\langle E^2 \rangle = \frac{128J^2}{Z}\left[e^{-\beta 8J} + e^{\beta 8J}\right] \tag{13}$$

By inserting the mean energy and mean squared energy results in equation (5), the specific heat capacity becomes

$$C_V = \frac{128J^2}{k_B T^2 Z}\left(\left[e^{-\beta 8J} + e^{\beta 8J}\right] - \frac{2}{Z}\left[e^{-\beta 8J} - e^{\beta 8J}\right]^2\right) \tag{14}$$

The magnetization expectation values are

$$\langle \mathcal{M} \rangle = 0 \tag{15}$$

$$\langle \mathcal{M}^2 \rangle = \frac{32}{Z}\left[1 + e^{\beta 8J}\right] \tag{16}$$

$$\langle |\mathcal{M}| \rangle = \frac{8}{Z}\left[2 + e^{\beta 8J}\right] \tag{17}$$

By inserting the mean magnetization and the mean square magnetization results in equation (8), the susceptibility becomes

$$\chi = \frac{1}{k_B T}\frac{32}{Z}\left[1 + e^{\beta 8J}\right] \tag{18}$$

2.3 Phase Transitions

A phase transition can occur when external changes, like an increase in temperature T, causes abrupt macroscopic changes in the system. The point where a phase transition occurs is called a critical point, and in our project, the Ising model undergoes a second order phase transition. The system goes from an ordered state (spins are mostly aligned) to a disordered state (random spin values). When the temperature in the system below a critical temperature T_C, we have an ordered state which exhibits spontaneous magnetisation. This does not occur in the disordered state, when the temperature is above T_C. From this vi have that the mean magnetisation should be zero when $T \geq T_C$ and nonzero for $T \leq T_C$ [2].

When the temperature is close (but below) to T_C, the thermodynamic statistical properties all behave according to power laws, where $\mathcal{M}$, C_V and χ behave according to

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \tag{19}$$

$$C_V(T) \sim |T_C - T|^{\alpha} \tag{20}$$

$$\chi(T) \sim |T_C - T|^{\gamma} \tag{21}$$

The critical exponents for the 2-dimensional system is β=1/8, α=0 and γ=7/4. An important feature of the critical point is the correlation length ξ, which are given by

$$\xi \sim |T_C - T|^{-\nu}, \tag{22}$$

where $\nu = 1$ is a critical exponent. ξ is a measurement of how strong the spins correlate, and ξ increases when the temperature nears T_C. In the 2-dimensional system with periodic boundary conditions, the lattice is finite with size L, which means that T_C will deviate slightly from that of an infinite lattice. With finite size scaling, T_C becomes

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{23}$$

where a is a constant. The deviation also affects the statistical properties, so by inserting equation (23) into equations (19), (20) and (21), they become

$$\langle \mathcal{M}(T) \rangle \approx L^{-\beta/\nu} \tag{24}$$

$$C_V(T)^{-1} \approx L^{\alpha/\nu} \tag{25}$$

$$\chi(T)^{-1} \approx L^{\gamma/\nu} \tag{26}$$

All equations are from the lecture notes [3].

The exact result for T_C were derived by Lars Onsager (1944) [9] to be

$$\frac{T_C k}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269 \tag{27}$$

2.4 Effective computations

There are a number of simplifications that can be employed in order to decrease the number of computations needed to get good results for these simulations. First we can exploit the fact that the energy E for any given spin can only be a discrete value listen in table 1. So when we are to compute the probability $w = e^{-\beta}$ we do not have to do it for every single spin state we iterate over, but rather compute them all beforehand and reference it. Secondly we can simplify the expression for computing the energy difference for a given microstate, that depends on its nearest neighbors, according to (9). It is only the one spin that flips in our algorithm, the surrounding neighbors remain in their configuration. The superscipt denotes different microstates. From the lecture notes [5], we have that

$$\begin{aligned}
\Delta E &= E_2 - E_1 \\
&= -J \sum_{\langle kl \rangle}^{N} s_k^2 s_l^2 - \left(-J \sum_{\langle kl \rangle}^{N} s_k^1 s_l^1 \right) \\
&= -J \sum_{\langle kl \rangle}^{N} \left(s_k^2 s_l^2 - s_k^1 s_l^1 \right) \\
&= -J \sum_{\langle kl \rangle}^{N} s_k \left(s_l^2 - s_l^1 \right)
\end{aligned} \tag{28}$$

Where we have used that $s_k^1 = s_k^2$ in the last step. Further, flipped spins means that we have $s_l^1 = -s_l^2 \equiv s_l^l$, so $s_l^2 - s_l^1 = -2s_l^l$. Putting this into equation (28) we get

$$\Delta E = 2J s_l^l \sum_{\langle k \rangle} s_k \tag{29}$$

We can find a similar compact expression for the magnetization.

$$\begin{aligned}\Delta M &= M_2 - M_1 \\ &= \sum_{k=1}^{N} s_k^2 - \sum_{k=1}^{N} s_k^1 \\ &= \sum_{k=1}^{N} \left(s_k^2 - s_k^1 \right) \\ &= s_k^2 - s_k^1\end{aligned}$$

Magnetization does not sum over neighbors, so the sum becomes a simple difference in the last step. Also we have that $s_k^2 = -s_k^1$. Then we get

$$\Delta M = 2s_k \tag{30}$$

2.5 Parallelization and CPU

When a large amount of MC-cycles have to be run, we need a large amount of computational power. As this project code are to be run on laptops, heavy parts of the code must be optimized and loops in the code should be parallelized. This will reduce CPU time significantly, and are achieved by implementing the **jit**-function from the Numba library in Python [7][8], with additional arguments such as nopython=True and parallel=True.

3 Method

The aim of this project is to study the phase shift in a system. We do this by considering the specific heat capacity C_V and magnetic susceptibility M as functions of temperature T. In order to compute these quantities, we need the 1st and 2nd moments of the energy and magnetization, that is the expectation values $\langle E \rangle$, $\langle E^2 \rangle$, $\langle M \rangle$ and $\langle M^2 \rangle$. We obtain these by using the Metropolis algorithm.

3.1 The Metropolis algorithm

THe Monte-Carlo methods is useful when the physical system has many degrees of freedom. It only requires a probability distribution function (PDF) that is proportional to the actual distribution, meaning we do not have to consider the normalization factor. The Metropolis algorithm needs only a probability distribution P to draw values from. In our study of the Ising model we will draw from the Boltzmann distribution (1). Because we can disregard the normalization factor, we do not have to concern ourselves with the partition function Z.

