Studies of Phase Transitions in Magnetic Systems

Modelling the two dimensional Ising model according to the Monte Carlo method using the Metropolis algorithm

Elias Tidemand Ruud, Bendik Nyheim & Mira Mors

Computational Physics I FYS3150/FYS4150

Department of Physics
University of Oslo
Norway
November 2020

Abstract

This report has the aim of determining the critical temperature of an infinity lattice based on the two dimensional Ising model. Computations are first done for a 2×2 which serve as a benchmark. Using a 20×20 lattice, it is shown that an ordered spin configuration is most stable at low temperatures with an average magnetization not zero. Whereas, a random spin orientation is stabilised at high temperatures where the averaged magnetization decays to zero. Based on computations for a $40^2, 60^2, 80^2$ and 100^2 lattice, the critical temperature for an infinite lattice is estimated to be 2.2699. According to Lars Onsager the analytical value is ~ 2.2692. Natural units were used. When ran in parallel on eight threads, the runtime was sped up by a factor of ~ 3.5. The code can be found here Github repository.

Contents

1 Introduction

Ferromagnetism is an interesting phenomenon in solid state physics. Until today, the Ising model is the only semi-realistic model that can be studied accurately in statistical physics for up to two dimensions. Furthermore, the Ising model is perhaps the simplest model for a system with interactions and is usually used to study ferromagnetism. Despite its simplicity, it can quantitatively describe many properties of systems undergoing phase transitions. A phase transition is defined as a fundamental change in the properties of the material at a critical point. This change often implies a change in order and symmetry. A well known example is the transition from ice to water at 0 °C. Ferromagnetic materials posses a spontaneous magnetisation without an external magnetic field. This is based on the ferromagnetic coupling of parallel aligned spins. However, the spontaneous magnetisation decreases with increasing temperature and thus works against the alignment. The Ising model is used to calculate the magnitude of the spontaneous magnetisation and thus allows to determine the critical temperature. At this and higher temperatures, the system is paramagnetic with an average magnetization decaying to zero. The main aim of this report is to determine the critical temperature.
The report first introduces the two dimensional Ising model with the most important thermodynamical quantities. Next, the phase transition is explained in more detail. Thereafter, it is shown how the Monte Carlo method, using the Metropolis algorithm as a sampling rule, can be used to solve the Ising model. Code optimization is also addressed. Calculations are done for different lattice sizes $N = \{2, 20, 40, 60, 80, 100\}$. Using $N = \{40, 60, 80, 100\}$, the critical temperature for an infinite lattice is estimated. Finally, the results are presented and discussed.

2 Methods

The following explanations are based on [1], [2]. [3], and [5].

2.1 Ising model - two dimensions

The starting point for the two dimensional Ising model is a square lattice of $N \times N$ spins s. Each spin can either point up or down, represented by the values $+1$ and -1 respectively. In our case, the spins stand for the electrons in the sample. Electrons are fermions having a half odd integer spin. Furthermore, we assume that the orientation of a spin at an arbitrary position is only influenced by its nearest neighbours. For a given square lattice, the number of possible spin configurations is $2^{N \cdot N}$. Furthermore, the energy of the system, thus the Hamiltonian is given by

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

where J is the coupling constant considered to be independent of lattice position and is set to $J = 1$. Furthermore, a spin is assumed to be dimensionless. In other words, we calculate the sum over all $N \times N$ lattice spins, s_k, and their nearest neighbours, indicated by $< kl >$. Note that we neglect the energy contribution from an external magnetic field.

2.1.1 Periodic Boundary Conditions

Given an infinite lattice, each spin has four nearest neighbours. For a finite lattice, we define the nearest neighbours as shown in figure 1. Given an arbitrary spin, shown as a red point, not located at the lattice edge it has four nearest neighbours, depicted in blue. If a spin is positioned at the edge, the missing nearest neighbour is considered to be the one from the opposite side of the grid. This implementation is known as periodic boundary conditions.

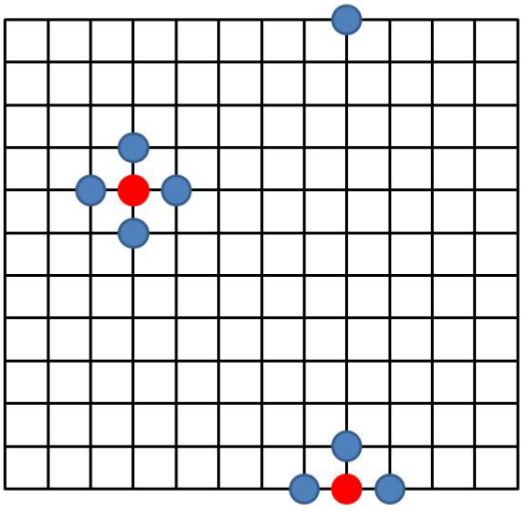


Figure 1: Lattice for Ising model in two dimensions using periodic boundary condition: The blue points are the nearest neighbours of an arbitrary spin (red) in the lattice. Ref [4]

2.1.2 Thermodynamical quantities at equilibrium

The Ising model can be considered as a physical system in a heat bath at a given temperature. At thermal equilibrium, the system can also be referred to as a canonical ensemble. Now, let p_i describe the probability of the system having a certain spin-configuration. The probability is given by the Boltzmann probability distribution

$$p_i = \frac{1}{Z} e^{-\beta E_i}, \qquad \beta = \frac{1}{k_B T}, \tag{2}$$

where k_B is Boltzmann constant, T the temperature (units k_B/J) and E_i the system's energy for this spin-configuration. We shall use natural units, such as $k_B = 1$. Z represents the partition function, defined as the sum of the Boltzmann factor for all possible orientations of all individual spins, referred to as microstates S

$$Z = \sum_{i=1}^{S} e^{-\beta E_i}. \tag{3}$$

Remember that the number of microstates is given by the number of lattice points.
Subsequently, the energy of the system is an expectation value given by the probability distribution

$$\langle E \rangle = \sum_{i=1}^{S} E_i p_i(\beta) = \frac{1}{Z} \sum_{i=1}^{S} E_i e^{-\beta E_i}. \tag{4}$$

It can be shown that the energy is proportional to the first derivative of the potential defined by Helmholtz' free energy (see section 6.1.1). Consequently, the expression for the variance is

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^{S} E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{S} E_i^2 e^{-\beta E_i} \right)^2. \tag{5}$$

