Numerical analysis of 2D Ising model: phase transition & critical temperature

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Abstract

In this text, there will be presented numerical results based on 2D Ising model of a finite lattice. One of the main goals was to estimate the curie temperature of a system with a finite lattice size, as well as discover when phase transition occurs. One needed to find a good equilibrium for our system in order to get reliable results. In agreement to Lars Onsager's [1] exact value of T_C, we ended up with an good estimate of the curie temperature $T_C \approx 2.268 \pm 0.005$ which yields a relative error of $\epsilon_{rel} \approx 0.040\%$. Finite dimensions of L = [40,60,80,100], was used to estimate the curie temperature.

I. Introduction

The study of phase transitions and statistical analysis is a fundamental part of physics, in this article we will look at the phase transitions through the two dimensional Ising model as well as statistical analysis of the system. This model exhibits a phase transition at some critical temperature, where it goes from magnetic phase to a phase of zero magnetization. The two dimensional Ising model, is a model based on a two dimensional lattice, consisting of electronic spins $\{\uparrow\downarrow\}$. This is called an binary system where each lattice position only can take two values. The energy formulated by the Ising model, can in its simplest form be expressed as:

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

The applied magnetic field $\mathscr{B}$ is disregarded in this text, for simplifications. Where $s_k = \pm 1$ indicating spin orientation. The quantity N represents the total number of spins, and J is the coupling constant expressing the strength between the neighbouring spins. $< kl >$ is says that the sum only goes over the neighbouring spins. By assuming a ferromagnetic ordering all spins is in an ordered arrangement, this will be one of the starting points in this text, as well as random spin configuration which is a paramagnetic ordering. These two states is what will be studied during this text.

The Ising model is a powerful model which describes a variety of physical properties and applications. In this text the main focus lies in statistical analysis of the system as well as phase transitions. The 2D Ising model has analytic solutions for several expectations values, such as $\langle E \rangle$ and $\langle \mathscr{M} \rangle$, where these corresponds to mean energy and mean magnetic moment respectively. Solutions in this text will be accessed through the use of periodic boundary conditions and metropolis algorithm, which will be discussed in the upcoming sections.

II. Theoretical insight

i. *Boltzmann statistic*

An introduction to Boltzmann statistics is necessary to fully understand the problem at hands. The Boltzmann factor plays a fundamentally important part of physics. It is a simple formula which manage to describe the probability of finding a system in a certain microstate. The Boltzmann factor is described as follows:

$$Boltzmann\ factor = e^{\frac{-E_i}{k_B T}} \tag{2}$$

Where we define $\beta = 1/k_B T$. This is unfortunately not enough to describe the probability of a certain state. We need to define the so-called partition function. This function takes into account the probability of all states, and is named Z [2].

$$Z(\beta) = \sum_i e^{-\beta E_i} \tag{3}$$

The partition function is then a sum over all Boltzmann factors for all possible states. We then end up defining the probability of finding the system at a state E_i as:

$$P_i = \frac{1}{Z} e^{-\beta E_i} \tag{4}$$

The partition function acts as a factor which normalize or converts the Boltzmann factor into a probability. By now we have managed to find the probability of a system being at a certain state. We can now find the mean values of desired quantities such as E and M

The mean energy is possible to extract with the help from the probability distribution described above. We may define the mean energy as a sum over energies E_i times the probability $P(i)$ of this energy at a given state $\{i\}$. This gives the mean energy [2]:

$$\langle E \rangle = \sum_i E_i P_i \tag{5}$$

We already know that the probability of a given state may be expressed as eq 4, simply inserting this into the equation above gives the mean energy:

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} \tag{6}$$

This is a neat expression for the mean energy, but it can be generalized for any variable Γ giving:

$$\langle \Gamma \rangle = \frac{1}{Z} \sum_i \Gamma_i e^{-\beta E_i} \tag{7}$$

By this we also find the mean absolute magnetic moment $\langle |\mathscr{M}| \rangle$:

$$\langle |\mathscr{M}| \rangle = \frac{1}{Z} \sum_i |\mathscr{M}_i| e^{-\beta E_i} \tag{8}$$