The Metropolis algorithm is very common in Monte Carlo simulations. It is an elegant algorithm, based on the ratio of probabilities, as explained in chapter 12.5 in the lecture notes [4]. Here follows a rough outline of the algorithm:

1. Define number of MC-cycles, T and L

2. Choose a random spin in the lattice with energy E_1, computed according to (9). Purpose as state where the spin is flipped, and then has energy E_2. Calculate the change in energy $\Delta E = E_2 - E_1$, equation (29). The number of available energy values are limited, see table 1.

3.
   - **if** $\Delta E \leq 0$: The new configuration is accepted, spin is flipped. The system has now gone to a lower energy state. Move directly to step 4.
   - **elif** $\Delta E > 0$: Calculate the probability $w = e^{-\beta \Delta E}$. Which is (1) without the normalization factor.
     Draw a random number $r \in [0, 1]$.
     - **if** $r \leq w$: The new configuration is accepted, spin is flipped. Calculate ΔM (30). Go to step 4.
     - **else**: Keep the initial state with energy E_1.

4. Update the expectation values, begin with step 2. Repeat until the number of MC-cycles is completed.

As mentioned before, $w = e^{-\beta}$, do not have to be calculated every time, but because of syntax error with Numba, we had to do so.

3.2 The Ising model for a 2×2 lattice

For the case of a 2×2 square lattice, it is possible to calculate the analytical solutions for $\langle E \rangle$, $\langle M \rangle$, $\langle |M| \rangle$, specific heat (C_V) and the susceptibility χ . The expressions for calculating these solutions are described in B. To test that our ising model worked properly, we implemented a method that computed the expected values of these features for a 2×2 lattice and temperature $T = 1.0$ [kT/J]. Then we ran 10 simulation of our implemented ising model, where each simulation had a maximum number of Monte-Carlo cycles of:

[5.e+02 1.e+03 5.e+03 1.e+04 5.e+04 1.e+05 5.e+05 1.e+06 5.e+06 1.e+07].

The computed analytical, and a selection of the numerical, values are listed in table 2.

To further visualize the agreement between the analytical and numerical values, we created methods for plotting the error ($|analytical - numerical|$) of $\langle |M| \rangle$ [1], and the spread of $\langle M \rangle$ (figure 1), as a function of number of Monte-Carlo cycles. The latter was created by running each simulation of maximum Monte-Carlo cycles a number of 30 times.

3.3 The Ising model for a 20×20 lattice

We continued our studies with a 20×20 lattice. In the previous exercise we did not study carefully how many Monte-Carlo cycles were needed in order to reach the most likely state. This is important knowledge one should know before calculating the expectation values. So, in this experiment we implemented algorithms to study the "time" (in practice the number of Monte-Carlo sweeps per lattice) needed before an equilibrium situation is obtained.

For this experiment we investigated the impact of the initial state of the spin matrix and temperature. As in the previous experiment, we first used an ordered initial state (all spins equal in one direction, here set to 1). For the second configuration, we used a disordered initial state by setting random indices of the lattice to -1 instead of 1. We used the "low temperature" of $T = 1.0$ [kT/J] from the previous experiment, but also included a "high temperature" situation with $T = 2.4$ [kT/J]. Thus, by looping over the two initial spin matrices and running the simulation for each temperature, we investigated a total of 4 different cases in this experiment.

For each combination of initial spin matrix and temperature, we plotted the expectation values for $\langle E \rangle$ (figure 2), $\langle |M| \rangle$ (figure 3), C_V (figure 4) and χ (figure 5) as a function of Monte-Carlo cycles, to investigate at which time an equilibrium situation appeared. We used a maximum number of Monte-Carlo cycles of 10^6. We also counted the number of accepted configurations for each lattice sweep, which result is illustrated by figure 6.

3.4 Probability distribution for a 20×20 lattice

We continued the study of the 20×20 lattice by now looking at the probability distribution P(E) for the system. Using an ordered initial spin configuration and a maximum number of Monte-Carlo cycles of 10^6, we obtained the values of the energy (E) from the Monte-Carlo algorithm. Then, starting at the time of equilibrium (steady state), we counted the number of times the different energies appeared. To vizulaize the probability, we created a histogram of the counted energies for the case of $T = 1.0$ (7) and $T = 2.4$ (8). The variance in energy,σ^2, was also computed in each case and included in the corresponding figures.

3.5 Phase transitions

When simulating phase transitions we wanted to study the behavior of the 2D Ising model close to the critical temperature, as a function of the lattice size. We calculated and plotted the expectation values, C_V and χ, where the only change we made to the algorithm were to use $\langle |\mathcal{M}| \rangle$ when calculating χ.

We made a loop, where we for each L value calculated the expectation values, C_V and χ for all temperature steps, before the results were plotted in four different figures. Each figures were made to include the current expectation values, C_V or χ for all $L = [40, 60, 80, 100]$ values as a function of temperature. The temperature interval were set to $T \in [2.0, 2.3]$ with $\Delta T = 0.02$, as we knew the analytical critical temperature from (27).

While running the code with 10^7 MC-cycles, we quickly realised that the CPU time for the simulation would be a problem. We initially intended to parallelize the code as explained in section 2.5, in addition to the implemented just-in-time (jit) compilation with Numba, but we ran into problems when setting the parallel option for **jit()**.

4 Results and Discussion

4.1 The Ising model for a 2×2 lattice

In table 2 we have the expectation values for the mean energy and the mean (and absolute) magnetisation, specific heat and the susceptibility. We can see from the table that the simulation needs 10^7 MC-cycles to achieve a good agreement, to get $\langle \mathcal{M} \rangle$ close to zero. If we disregard this value, we reach a good agreement with 10^5-10^6 MC-cycles.

Table 2: The table contains the calculated and analytical expectation values for $\langle E \rangle$, $\langle \mathcal{M} \rangle$ and $\langle |\mathcal{M}| \rangle$, as well as for specific heat C_V and the susceptibility χ, as a function of MC-cycles.

MC cycles	$\langle E \rangle$	C_V	$\langle \mathcal{M} \rangle$	$\langle \lvert\mathcal{M}\rvert \rangle$	χ
Numerical					
10^3	-2.000000	0.000000	1.000000	1.000000	0.000000
10^4	-1.996400	0.028748	0.716700	0.998900	1.939564
10^5	-1.996040	0.031617	0.224325	0.998675	3.792103
10^6	-1.996158	0.030677	-0.022934	0.998737	3.991528
10^7	-1.995993	0.031997	0.016795	0.998665	3.992194
	(12)	(14)	(15)	(17)	(18)
Analytical	-1.995982	0.032082	0.000000	0.998661	3.993304

In figure 1, we have plotted the spread of expected mean magnetisation with $T = 1.0$, as a function of Monte Carlo cycles. The analytic value is zero, as seen in table 2, which the graph shows a clear tendency towards with increased MC-cycles. This indicates that the algorithm successfully simulates the Ising model.