The specific heat at constant volume

$$C_V = \frac{1}{k_B T^2} \sigma_E^2. \tag{6}$$

The total magnetisation of a given spin-configuration, M_i, is determined by summing over all values of the spin variables s_i

$$M_i = \sum_i s_i. \tag{7}$$

Further, the thermal expectation value reads

$$\langle M \rangle = \sum_i p_i M_i = \frac{1}{Z} \sum_i M_i e^{-\beta E_i}, \tag{8}$$

with a variance of

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2 = \frac{1}{Z} \sum_{i=1}^{S} M_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{S} M_i^2 e^{-\beta E_i} \right)^2. \tag{9}$$

From this results the magnetic susceptibility χ

$$\chi = \frac{1}{k_B T} \sigma_M^2. \tag{10}$$

In section 6.1.2, the above observation values are analytically calculated for a 2×2 lattice. They will serve as benchmark calculations when proceeding to bigger lattices.
Furthermore, a 20×20 lattice shall be studied determining the number of Monte Carlo cycles needed before reaching an equilibrium situation. Note that only after having reached equilibrium, it is plausible to compute the various expectations values. In addition, we compute the probability, $p(E)$. The analysis shall be done for $T = 1.0$ and $T = 2.4$ with both ordered (all spins pointing in one direction) and a random spin orientation as a starting point.

2.1.3 Phase transition and critical phenomena

The macroscopic properties of a system may abruptly change as the external parameters are changed. The system is said to undergo a phase transition. There are two types of phase

transitions: a first-order and a second-order transition. Further, the point of transition is referred to as critical point. Here, the thermodynamical functions show a discontinuous behaviour and two or more states can coexist. For the Ising model, the changing parameter is the temperature causing a second-order phase transition. The overall aim of this report is finding the critical temperature.

Another characteristic quantity is the correlation length, ξ. Generally, the correlation length is a measure for the length scale at which the overall properties of a material start to differ from its bulk properties. Hence, it describes the distance over which the fluctuations of the spins significantly correlate with each other. In thermal equilibrium, the spins form domains of a given size, determined by the temperature.

If the temperature is close to the critical temperature, T_C, the correlation length is expected to be of the order of the lattice spacing. With increasing temperature, the correlation length increases. At the critical point, the correlation length diverges and be estimated to be

$$\xi(T) \sim |T_C - T|^{-\nu}, \tag{11}$$

where ν is a constant. Now, the system is in a unique critical phase as the fluctuations correlate over all distance scales. It follows that the spontaneous mean magnetisation, due to aligning of spins (domains), approaches zero. The sample is said to go over from a *ferromagnetic* (mean magnetisation is nonzero) to a *paramagnetic* state (mean magnetisation is zero). For temperatures below the critical temperature, T_C, the mean magnetisation turns out to be

$$\langle M(T) \rangle \sim (T - T_C)^{\beta}, \tag{12}$$

where $\beta = \frac{1}{8}$ is called the critical exponent.

Likewise, the heat capacity and the susceptibility can be approximated with

$$C_V(T) \sim |T_C - T|^{-\alpha} \qquad \alpha > 0, \tag{13}$$

$$\chi(T) \sim |T_C - T|^{-\gamma} \qquad \gamma = -\frac{7}{4}. \tag{14}$$

Note that second-order phase transitions are generally difficult to comprehend and thus to model. Therefore, the reason why the the correlation length can extend to the macroscopic size is not yet well understood. Nevertheless, our model is always limited to a finite lattice. Thus, the correlation length will remain proportional to the size of the lattice at the critical point.

Using finite size scaling relations, the behaviour of finite lattices can be related to the results for an infinitely large lattice. Accordingly, the critical temperature scales as

$$T_C(N) - T_C(N = \infty) \propto aN^{-1/\nu}, \tag{15}$$

where a and ν are constants.

Hence, the critical temperature can be found by solving the above linear equation for $T_C(N = \infty)$.

For $T = T_C$, the magnetisation, heat capacity and susceptibility can now be expressed as

$$\langle M(T) \rangle \sim (T - T_C)^{\beta} \propto N^{-\beta/\nu}, \tag{16}$$

$$C_V(T) \sim |T_C - T|^{-\alpha} \propto N^{-\alpha/\nu}, \tag{17}$$

$$\chi(T) \sim |T_C - T|^{-\gamma} \propto N^{-\gamma/\nu}. \tag{18}$$

According to Lars Onsager, the exact analytic result for the critical temperature is $k_B T_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ with $\nu = 1$. Thus, looking at equation (17), we can use computed values for the heat capacity to determine $T(N = \infty)$. More precise, we find the critical temperature where the heat capacity has its maximum given different lattice sizes, $T_C(N)$. In other words, we let $T(N)$ range from $T \in [2.0, 2.35]$ with $\Delta T \leq 0.05$ for $N = \{40, 60, 80, 100\}$ in order to determine the critical temperature.

2.2 Monte Carlo method

Usually, the Monte Carlo simulation is used to determine the expected value of a physical observable. Given the probability distribution in equation (2) as the sampling function, the expectation value for the observable, O, reads

$$\langle O \rangle = \sum_{i=1}^{S} p_i O_i = \frac{1}{Z} \sum_{i=1}^{S} e^{-\beta E_i} O_i = \frac{\sum_{i=1}^{S} e^{-\beta E_i} O_i}{\sum_{j=1}^{S} e^{-\beta E_j}}, \tag{19}$$

where we sum over all the microstates S.
Note that for a small lattice size, equation (19) can be calculated analytically. For a two dimensional lattice with 50×50 spins, more than $2^{2500} \approx 10^{753}$ configurations must be summed over. Thus, a direct summation of the partition function is impossible due to the long computing time. Moreover, a naive random sampling of the spin configurations will not give accurate results. The relevant region in the high-dimensional phase is relatively narrow. Thus, the region is seldom hit by random sampling. The solution to this problem is *importance sampling* which is based on drawing configurations according to their Boltzmann weight. In order to understand the principle, two terms must be defined: *Markov chain* and *ergodicity*.
A Markov chain is a stochastic sequence of configurations where each element depends only on its direct predecessor.
If a system is ergodic, in principal every state can be reached from any other state.

Let us look at an example. Imagine you have two dice. You probably obtain two different states by rolling them twice. These two states are independent of each other. If, however, you role the two dice once and then turn one of the two dice over, this configuration is dependent on the direct predecessor. This is a Markov chain. Since all possible configurations can be reached by turning the dice, the system is ergodic.