These expressions is perfectly fine, but there is a more compact way of expressing the mean values:

$$\langle \Gamma \rangle = -\frac{\partial ln Z}{\partial \beta} \tag{9}$$

We can easily see that this is equivalent to the mean values described above. We can now move forwards, by finding the heat capacity. The heat capacity describes how the energy changes as the temperature changes. This can easily be expressed as the derivative of the energy with respect to the temperature. Further more we may use the equation 6 as the energy for describing the heat capacity:

$$C_V = \left(\frac{\partial \langle E \rangle}{\partial T} \right)_{V,N} \tag{10}$$

By inserting the mean energy in the form as described in equation 9, and changing variables we end up with the heat capacity [3]:

$$C_V = \frac{1}{k_B T^2} \frac{\partial^2}{\partial \beta^2} ln Z \tag{11}$$

Another way of expressing the heat capacity is with the help of variance expressed in terms of energy:

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{12}$$

Which further gives us a formula for the heat capacity:

$$C_V = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{13}$$

The same way can be done, if one needs to calculate the susceptibility. Firstly one calculates the magnetic variance $\sigma_{\mathscr{M}}^2$:

$$\sigma_{\mathscr{M}}^2 = \langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2 \tag{14}$$

$$\chi = \frac{1}{k_B T}(\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2) \tag{15}$$

ii. *Phase transition*

Phase transition is an important aspect to look at when studying magnetization. In this text we look at the second order phase transition that occurs for the 2D Ising model. One of the most important parameters is the curie temperature. This critical temperature determines when the system exhibits a phase transition. According to the Norwegian theoretical physicist and chemist Lars Onsager, there exist a theoretical value of the curie temperature when the lattice dimension goes to infinity, he calculated the critical temperature to be $kT_C/J = 2/ln(1+\sqrt{2} \approx 2.269)$ [1]. Further on the system will be in a ferromagnetic state for low temperatures and make a phase transition to a paramagnetic phase when it reaches the critical temperature. This is when the ferromagnetic state has no external field applied to it, also at the paramagnetic phase it looses its ability to self-magnetize.

It is possible to describe many of the physical quantities by a power law behaviour near the critical temperature T_C, for the Ising model the mean magnetization can be written as:

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

where $\beta = 1/8$ is a so-called critical exponent. A similar relation applies to the heat capacity

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

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{16}$$

with $\alpha = 0$ and $\gamma = 7/4$. It is possible to relate the behavior at finite lattices with the results for an infinitely large lattice as done by Lars Onsager [1]. The critical temperature scales then as:

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{17}$$

Where a is a constant. We set $T = T_C$ and obtain a mean magnetisation

$$\langle \mathscr{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu}, \tag{18}$$

Whwere $\nu = 1$, and the heat capacity:

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \tag{19}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu}. \tag{20}$$

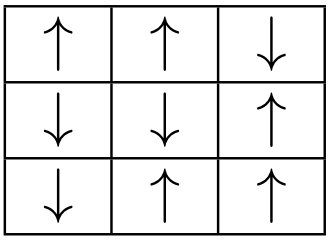
III. Method

i. *Periodic boundary condition*

When implementing the Ising model we need to apply periodic boundary conditions to the given lattice. In our case we will restrict ourself to a 2D-model. Which means that we will have a spin configuration of up and down in a two dimensional lattice. In this subsection we will be confined to a 3×3-lattice, for simplicity.