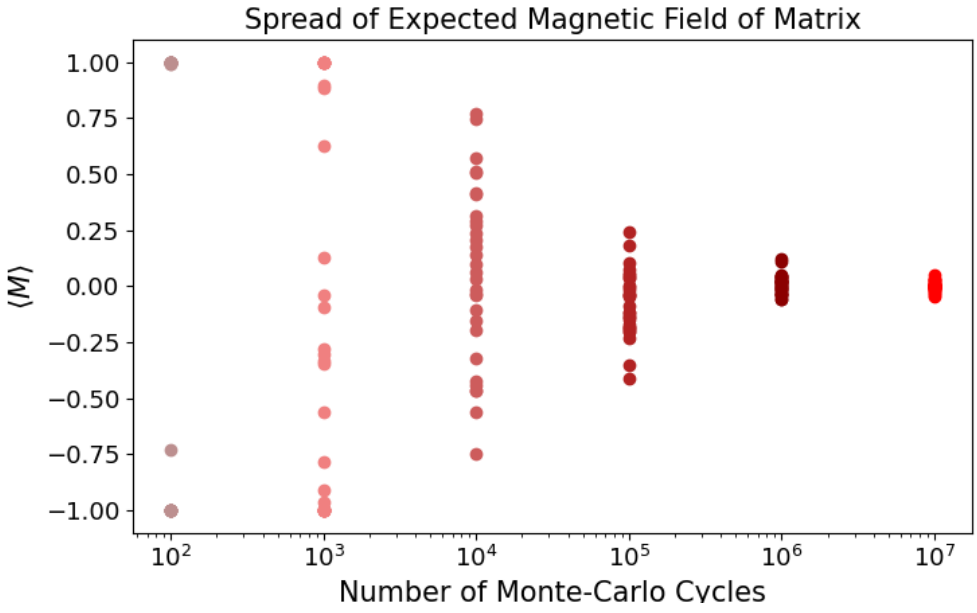

Figure 1: Spread of expected $\langle \mathcal{M} \rangle$ for the 2×2 lattice with $T = 1.0$, as a function of MC-cycles.

4.2 The Ising model for a 20×20 lattice

The results from the experiment with the 20×20 lattice are in figures 2-5. In figure 2 we observe the evolution of the mean energy of the system, as a function of MC-cycles along the x-axis. The evolution is shown for two temperatures, with the two initial configurations ordered and disordered, as explained in section 3.3. We note that the systems with different temperatures converge toward different mean energies. The higher temperature ($T = 2.4$) has a higher energy than the lower. We have the same evolution for the mean absolute magnetisation in figure 3. Here we see that a high temperature yields a lower magnetization than the lower one. This is because a higher temperature means more random orientations of the spins, and thus the net magnetic momentum is decreased.

The specific heat and the susceptibility are shown in figure 4 and 5. Common for all figures except for C_V (figure 4) is that the low temperature simulations ($T = 1.0$) show more stable tendencies in their convergence to their equilibrium states. In the case of C_v simulation with the disordered starting configuration varies wildly before converging around 10^5. Lower temperature systems generally reach equilibrium with a lower number of MC-cycles.

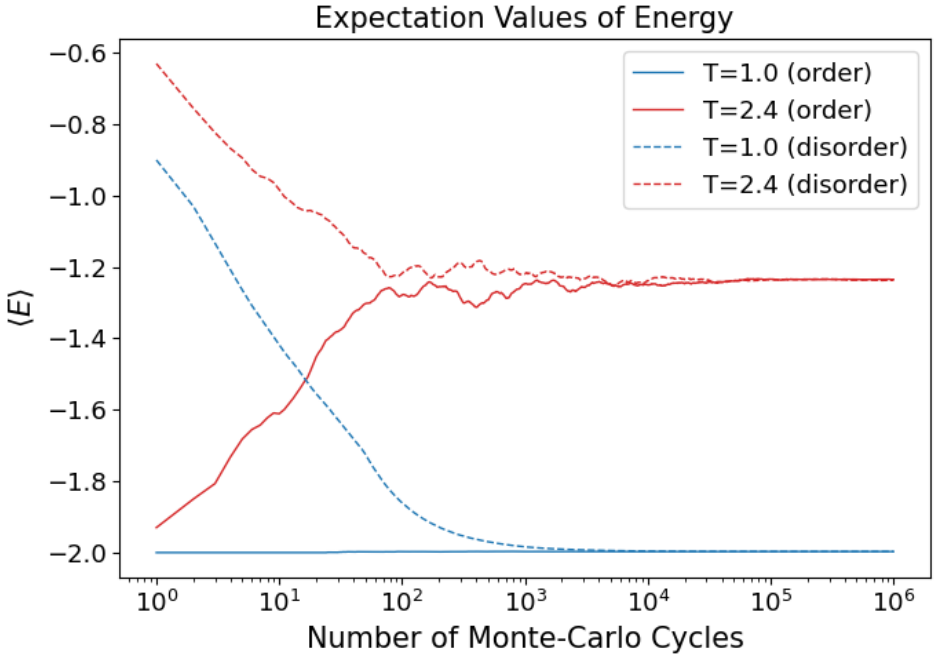

Figure 2: Evolution of $\langle E \rangle$ per spin of the 20×20 Ising system with two starting configurations (order and disorder), for $T = 1.0$ and $T = 2.4$ [k_BT/J].

From figures 2 and 3 we can see that the simulations converge to an equilibrium values after 10^4 MC-cycles for $T = 1.0$. While for $T = 2.4$, they reach stable values after 10^5 MC-cycles. This indicates that the system is more chaotic for higher temperatures, that is the tendency to converge is lower. In figure 4, the equilibrium is reached after $5 * 10^4$ MC-cycles for C_V at $T = 1.0$ and 10^4 MC-cycles at $T = 2.4$. For χ, as shown in figure 5, we get stable values after 10^4 cycles for $T = 1.0$ and a little above 10^5 for $T = 2.4$.

Overall, we have reached equilibrium for all quantities when we use at least 10^5 Monte Carlo cycles in our simulations.

Figure 6 displays the acceprance rate for the two temperatures as a function of MC cycles. We observe that for the lower temperature, the acceptance rate is constant and significantly lower than for the high temperature, for both initial configurations. We also observe that the initial configurations have almost none impact on the convergence to the equilibrium value.