Given an ergodic system, it can be shown that a Markov chain can be generated if the transition probability from one state to another, $P(i \to j)$, is chosen appropriately. At steady state, we

must have a *detailed balance* meaning that it is equally probable to go from one state to another as the other way round

$$p(i)P(i \to j) = p(j)P(j \to i), \tag{20}$$

where p represents the probability of being in a certain state, given by Boltzmann's distribution. Defining $P(j \to i) \equiv 1$, the transition probability $P(i \to j)$ reads

$$P(i \to j) = \begin{cases} \frac{p(j)}{p(i)} : \ p(j) < p(i) \\ \\ 1 \quad : \text{ else} \end{cases} \tag{21}$$

Thereby, the transition probability generates a Markov chain which strives as quickly as possible against the expected value. Note that the probability is normalised, hence the condition $p(j) < p(i)$. The expectation value is then given by the K^{th} element of the Markov chain

$$\langle O \rangle \approx \frac{1}{K} \sum_{i}^{K} O(p_i), \qquad K \to \infty. \tag{22}$$

2.2.1 Metropolis algorithm

The Metropolis algorithm allows the application of the Monte Carlo method to our spin lattice. We remind that the probability of having a certain spin configuration, p_i, is given by the Boltzmann distribution defined in equation (2). The transition probability, that is the probability of flipping a spin, given in equation (21), can be rewritten to

$$P(i \to j) = \begin{cases} e^{-\beta \Delta E} : \ \Delta E > 0 \\ \\ 1 \qquad : \ \Delta E < 0 \end{cases} \tag{23}$$

Note that the sum of the partition function is cancelled. Furthermore, the probability of a spin-flip is solely dependent on the energy-difference of the two considered states, $\Delta E = E_i - E_j$. Consequently, only the nearest spin-neighbours are relevant with regard to the spin-flip probability. Apparent from equation (23), the system tries to reach the lowest energy state. If a spin-flip results in $\Delta E < 0$, the flip is immediately accepted. Whether a spin-flip resulting in $\Delta E > 0$, is accepted, depends on the probability.
In our simulation, a possible accepted spin-flip is determined by comparing the Boltzmann factor, $e^{-\beta \Delta E}$, with a uniformly distributed random number, $r \in [0, 1]$. If the Boltzmann's factor is larger than or equal to r, the spin-flip is accepted. Note that if $\Delta E < 0$, the Boltzmann factor reads $e^{-\beta \Delta E} > 1$ and thus is always larger than r. Moreover, the higher the temperature, the higher is the probability that the system escapes the low energy state.

Possible changes in energy For the two dimensional Ising model, there are five possible changes in energy when flipping one arbitrary spin at a time. Consider a system with five spins, just as the red and blue points in figure 1; one spin pointing up at the centre with four neighboring spins with an arbitrary orientation. The number of up and down spins determines

the energy of that system, and all the possible configurations only yields five different possible energies. When flipping the spin at the centre, the total energy of the system switches the sign. Since there are only five different absolute values for the total energy, there are only five possible changes in energy too (when flipping the spin at the centre). Given the temperature of the system, these values can be precalculated. An example on how to calculate the energy for a 2×2 lattice is given in section 6.1.2.

Basic implementation of the code A basic implementation of the code for the two-dimensional Ising model, using the Monte Carlo method and Metropolis algorithm as sampling rule, is given below. A more detailed implementation can be found here: Github repository. The critical temperature can be determined by repeating the Monte Carlo cycle for a range of temperatures, for example $T \in [2.0, 2.4]$.

Algorithm 1: Metropolis Algorithm for the two-dimensional Ising model

Result: Mean observables: (including energy E, magnetisation M, heat capacity C_V and susceptibility χ)

Initialization:
    Set up initial spin matrix with given size at a given temperature
    Compute system's E_i, M_i, C_{Vi} and χ_i
for *MCs = 1, ..., Final cycle* **do**
    `// One Monte Carlo cycle comprises` N^2 `attempts to flip a spin`
    Pick new microstate by flipping one arbitrary spin and find new E_j
    Metropolis Test:
    Calculate random number $r \in [0, 1]$
    if $r \leq e^{-\beta(E_i - E_j)}$ **then**
        Accept spin-flip and update spin matrix
        Update $E_i = E_i + (E_i - E_j)$
        Update M_i, C_{Vi}, χ_i
    else
        Reject spin-flip
    end
end
Final averages $E = \frac{E}{MCs}$ `// E is the sum of energies for every accepted spin-matrix flip`

Optimizing the code Computations for the different temperatures can be parallelized, reducing the run-time significantly. Usually when you run a program, it uses one thread. It is common to have four or eight threads in a CPU, and some even have 16. In this project, we are running a simulation of the Ising Model for many different temperatures. An easy way to speed up the code significantly, is to make use of all the threads in the CPU. We did this by splitting the simulation for each temperature on all the available threads. If the CPU has eight threads, it can in theory speed up the simulation for eight different temperatures by a factor of eight. Another way to speed up the code is to reduce the number of operations. This is of course not as effective as parallelizing the code, but when the duration of the simulation is multiple days,

all operations count. For example, we had a for-loop with hundred of millions of iterations, and we wanted to start calculating expectation values after 10% of the iterations. One way to do this, is to use an if-statement, but that means executing an if-statement hundred of millions of times. What we did instead, was splitting first having a loop with the first 10% of the iterations, and then a loop with the last 90% of them.
Other things to look for is the same calculation being done multiple times, or just unnecessary calculations in general. For instance, $e^{\beta\Delta E}$ can be precalculated, since there are only five different ΔE (see 2.2.1). Thus, the exponential function need not be computed every time the Metropolis test is run.
An important thing to keep in mind, is that one operation is insignificant, but when you add all small optimizations together, the impact may be significant.