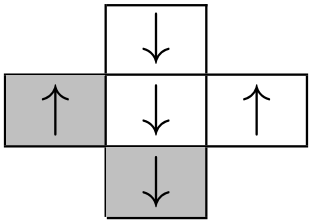
$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{21}$$

Table 1: Random spin configuration of a 3×3-lattice



As seen by table 1, there is a 3×3-lattice which consist of spins up and down. As we know from equation 21, we are only interested in the closes neighbours to a certain spin-configuration. Let us say we look at the spin, which is placed in the center of the lattice. At this position it is easy to find the nearest neighbours. We define the spins as a matrix $\mathbf{S}^{n \times n}$, by this we see that the closest neighbours of $s_{2,2}$ is the set of spins $\{s_{1,2}, s_{2,1}, s_{2,3}, s_{3,2}\}$. All this is fine, and we can easily extract various expectation values that we are interested in. The exceptions occurs at the boundaries, here there is a simple implementation which takes care of the problem. We simply define some spin-configuration in the non-existing lattice place to the right, left or above, beneath, and place a spin which is equal to the symmetric counterpart. More easily said, if we look at $s_{1,1}$ we have two spins which all points upwards as the closest neighbours. In order to apply the periodic boundary condition we define an imaginary spin above and to the left of the lattice.

Table 2: Visualization of Periodic boundary condition: Grey cells is the imaginary spins as a result of the boundary condition at the bottom left corner.



As seen by table 2, there is been a creation of new spins which is equivalent to the opposite spins. The periodic boundary condition will be applied to all cases at the edges, by this we know that for

the 2D-model we only have four spins to take into consideration. In the upcoming subsection we will dive in to the Ising model confined to the two dimensional case.

ii. *2D-Ising Model*

We will as said previously restrict ourself to the 2D-Ising model. In this case we look at an 2D-lattice which have spins of up and down in the lattice-sites. The Ising model is a model that allows for identification of phase transitions. As we have seen above the energy may be expressed as:

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{22}$$

Where the external magnetic field $\mathscr{B}$ is zero. This equation takes into account the nearest neighbours of the spin we are looking at. Where the variables s_k and s_l takes the values ± 1, spin up and spin down. We are however also interested in mean energy $\langle E \rangle$ and magnetization $\langle |\mathscr{M}| \rangle$. By using the canonical ensemble we can determine $\langle E \rangle$ and $\langle |\mathscr{M}| \rangle$ by a probability distribution. Using Boltzman distribution yields the probability a state being in an energy E_i. :

$$P_i(\beta) = \frac{e^{-\beta} E_i}{Z} \tag{23}$$

As done in the previous section we found the general expressions for both mean energy and mean absolute magnetic moment. The 2D-ising model is a reliable method for determining multiple physical values in a 2D-lattice consisting of spins of up and down.

iii. *Metropolis-Hasting algorithm*

So far we have talk about probability distributions and the Ising model. The Ising model provides a fairly simple model to calculate the energies of the spins in a 2D lattice. To fully calculate the spins throughout the lattice one need to sweep through the lattice. Firstly we implement Monte Carlo algorithm [See Project.3]. Once we have implemented Monte Carlo algorithm, we can start sweeping through the lattice. Selecting a state within the lattice via a probability selection, this is a probability that tells which state is being picked out of all states in the lattice. Once the a spin has been picked out we want to check if it satisfy the so-called acceptance probability. This is basically the probabillity of one state being transferred to another, spin up flips down and vica versa $\{(\uparrow) \Longrightarrow (\downarrow)\}$,$\{(\downarrow) \Longrightarrow (\uparrow)\}$

$$\frac{P_i(\beta)}{P_j(\beta)} = \frac{\frac{1}{Z} e^{-\beta E_i}}{\frac{1}{Z} e^{-\beta E_j}} = e^{-\beta \Delta E} \tag{24}$$