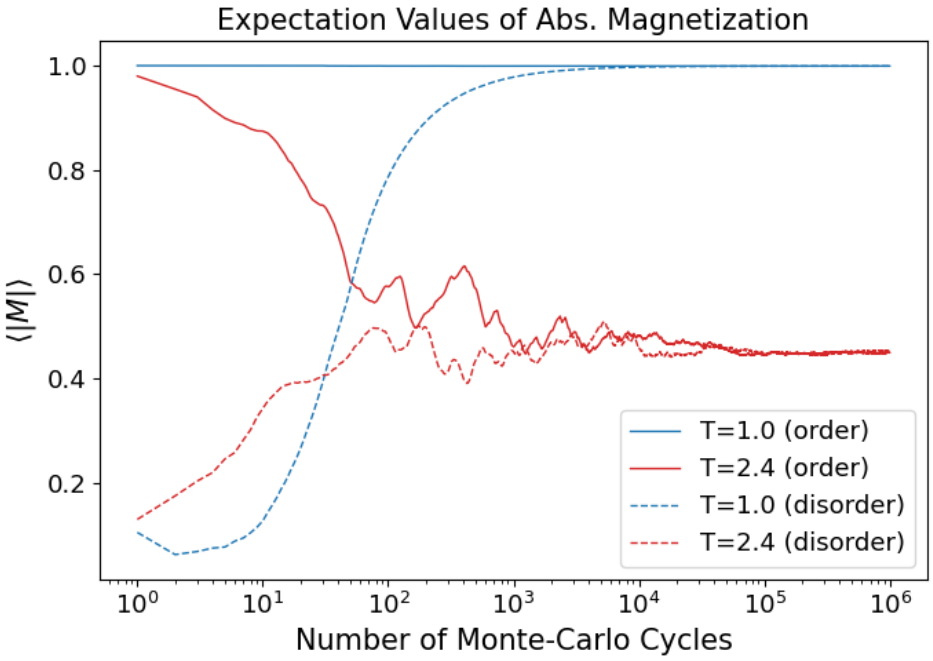

Figure 3: Evolution of $\langle|\mathcal{M}|\rangle$ per spin of the 20×20 Ising system with two starting configurations (order and disorder), for $T = 1.0$ and $T = 2.4$ [k_BT/J].

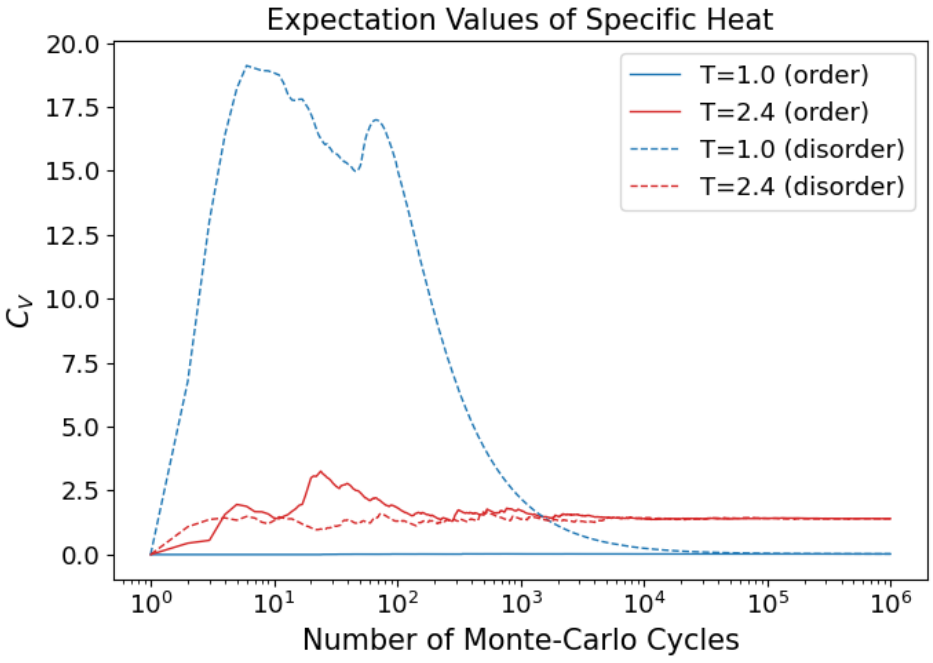

Figure 4: Evolution of C_V of the 20×20 Ising system with two starting configurations (order and disorder), for $T = 1.0$ and $T = 2.4$ [k_BT/J].

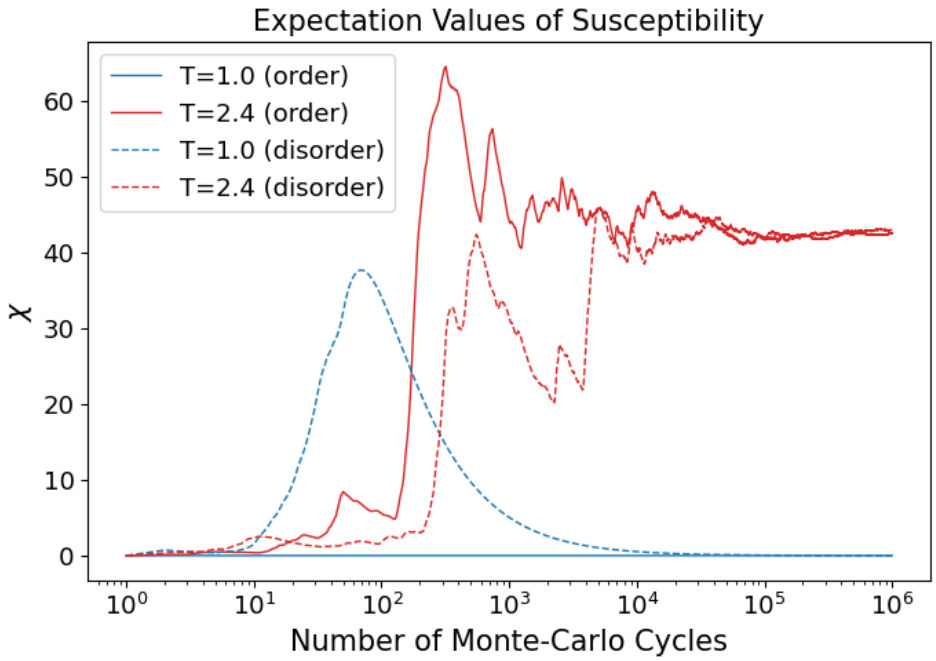

Figure 5: Evolution of χ of the 20×20 Ising system with two starting configurations (order and disorder), for $T = 1.0$ and $T = 2.4$ [k_BT/J].