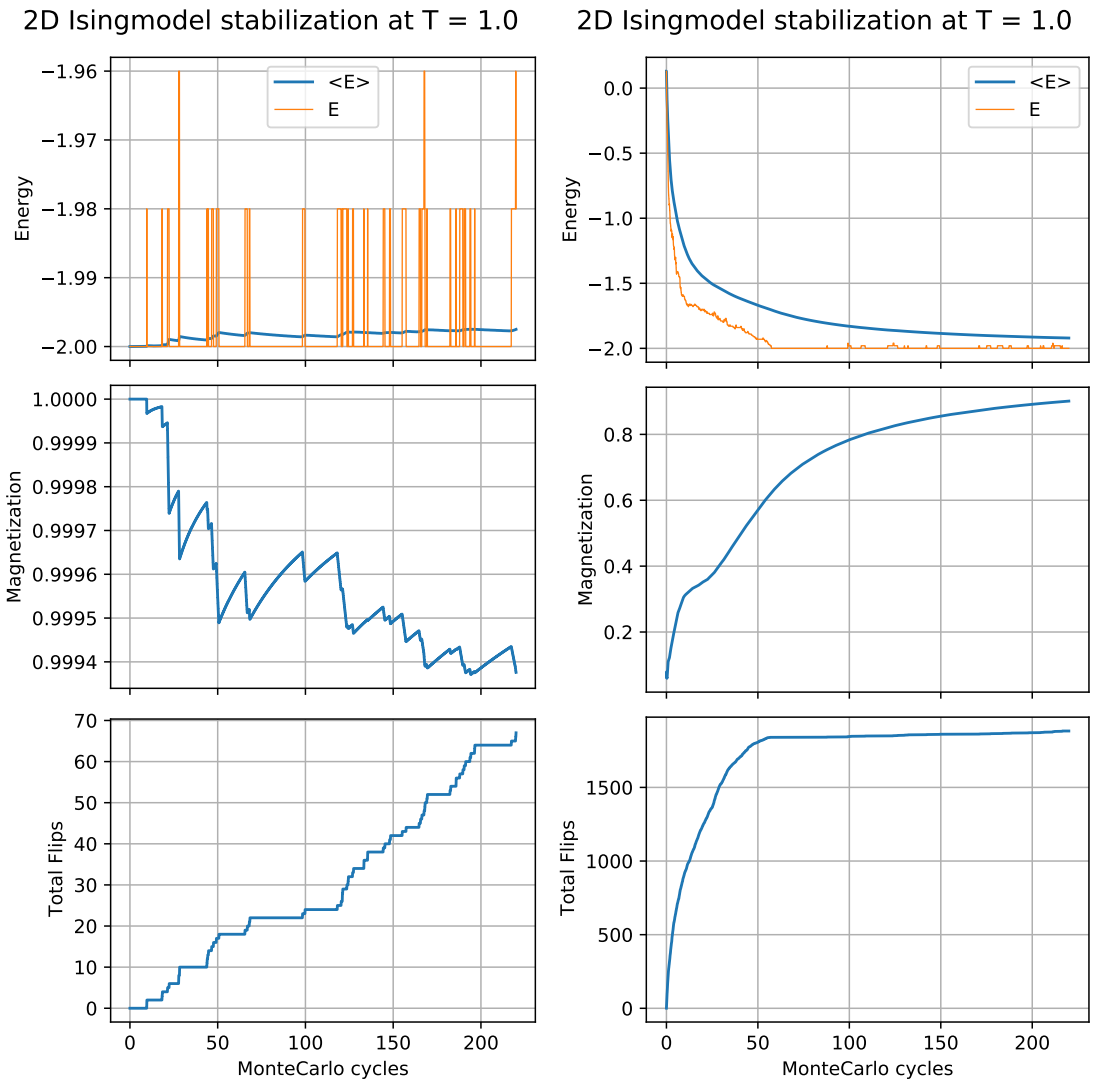
3 Results

3.1 20×20 lattice

In the following the two dimensional Ising Model for a 20×20 lattice is studied.

3.1.1 Most likely state

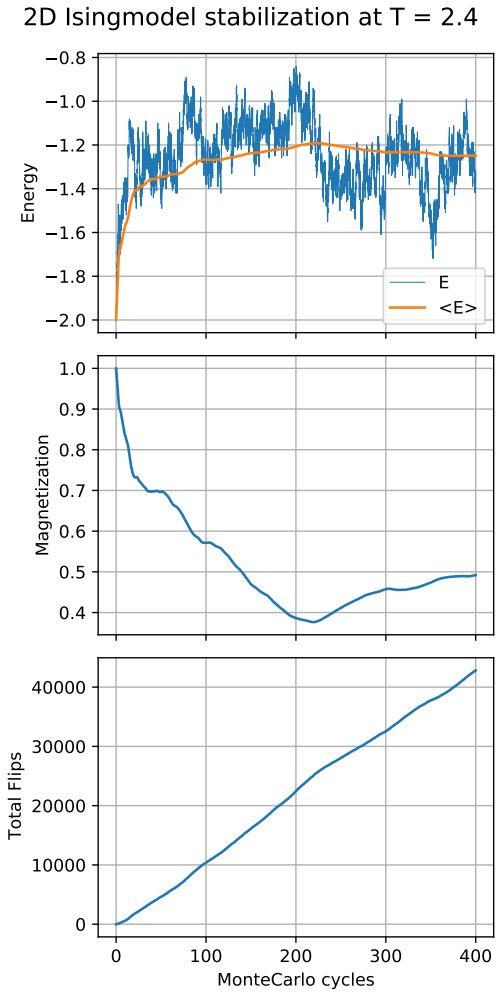
First, we are interested in how many Monte Carlo cycles are needed in order to reach the most likely state, thus equilibrium. Figure 2 shows the stabilization process for $T = 1.0$ starting with a (2a) ordered and (2b) random spin-matrix. Likewise, figure 3 displays the results for $T = 2.4$.



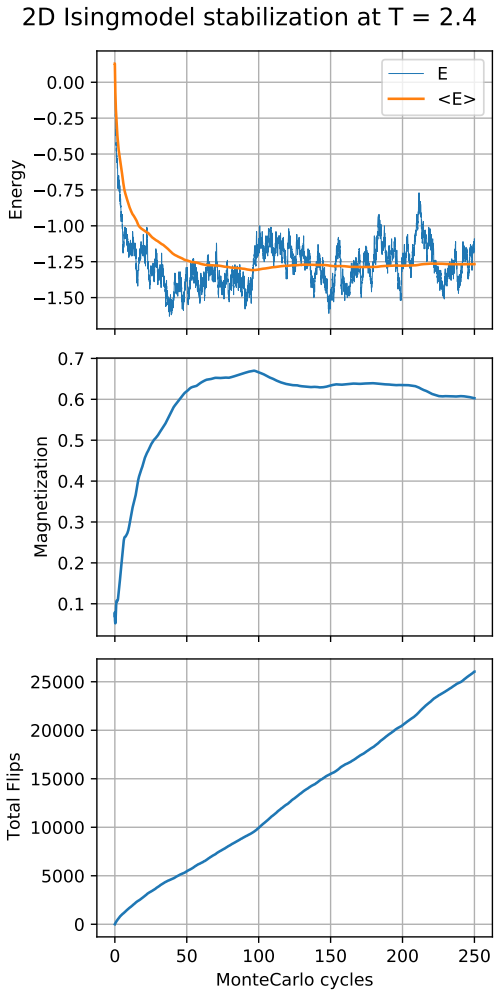
(a) Spin-up orientation as the starting configuration

(b) Random spin orientation as the starting configuration

Figure 2: Two dimensional Ising model for a 20×20 lattice: Energy and mean energy per spin, absolute magnetisation per spin and total flops as a function of Monte Carlo cycles at temperature $T = 1.0$ using natural units.