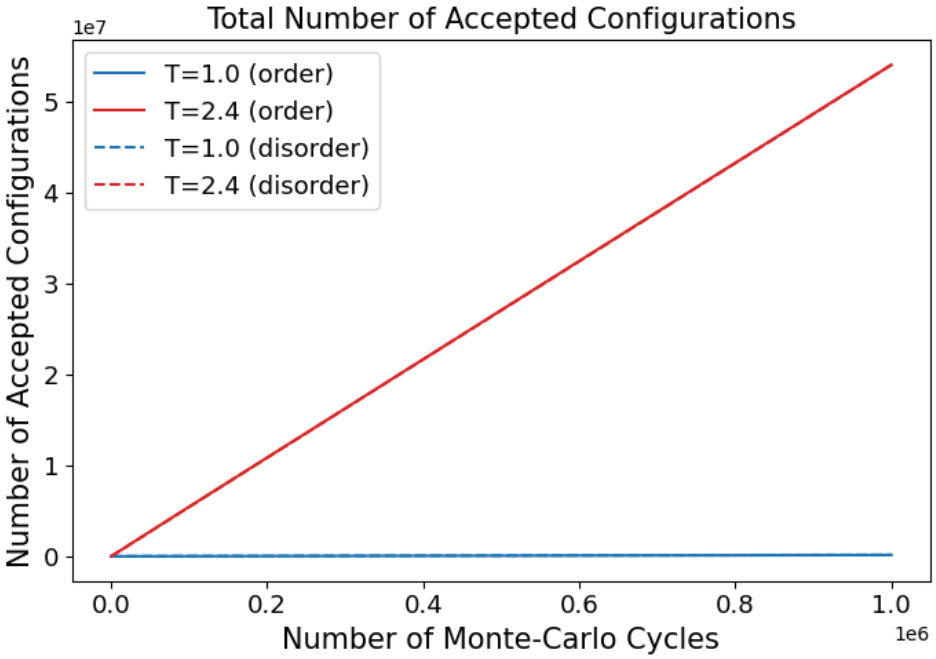

Figure 6: Total number of accepted configurations with two starting configurations (order and disorder), for $T = 1.0$ and $T = 2.4$ [k_BT/J].

4.3 Probability distribution for a 20×20 lattice

After the system reaches equilibrium, the normalized histograms in figure 7 and 8 show the frequencies of energies that appear in the simulation, for $T = 1.0$ and $T = 2.4$ respectively. We observe that the probability distribution for the low temperature seems to be exponential and around $E = -2.0$, while the higher temperature seems to have an Gaussian probability distribution around $E = -1.2$. This seems to suggest a sharp "cut off point" for the energies for the lower temperature.

We can see from the variance σ^2 in the figures that with increased temperature, the variance is higher. This is as expected, since we observe higher fluctuations in the energy when the temperature is higher. As shown energies take longer to converge and their paths are less stable, so the fluctuations about the equilibrium give rise to the Gaussian form of the probability distribution if their energies.

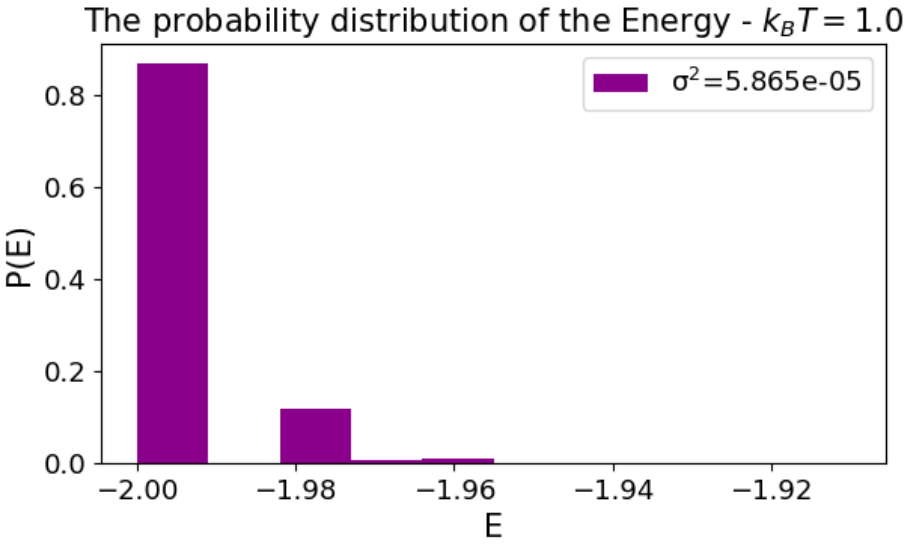

Figure 7: Frequency of certain energies for a 20×20 lattice with $T = 1.0$ [k_BT/J]

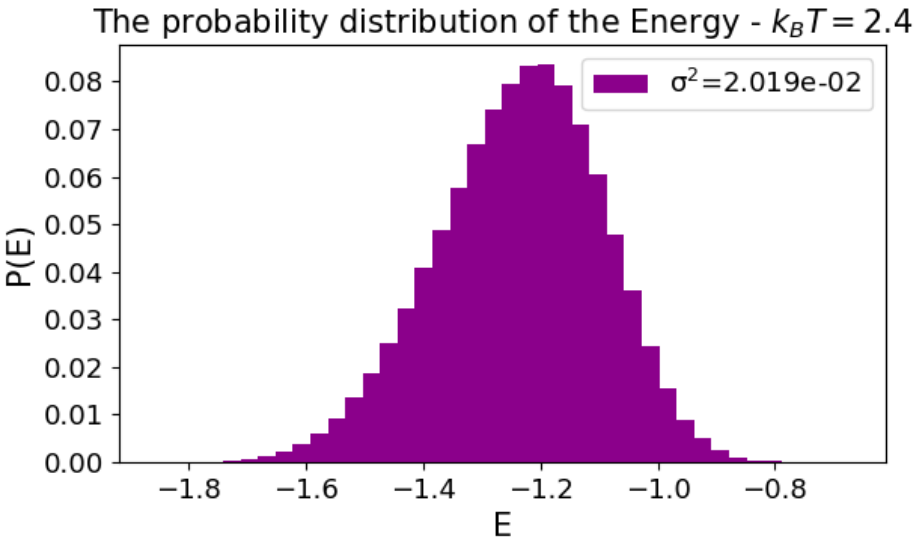

Figure 8: Frequency of certain energies for a 20×20 lattice with $T = 2.4$ [k_BT/J]

4.4 Phase transitions and critical temperature

In order to study the phase transitions in a thermodynamical system, we made plots that shows $\langle E \rangle$, $\langle M \rangle$, C_V and χ as functions of temperature T. We know that C_V and χ will diverge to infinity at the critical temperature. This does not happen in our simulations, because we do not have an infinite lattice. Instead we can only study the tendency when we increase the size by increasing L.

Figures 9 and 10 show the mean energy and magnetization respectively. As expected it shows that energy increases approximately linearly with higher temperatures, and that the increased energy gives a more disordered configuration of the spins, so the magnetization decreases. There is no great variation with the increase of L except around the temperature $T \approx 2.75$.

Figures 11 and 12 show C_V and χ. As discussed above, these are expected to diverge around the critical temperature T_C, and indeed we see a peak forming around $T_C \in [2.26, 2.28]$, and the peak is higher with increasing L, meaning our model becomes more realistic when our lattice is larger.

From equation (27), we have that the analytical critical temperature is $T_C k_B / J \approx 2.269 \approx 2.27$, which is in good agreement with our estimation from the simulations.

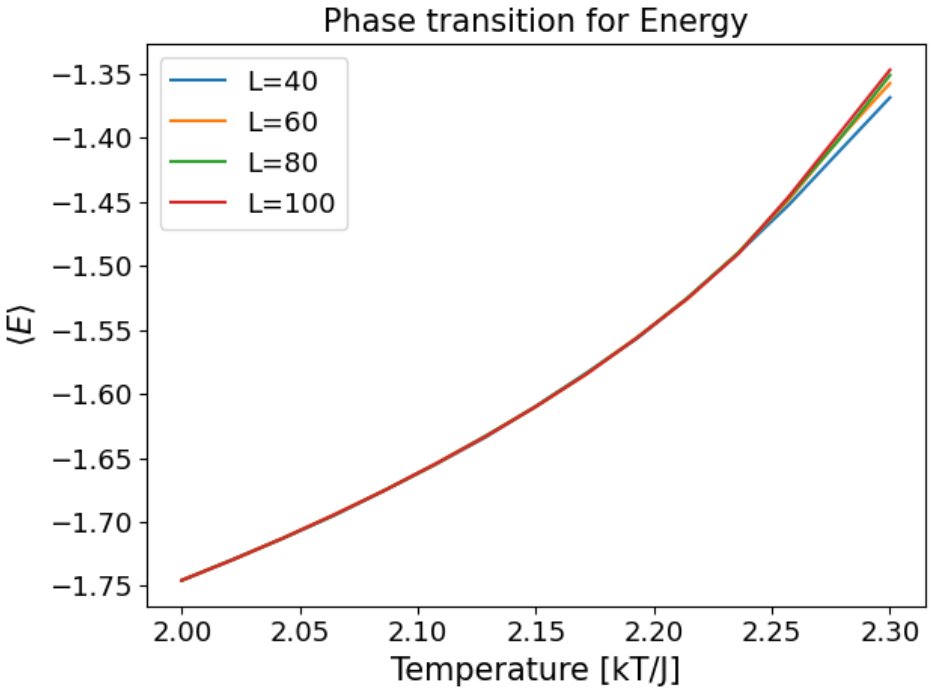

Figure 9: Phase transition for mean energy (per spin) in the system, as a function of temperature [k_BT/J], for $L = [40, 60, 80, 100]$ and $\Delta T = 0.02$.

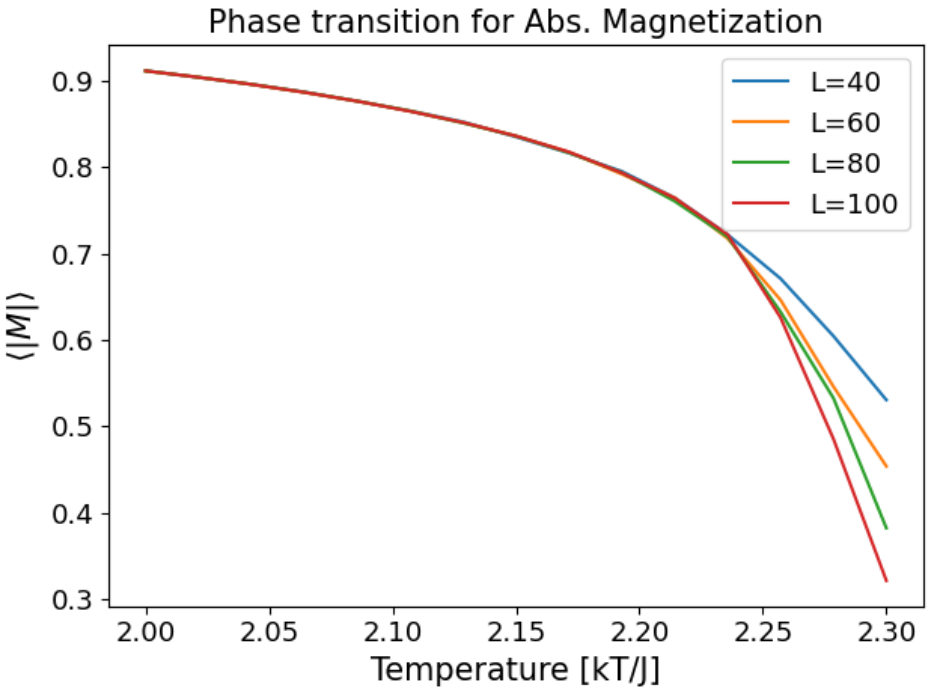

Figure 10: Phase transition for mean absolute magnetisation (per spin) in the system, as a function of temperature [k_BT/J], for $L = [40, 60, 80, 100]$ and $\Delta T = 0.02$.

In figure 11 we have the phase transition for the specific heat (per spin) as a function of temperature. We observe that C_V increases with higher temperatures, reaching a peak we assume to be the critical point. The exact peak location vary slightly in temperature, and more in specific heat. We observe that the critical point are right around the analytical critical temperature. From reading the critical temperature from the figure directly, we estimate it to be right around $T = 2.27$ as expected. As the peaks are slightly off from each other for the various L values, and an exact reading is difficult, we would say $T_C \in [2.265, 2.275]$.

These estimations of T_C are very crude, but they do approximate the value for the analytical T_C. The CPU times for these simulations were significant, around 4-5 hours, which put limitations on what we could work with in the time given. More accurate estimates of T_C should be made for a better assessment of the quality of the simulations.