(a) Spin-up orientation as the starting configuration



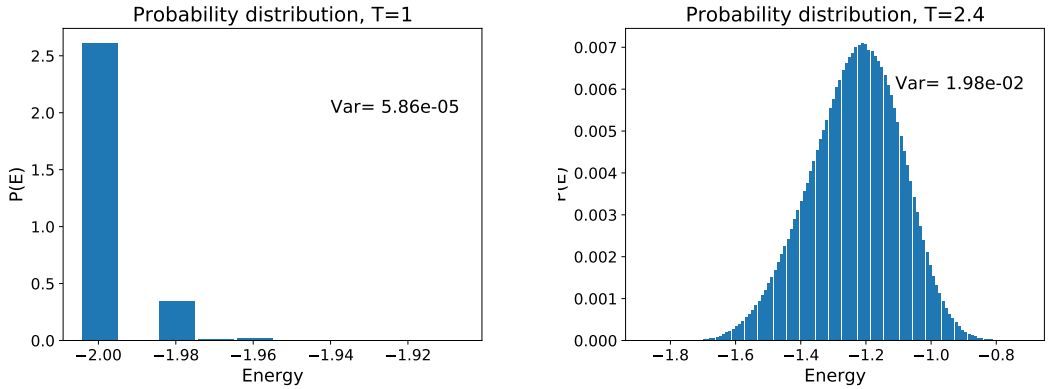
(b) Random spin orientation as the starting configuration

Figure 3: Two dimensional Ising model for a 20×20 lattice: Energy and mean energy per spin, absolute magnetisation per spin and total flops as a function of Monte Carlo cycles at temperature $T = 2.4$ using natural units.

3.1.2 Analyzing the probability distribution

In order to analyze the probability, p, defined in equation (2), the number of times a given energy appears in the computation was counted after the steady state had been reached. As a rule of thumb, the values obtained from the first 10% of cycles are not considered. The results for a simulation using $100,000$ Monte Carlo cycles are summarized in a histogram in figure 4. Figure 4a shows the energy distribution for the ordered spin configuration as starting point at $T = 1.0$ and 4b for a random configuration at $T = 2.4$.

Table 1 lists the computed variance of the energy using both a random and ordered configuration as a starting point for $T = 1.0$ and $T = 2.4$.



(a) Spin-up orientation as starting configuration, $T = 1.0$

(b) Random spin orientation as starting configuration, $T = 2.4$

Figure 4: Two dimensional Ising Model for a 20×20 spin-matrix: probability distribution for the energy per spin after $100,000$ Monte Carlo cycles cutting of the first 10% using natural units.

Table 1: Two dimensional Ising Model for a 20×20 lattice: variance of energy for different temperatures after $100,000$ Monte Carlo cycles minus 10% equilibration time

Spin orientation	Temperature	σ_E^2
ordered	1.0	0.0234551
random	1.0	0.0238206
ordered	2.4	8.15286
random	2.4	7.93062

3.2 Numerical study of the 2nd order phase transition

The aim is to compute the critical temperature where the ferromagnetic state is replaced by the paramagnetic state as a function of lattice size.

3.2.1 Time analysis

Table 2 shows the total and average per thread runtime, for a simulation. The laptop the results were obtained from has four processor cores and eight threads.

Table 2: Simulation run for eight temperatures, with different number of threads.

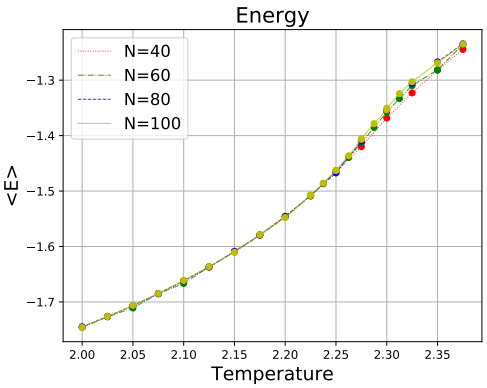
# of threads	Avg. thread time	Total runtime
1	$17.81s$	$142.6s$
2	$21.0s$	$85.2s$
4	$27.6s$	$56.3s$
8	$39.1s$	$40.3s$

3.2.2 Computed observables and critical temperature

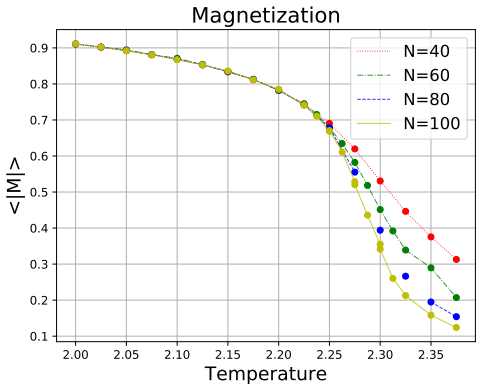
The observables (mean energy, mean absolute magnetization, susceptibility and heat capacity) for four different lattice matrices, $N = \{40, 60, 80, 100\}$, were computed and are presented in figure 5. The simulations were done for $15,000,000$ Monte Carlo cycles and $\Delta T \leq 0.05$. For better resolution, additional datapoints were computed for $T \in [2.2, 2.3]$.
Next, for each lattice size, the temperature, $T_C(N)$, for the maximum value of the heat capacity were extracted using polynomial approximation (see section 6.1.3 for further details).
Based on equation (15) and (17), the obtained $T_C(N)$ were plotted as a function of the inverse of lattice size. The results are presented in figure 6. A linear regression was also run on the data with the following equation

$$T = 0.9095N^{-1} + 2.2699. \tag{24}$$

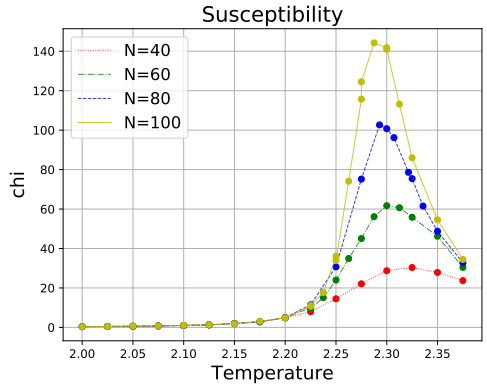
Therefore, the computed critical temperature is $T_C(\infty) = 2.2699$.