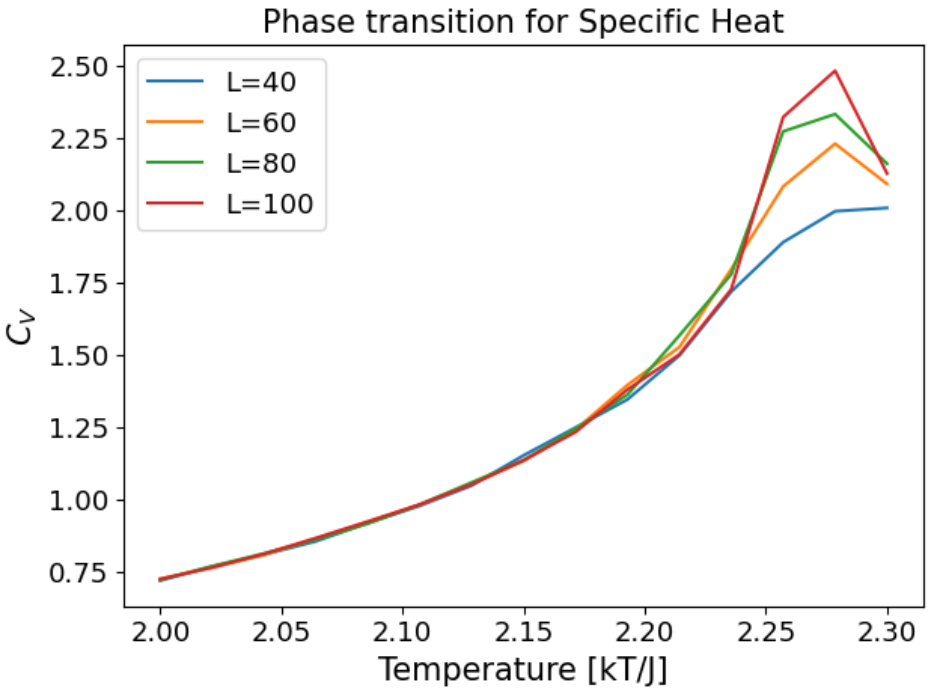

Figure 11: Phase transition for specific heat (per spin) in the system, as a function of temperature [k_BT/J], for $L = [40, 60, 80, 100]$ and $\Delta T = 0.02$.

Our approach on calculating the critical temperature uses equation (23) and $\nu = 1$

$$T_C(L = \infty) = T_C(L) - aL^{-1},$$

Where we can calculate the constant a by

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1} - L_2^{-1}}$$

Using the equation above, using the results from the C_V-simulation and $L_1 = 40$ and $L_2 = 100$, we get

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1} - L_2^{-1}} = \frac{2.265 - 2.27}{40^{-1} - 100^{-1}} = -0.33$$
$$T_C(L = \infty) = T_C(L_2) - aL_2^{-1} = 2.27 + 0.33 * 100^{-1} = 2.273$$

This T_C is relative close to the theoretical value. We choose $L = 100$ as the best L for calculating the critical temperature, as it got the highest and narrowest peak.

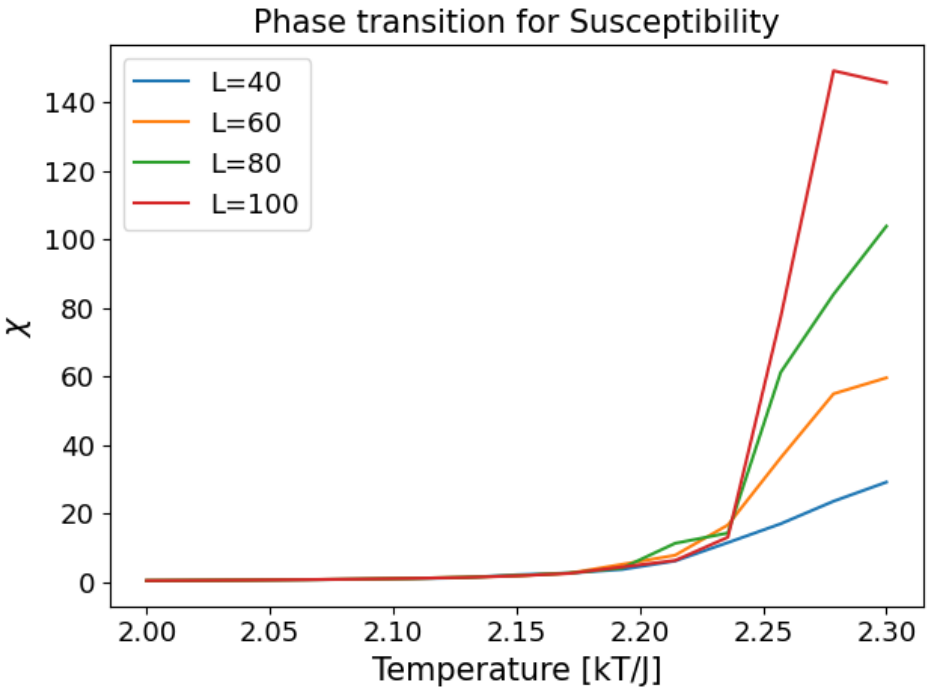

Figure 12: Phase transition for mean susceptibility (per spin) in the system, as a function of temperature [k_BT/J], for $L = [40, 60, 80, 100]$ and $\Delta T = 0.02$.

Conclusion

By using the Ising model in two dimensions, we have looked at the binary system consisting up spins pointing up (equal to 1) or down (equal to -1), and performed different experiments which have been evaluated by E, $\langle E \rangle$, $\langle M \rangle$, $\langle |M| \rangle$, C_V and χ.

We have seen that the implemented algorithms performs well in our studies, by getting several expected results. In addition, we have established that the initial state of the spin matrix have little impact on the time of reached equilibrium, since they converged at approximately the same time. For the lower temperature case, the expectation values have shown a tendency of more "stable" paths towards the equilibrium. The higher temperature case needed in general a little more time to reach a steady state. Therefore, the overall needed number of Monte-Carlo cycles was found to be about 10^5.

Although the implemented algorithms for the Ising model in most cases yielded expected and/or reasonably results, there have been some problems during the process. To be able to compute the experiments with the required number of Monte-Carlo cycles within a satisfying computation time, the main algorithms have been dependent on some additional optimization tools. For this project, we ended up using the just-in-time compiler provided by Numba, which automatically contributed to a significantly lower computation time in most situations. Being new to Numba and this sort of required code optimization, we have improved our understanding of this subject. For instance, large parts of the code must have been written in such a way that the code could be compiled in "no python" mode to achieve good enough speed-up of the computation. However, when encountering the phase transition experiment, our

Ising model did not perform as fast as desired. This will hopefully be solved in the near future, by rewriting some parts of the code, so that the argument "parallel=True" can be passed to njit() without causing any conflicts.

In addition, to estimate the critical temperature better, it would be smart to run the simulation for a narrower temperature interval around $T = 2.27$. This would give more datapoints around the analytical T_C, and the critical point would potentially stand out more.

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Appendix A 2×2 Ising Model: Spin configurations

In table 3 we have an overview of all 16 possible spin arrangements of the 2×2 Ising model. From this information we can fill up the degeneracy column in table 1. There is only 1 occurrence where all four spin states are up ($E = -8J$). The same occurs for when all spin states are down ($E = -8J$). There are 4 occurrences where tree spin states are up ($E = 0$), and 4 occurrences where tree spin states are down ($E = 0$). For the 6 occurrences where we have two spin-up and two spin-down states, we have to look closer at which positions the up- and down states are in the matrix. There are 2 cases where the flipped spins are not neighbours, meaning there will be no interaction between them. We then have $E = 8J$. For the four other occurrences, we have $E = 0$.