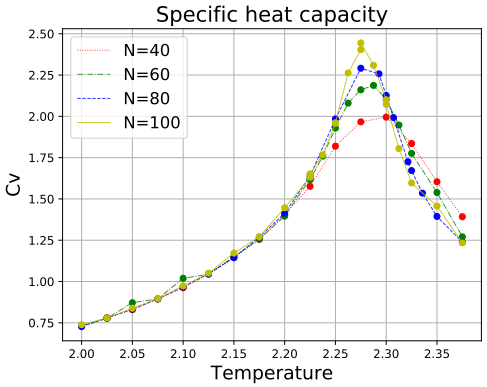
(a) Mean Energy



(b) Mean absolute value of magnetization



(c) Susceptibility



(d) Heat capacity

Figure 5: Two dimensional Ising Model for different sized spin-matrices: Observables per spin obtained after $15,000,000$ Monte Carlo cycles as a function of temperature using natural units

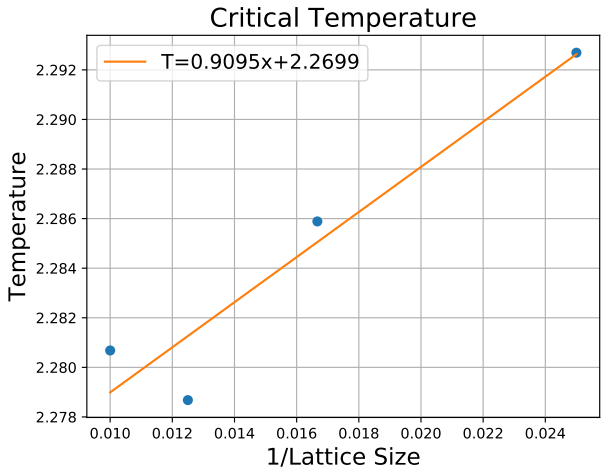


Figure 6: Linear regression of the critical temperature for the heat capacity found for a given lattice size according to equation (15)

4 Discussion

4.1 20×20 lattice

To begin with, the results for the 20×20 lattice will be discussed.

4.1.1 Most likely state

The low temperature state, $T = 1.0$, implies an ordered spin configuration to be stable. Apparent from Figure 2a where the spins start out with an ordered configuration, the steady state is reached almost at once. Unlike, the random start configuration (Figure 2b) needs about 50 Monte Carlo cycles per spin in order for the energy, E, to be stabilized. Moreover, the total number of flips after 200 cycles is 28 $\times$ higher for the random configuration. This stabilisation is also visible in the number of total flips. The number of flips per Monte Carlo cycle is significantly reduced after equilibrium is reached. If the simulation is done for more than 200 Monte Carlo cycles, also the random start configuration reaches the equilibrium value for $\langle E \rangle$. It takes more cycles for the mean magnetization to be stabilized. Note that the absolute value of the mean magnetization is displayed. It takes even more time for the magnetisation (not absolute value) to become stabilized. For the ordered case, it takes about 800 cycles for the mean magnetization to reach equilibrium. For the random case, it takes about 5000 cycles (not shown in the Figure). For $T = 2.4$, the opposite is true. Now, a random spin configuration is expected to be more stable. Indeed, figure 3b shows that the mean energy is stabilized after 50 Monte Carlo cycles for the random start configuration. Given an ordered start configuration, the mean energy is stabilized after around 200 cycles. As the temperature is higher, $\langle E \rangle$ gets closer to zero.
Noteworthy, the number of total flips per cycles increases with increasing temperature. For equilibrium to be reached at the low temperature state, in total about 20 and 2000 flips are needed for the ordered and random case respectively. At $T = 2.4$, respectively about 5000 and

more than $20,000$ flips are needed. This makes sense, as the exponential function (equation (23)) gets less steep. Intuitively, the higher the temperature, the more energy each spin has and thus the higher the probability for the spin to change its orientation.

4.1.2 Analyzing the probability distribution

As figure 4a shows, the most likely energy state for temperature $T = 1.0$ is $E = -2$. Note that is energy per particle. Because the temperature in this simulation is very low, it is expected that the most likely state is the one with the least energy, which is exactly what the figure shows. When the temperature is high on the other hand, the transition probability increases, which means we expect a broader range of likely energy states. Figure 4b shows exactly this. Table 1 shows us the variance of the energy distribution, which matches the two figures well. Note that the variance values in the table must be divided by N^2 in order to get the variance values displaced in the figure label.
Furthermore, the most likely energy state corresponds to the mean energy which are given in figure 3 for the high temperature case and figure 2 for the low temperature case. Even though the start configuration is specified in the figures 4a and 3a, it does not affect the results. This is because we do not start sampling until the system has reached the equilibrium state.

4.2 Numerical study of the 2$^{\text{nd}}$ order phase transition

The results in order to determine the critical temperature are discussed below.

4.2.1 Time analysis

From table 2, we can clearly see a significant speed-up when the code is run in parallel, even though the average runtime per thread is increased significantly as well. We do not know the reason why a thread works so much slower when the number of threads in use increases. It may have to do with other processes on the computer. It may also have to do with how the program is executed when ran in parallel. We ran into a problem with the random number generator. In the earlier stages of the project, the random number generator used was not thread safe, which meant the code block associated with generating random number, could only be executed by a single thread at a time. Considering that one of the biggest parts of the simulation is generating random numbers, there is no surprise this made the code really slow. The random number generator we switched to was much slower, than the non thread safe one. That means that the code is now very slow when only one thread is in use, but is faster when using multiple threads.

4.2.2 Computed observables and critical temperature

Apparent from figure 5a, the mean energy per spin increases almost linearly with temperature as expected. The higher the temperature, the more the spins are randomized and the sum given in equation 1 gets smaller.
As also described in section 2.1.3, more randomized spins cause the mean magnetization to decay to zero. The ferromagnetic state is replaced by the paramagnetic state. Figure 5b shows that the mean magnetisation per spin decreases with increasing temperature for all lattice sizes.

Furthermore, equations (16) to (18) state that the mean magnetization, heat capacity and susceptibility depend on the lattice size. This is the reason why figures 5b, 5c and 5d show different curves for the different lattice sizes. Both the heat capacity and susceptibility diverge at the critical temperature given an infinite lattice. In our case, a larger lattice implies a larger value of the two observable at that point. More precise, the maximum shifts to the left with the smallest lattice having the broadest peak.
The computed critical temperature for the second order phase transition (described in section 2.1.3) is $T_C(\infty) \approx 2.2699$ compared to the analytical value of ~ 2.2692. Thus, the computed result match very well the analytical one.
As described above, the datapoints for the critical temperature for the different lattice sizes were computed using $15,000,000$ Monte Carlo cycles and $\Delta T \leq 0.05$. Here, the equilibration time was set between 10% and 15% of the total number of Monte Carlo cycles. A few obtained datapoints were removed as they showed no reasonable values. This is the reason why the equilibration time was increased to 15%. We remind that the obtained data can be found on Github repository.