Table 3: All 16 configuration of the 2×2 Ising model on a 2D lattice. Each spin is allowed to occupy a spin-up state ($\uparrow$) or a spin-down state ($\downarrow$).

$\uparrow\uparrow$ $\uparrow\uparrow$	$\downarrow\uparrow$ $\uparrow\uparrow$	$\uparrow\downarrow$ $\uparrow\uparrow$	$\uparrow\uparrow$ $\uparrow\downarrow$
$\uparrow\uparrow$ $\downarrow\uparrow$	$\uparrow\uparrow$ $\downarrow\downarrow$	$\downarrow\downarrow$ $\uparrow\uparrow$	$\uparrow\downarrow$ $\uparrow\downarrow$
$\downarrow\uparrow$ $\downarrow\uparrow$	$\downarrow\uparrow$ $\uparrow\downarrow$	$\uparrow\downarrow$ $\downarrow\uparrow$	$\uparrow\downarrow$ $\downarrow\downarrow$
$\downarrow\uparrow$ $\downarrow\downarrow$	$\downarrow\downarrow$ $\downarrow\uparrow$	$\downarrow\downarrow$ $\uparrow\downarrow$	$\downarrow\downarrow$ $\downarrow\downarrow$

Appendix B Quantities for a 2×2 lattice grid

The appendix shows the detailed derivation of the analytical 2×2 lattice quantities. These equations/results will be used as benchmark calculations when building the numerical Ising model. The partition function is computed, using equation (2).

$$\begin{aligned} Z &= \sum_{i=1}^{M=16} e^{-\beta E_i} \\ &= \sum_{E} deg(E) e^{-\beta E} \\ &= 1e^{-\beta(-8J)} + 4e^{0} + 4e^{0} + 2e^{-\beta(8J)} + 4e^{0} + 1e^{-\beta(-8J)} \\ &= 2e^{8\beta J} + 2e^{-8\beta J} + 12 \end{aligned}$$

In the first step we change the sum from iterating over every microstate i to every energy level E instead. We then calculate the mean energy and mean squared energy with equation (3) and (4) respectively, and get

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} E_i e^{-\beta E_i} \\ &= \frac{1}{Z} \sum_{E} deg(E) E e^{-\beta E} \\ &= \frac{1}{Z} \Big[(-8J)e^{-\beta(-8J)} + 4(0)e^{0} + 4(0)e^{0} + 2(8J)e^{-\beta 8J} + 4(0)e^{0} + (-8J)e^{-\beta(-8J)} \Big] \\ &= \frac{16J}{Z} \left[e^{-\beta 8J} - e^{\beta 8J} \right] \end{aligned}$$

$$\begin{aligned} \langle E^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} E_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z} \sum_{E} deg(E) E^2 e^{-\beta E} \\ &= \frac{1}{Z} \Big[(-8J)^2 e^{-\beta(-8J)} + 4(0)^2 e^{0} + 4(0)^2 e^{0} + 2(8J)^2 e^{-\beta 8J} + 4(0^2) e^{0} + (-8J)^2 e^{-\beta(-8J)} \Big] \\ &= \frac{128J^2}{Z} \left[e^{-\beta 8J} + e^{\beta 8J} \right] \end{aligned}$$

By inserting the mean energy and mean squared energy results in equation (5), the specific heat capacity C_V becomes

$$\begin{aligned} C_V &= \frac{1}{k_B T^2} \left(\frac{128J^2}{Z} \left[e^{-\beta 8J} + e^{\beta 8J} \right] - \left[\frac{16J}{Z} \left[e^{-\beta 8J} - e^{\beta 8J} \right] \right]^2 \right) \\ &= \frac{1}{k_B T^2} \left(\frac{128J^2}{Z} \left[e^{-\beta 8J} + e^{\beta 8J} \right] - \frac{256J^2}{Z^2} \left[e^{-\beta 8J} - e^{\beta 8J} \right]^2 \right) \\ &= \frac{128J^2}{k_B T^2 Z} \left(\left[e^{-\beta 8J} + e^{\beta 8J} \right] - \frac{2}{Z} \left[e^{-\beta 8J} - e^{\beta 8J} \right]^2 \right) \end{aligned}$$

We calculate the mean magnetization and the mean square magnetization with equation (6) and (7) respectively, and get

$$\begin{aligned}\langle \mathcal{M} \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} \mathcal{M}_i e^{-\beta E_i} \\ &= \sum_{\mathcal{M}} deg(\mathcal{M}) \mathcal{M} e^{-\beta E} \\ &= \frac{1}{Z} \Big[4e^{-\beta(-8J)} + 4 * 2e^0 + 4(0)e^0 + 2(0)e^{-\beta 8J} + 4 * (-2)e^0 + (-4)e^{-\beta(-8J)} \Big] \\ &= 0\end{aligned}$$

$$\begin{aligned}\langle \mathcal{M}^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} \mathcal{M}_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z} \sum_{\mathcal{M}} deg(\mathcal{M}) \mathcal{M}^2 e^{-\beta E} \\ &= \frac{1}{Z} \Big[4^2 e^{-\beta(-8J)} + 4 * 2^2 e^0 + 4(0)^2 e^0 + 2(0)^2 e^{-\beta 8J} + 4 * (-2)^2 e^0 + (-4)^2 e^{-\beta(-8J)} \Big] \\ &= \frac{32}{Z} \Big[1 + e^{\beta 8J} \Big]\end{aligned}$$

By inserting the mean magnetization and the mean square magnetization results in equation (8), the susceptibility χ becomes

$$\chi = \frac{1}{k_B T} \left(\frac{32}{Z} \Big[1 + e^{\beta 8J} \Big] - 0^2 \right) = \frac{1}{k_B T} \frac{32}{Z} \Big[1 + e^{\beta 8J} \Big]$$

The expected mean absolute magnetisation $|M|$, is given by

$$\begin{aligned}\langle |\mathcal{M}| \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} |\mathcal{M}_i| e^{-\beta E_i} \\ &= \frac{1}{Z} \sum_{\mathcal{M}} deg(|\mathcal{M}|) e^{-\beta E} \\ &= \frac{1}{Z} \Big[4e^{-\beta(-8J)} + 4 * 2e^0 + 4(0)e^0 + 2(0)e^{-\beta 8J} + 4 * |-2|e^0 + |-4|e^{-\beta(-8J)} \Big] \\ &= \frac{8}{Z} \Big[2 + e^{\beta 8J} \Big]\end{aligned}$$