5 Conclusion

The calculations were done using natural units.
Using the $N = 20$ lattice as an example, we have shown that an ordered spin configuration is stabilized at low temperatures. Whereas, a random spin configuration is most probable at high temperatures. The equilibration time is dependent on the starting configuration. As a rule of thumb, the equilibration time can be set as $10\% - 15\%$ of the number of Monte Carlo cycles. Furthermore, the number of flips per cycle increases with temperature. In addition, at high temperatures ($T \approx 2.4$) more energy states, that is different spin configurations, are probable to exist. Here, the probability distribution of the mean energy looks like a Maxwell-Boltzmann distribution. At low temperatures ($T = 1.0$), the probability of a particle having energy $E = -2.0$, is more than 80%.
In order to compute the critical temperature, running the program in parallel for different temperatures is recommended as the run time gets reduced. Then a thread safe implantation is crucial. The total run time using 8 threads instead of one reduced the run time by more than three times.
The critical temperature was computationally estimated to be 2.2699 compared to the analytical one of ~ 2.2692.
Future analysis could for example include code optimization when running in parallel. Especially, the random number generator can slow down the program significantly. Generally, the more Monte Carlo cycles the better the results will become. Especially for larger lattice sizes, increasing the cycles has a positive effect as it takes longer for equilibrium to be reached. Further analysis could include how decreasing ΔT and increasing the number of Monte Carlo cycles influences the computed critical temperature. However, this increases the number of calculations. Moreover, having a large enough equilibration time can improve results as well.

6 Appendix

6.1 Ising model - two dimensions

6.1.1 Helmholtz free energy

Helmholtz' free energy relates the expectation value of the energy, E, to the entropy, S, at a given temperature, T

$$F = -k_B T ln(Z) = \langle E(T) \rangle - TS, \tag{25}$$

where F is the Helmholtz' theromdynamical potential, $ln(Z) = -F/k_B T$ and k_B the Boltzmann constant.
Apparent from the equation, there are two competing parameters: the strive towards an energy minimum and the drive towards higher entropy as temperature increases. As we will see, at a critical temperature the Ising model will go from a ferromagnetic to a paramagnetic state where the spins are randomly orientated. Thus, at higher temperatures the degree of disorder is larger which is equivalent to a higher entropy. The energy is defined by the second derivative of F

$$\langle E(T) \rangle = \frac{-\partial ln(Z)}{k_B T} = \frac{\partial(\beta F)}{\partial \beta} \qquad \beta = k_B T. \tag{26}$$

The heat capacity at constant volume is given by the second derivative of F

$$C_V = \frac{1}{k_B T^2} = \frac{\partial^2(\beta F)}{\partial \beta^2} \qquad \beta = k_B T. \tag{27}$$

For the Ising model, a second-order phase transition will be denoted by a diverging heat capacity. Similarly, the susceptibility is given by the second derivative of F with respect to the external magnetic filed which is zero in our case.

6.1.2 A simple 2×2 lattice

Analytic calculations Given a 2×2 lattice, there are a total of 4 spins. For this lattice, finding the analytical expressions for different quantities is not hard, and they will serve as benchmark calculations when proceeding to bigger lattices. First, we look at the different microstates for this system. Table 4 presents the energy and magnetization of all the different configurations for the 2x2 lattice. To give an example as to how this is calculated, we can consider a configuration where there are three spins up and one spin down. The degeneracy for this configuration is 4, because the down spin can be positioned in all four positions. The magnetization is $1 + 1 + 1 - 1 = 2$. The energy is found using 1, and we get $E = -J(1 \cdot 1 + 1 \cdot 1 + 1 \cdot (\text{-}1) + 1 \cdot (\text{-}1) = 0$. If we look at table 4, this is the results from the second row.

Table 3: The different microstates and corresponding values for the 2x2 lattice in the two dimensional Ising model

Number of spins up	Degeneracy	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

First, we find the partition function presented in (3). Because we only have two possible spins, up and down, the total number of configurations for the system is $2^4 = 16$ microstates. From table 4, we see that there are only three different energies for the 16 microstates. $E = 8J$ and $E = -8J$, which occurs two times each, and $E = 0$, which occurs 12 times. The sum in (3) now becomes quite simple, and we get

$$Z = 2e^{8J\beta} + 2e^{-8J\beta} + 12 = 4\cosh(8J\beta) + 12 \tag{28}$$

Other quantities that are useful to calculate and analyze, are the specific heat C_V (2.1.2) and the susceptibility χ (10). In order to calculate these quantities, we need to know the variance of energy (5) and mean magnetization (9) respectively. For the energy we get

$$\langle E\rangle = \sum_i p_i E_i = \frac{1}{Z}\left(2\cdot 8Je^{-8J\beta} - 2\cdot 8Je^{8J\beta}\right) = \frac{-32J\sinh(8J\beta)}{4\cosh(8J\beta)+12} = \frac{-8J\sinh(8J\beta)}{\cosh(8J\beta)+3} \tag{29}$$

and

$$\langle E^2\rangle = \sum_i p_i E_i^2 = \frac{1}{Z}\left(2\cdot(-8J)^2 e^{8J\beta} + 2\cdot(8J)^2 e^{-8J\beta}\right) = \frac{256J^2\sinh(8J\beta)}{4(\cosh(8J\beta)+3)} = \frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} \tag{30}$$

which makes the variance of energy

$$\sigma_E = \langle E^2\rangle - \langle E\rangle^2 = \frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} - \left(\frac{-8J\sinh(8J\beta)}{\cosh(8J\beta)+3}\right)^2 = \frac{64J^2(3\cosh(8J\beta)+1)}{(\cosh(8J\beta)+3)^2}. \tag{31}$$

With this, we can now calculate the specific heat capacity

$$C_v = \frac{1}{k_B T^2}\sigma_E = \frac{1}{k_B T^2}\frac{64J^2(3\cosh(8J\beta)+1)}{(\cosh(8J\beta)+3)^2} \tag{32}$$

We now do the same for the mean magnetization. The values for the magnetic moment for each of the microstates can also be found in table 4. Note that mean magnetic moment refers to the

absolute value of the magnetization.

$$\begin{aligned}\langle M\rangle &= \sum_i p_i M_i = \frac{1}{Z}\left(4e^{8J\beta} + 4\cdot 2e^0 + 4\cdot |\text{-}2|\cdot e^0 + |\text{-}4|\cdot e^{8J\beta}\right) = \frac{8e^{8J\beta}+16}{4\cosh(8J\beta)+12} \\ &= \frac{2(e^{8J\beta}+2)}{\cosh(8J\beta)+3}\end{aligned} \tag{33}$$

and

$$\begin{aligned}\langle M^2\rangle &= \sum_i p_i M_i^2 \frac{1}{Z}\left(4^2e^{8J\beta} + 4\cdot 2^2e^0 + 4\cdot |\text{-}2|^2\cdot e^0 + |\text{-}4|^2\cdot e^{8J\beta}\right) = \frac{32e^{8J\beta}+32}{4\cosh(8J\beta)+12} \\ &= \frac{8(e^{8J\beta}+1)}{\cosh(8J\beta)+3}\end{aligned} \tag{34}$$

which gives us the variance of the mean magnetization

$$\sigma_M = \langle M^2\rangle - \langle M\rangle^2 = \frac{8(e^{8J\beta}+1)}{\cosh(8J\beta)+3} - \left(\frac{2(e^{8J\beta}+2)}{\cosh(8J\beta)+3}\right)^2 = \frac{4(e^{-8J\beta}+3e^{8J\beta}+3)}{(\cosh(8J\beta)+3)^2}. \tag{35}$$

Finally, we can calculate the susceptibility

$$\chi = \frac{1}{k_BT}\sigma_M = \frac{4\beta(e^{-8J\beta}+3e^{8J\beta}+3)}{(\cosh(8J\beta)+3)^2} \tag{36}$$

In our simulations, we use $T = k_B = J = 1$. Inputing these values in the analytical expressions, we can calculate the values for these quantities. With these inputs, we get

$$\begin{aligned}C_v &= \frac{64(3\cosh(8)+1)}{(\cosh(8)+3)^2} \approx 0.12832 \\ \chi &= \frac{4\beta(e^{-8}+3e^{8}+3)}{(\cosh(8)+3)^2} \approx 0.01604\end{aligned} \tag{37}$$

Computational results Table 4 list the computed observables for the 2×2 lattice for different Monte Carlo cycles at $T = 1.0$. The analytical values are also stated. The spin matrix was initialized with both a uniform and disordered spin distribution. Generally, all computational values are of the same order as the analytical one. This implies that our implementation is correct. Given the randomness in the simulations, we expect the results to get closer to the analytical value if we run the simulation multiple times and calculate an average instead. Indeed, for both the disordered and ordered case, the values strive towards the analytical one with increasing number of cycles. As the temperature is low, we expect the ordered case to be more probably. Therefore, for 2000 Monte Carlo cycles, the results for the ordered case are quite close the the analytical ones.

Table 4: Two dimensional Ising Model for 2×2 spin-matrix: Computational values per spin for mean energy, E, mean magnetisation, M, heat capacity, C_V and susceptibility, χ. Spin matrix was initialized with both random and ordered orientation and the simulation was repeated for different numbers of Monte Carlo cycles, MC. Analytic values shown as $\sim \infty$.

Spin orientation	MCs	$\langle E \rangle / N^2$	$\langle \lvert M \rvert \rangle / N^2$	C_V / N^2	χ / N^2
ordered	$2,000$	-1.99500	0.99854	0.03989	0.00374
random	$2,000$	-1.98528	0.99486	0.11689	0.01600
ordered	$20,000$	-1.99681	0.99893	0.02551	0.00322
random	$20,000$	-1.99636	0.99813	0.02906	0.00348
ordered	$20,000,000$	-1.99560	0.99867	0.03194	0.00398
random	$20,000,000$	-1.99598	0.99866	0.03210	0.00401
	$\sim \infty$	-1.99598	0.99866	0.03208	0.00401

6.1.3 Numerical study of the 2nd order phase transition

When finding the maximum of the C_v vs T plots, we used the maximum of a 3rd degree polynomial fit of the datapoints. Figure (7) shows an example for $N = 100$. We did that because we don't have a large number of datapoints, and the maximum could be different from the maximum datapoint we have.

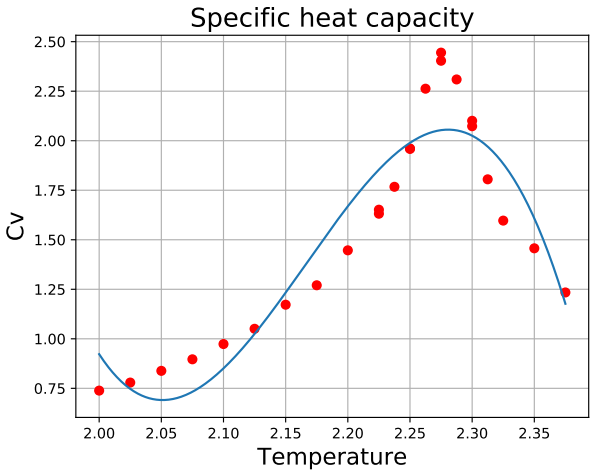


Figure 7: Polynomial fit of the datapoints from the specific heat capacity as a function of temperature.

References

[1] Bänz Bessir. *Ising-Modell mit Monte Carlo Methode*. 2007. URL: http://www.wiese.itp.unibe.ch/theses/bessire_bachelor.pdf. (accessed: 08.11.2020).

[2] Morten Hjorth-Jensen. *Computational Physics Lectures: Statistical physics and the Ising Model*. Aug. 2017. URL: http://compphysics.github.io/ComputationalPhysics/doc/pub/statphys/pdf/statphys-print.pdf. (accessed: 06.11.2020).

[3] Wolfhard Janke. *Monte Carlo Simulations of Spin Systems*. URL: https://www.physik.uni-leipzig.de/~janke/Paper/spinmc.pdf. (accessed: 08.11.2020).

[4] T. Judd. *Das Ising Modell und Phasenübergange*. URL: https://www.tat.physik.uni-tuebingen.de/~kley/lehre/cp-prakt/projekte/projekt-judd.pdf. (accessed: 07.11.2020).

[5] Thomas Schart. *Monte Carlo Simulation des 2-D Ising Modells*. May 2004. URL: https://perso.u-cergy.fr/~ahonecker/bs/semstat/ausarb/schart. (accessed: 09.11.2020).