By allowing each spin to interact with its closest neighbours, it is for Ising model, possible to calculate ΔE for all possible spin configuration, giving possible values of $\Delta E = \{-8J, -4J, 0J, 4J, 8J\}$. So already before doing the Metropolis sampling we can assemble an array containing all ΔE. Now to be able to flip the spin, it need to pass the metropolis acceptance probability:

$$\chi \leq e^{-\beta \Delta E} \tag{25}$$

Where χ is a random number generator, which provides random numbers between [0,1]. If this statement is fulfilled, the spin will flip, and the important values such as energy and magnetization will be updated, afterwards the process restarts. On the other hand, if this statement is not fulfilled the process restarts without updating the energy and magnetization. Usaly this process continues until some criteria is met, for our model it is often when the lattice becomes ferromagnetic, when all

the spins is ordered in one direction. By allowing each spin to interact with its closest neighbours, the metropolis acceptance probability tends to flip spins with lowest energy than those with high energy. This will in time provide an equilibrium to the system, however we can see by equation 25, that increased temperature will effect the system. Further results regarding temperature change of the system will be presented in the upcoming section

IV. Implementation

Programs used in this project can be found on https://github.com/patrykpk/FYS4150/tree/master/Project_4 and the "README.md" explains how to run the scripts. All calculations are done in C++, while the plotting is done in Python. Our C++ program is based on the codes found in the course's github repository https://github.com/CompPhysics/ComputationalPhysics/tree/master/doc/Projects/2019/Project4 and the content found in "Computational Physics Lecture Notes 2015" on 2D-Ising model and metropolis algorithm [3]. This section will include how we implemented the code and include some of the code:

i. *Initializing a $L \times L$ lattice*

When analysing a Lattice, one first need to create a lattice. In our code this is done by creating a $L \times L$ matrix. Two system is possible to initialize, either an ordered configuration of spins all spins pointing upwards, or an ordered matrix, where all spins is randomized. In this project we chose the Mersenne Twister pseudorandom number generator (mt19937_64)[1] found in the <random> library of C++ due to its high sample size.

Listing 1: C++ Initilizing ordered and unordered matrix

```
/*
Pseudocode for Initializing a LXL-matrix
*/
void Initialize(int L, mat& SpinMatrix, double& Energy, double& Magnetization,
    string SpinConfig){
    if (SpinConfig == "Ordered"){
        SpinMatrix.fill(1);          // Fills all elements with ones
    }
    else if (SpinConfig == "Unordered"){
        random_device rd;
        mt19937_64 gen(rd());
        uniform_real_distribution<double> RandomNumb(0.0, 1.0);
        for (int x = 0; x < L; x++){
            for (int y = 0; y < L; y++){
                if (RandomNumb(gen) >= 0.5){
                    SpinMatrix(x,y) = 1.0;
                }
                else{
                    SpinMatrix(x,y) = -1.0;
                }
            }
        }
    }
}
```

By now we have an simple $L \times L$ matrix which constitutes of $\{\pm 1\}$. This matrix is now our lattice which we will evaluate.

[1] http://www.cplusplus.com/reference/random/mt19937_64/

ii. *Metropolis-Hasting algorithm code implementation*

When implementing the Metropolis algorithm to the code, one needs to implement it into an for-loop of Monte Carlo cycles. For each Monte Carlo cycle the metropolis algorithm is being assessed. The outer loop is fairly simple:

Listing 2: C++ Looping through Monte Carlo cycles

```
/*
Pseudocode for looping through Monte Carlo cycles.
*/
void MonteCarloAlgorithm(int L, double Temperature, int MonteCarloCycles, string
    SpinConfig, int Equilibrium){
    mat SpinMatrix = zeros<mat>(L,L); //
    vec w = zeros<vec>(17);

    for (int dE = -8; dE <= 8; dE+=4){
        w(dE+8)=exp(-dE/Temperature);
    }
    double Energy = 0.0, Magnetization = 0.0;
    Initialize(L, SpinMatrix, Energy, Magnetization, SpinConfig);

    for (int Cycles = 1; Cycles <= MonteCarloCycles; Cycles++){
        Metropolis(L, SpinMatrix, Energy, Magnetization, w);
    }
```

For each Monte Carlo cycle we enter the metropolis algorithm, as mentioned in section method-Metropolis-Hasting algorithm. Initializing the energy and the magnetization to be zero, before entering the loop. As we also can see by the pseudocode above the energy difference ΔE is computed and stored away in an array consisting of $w(\Delta E + 8) = e^{-\beta \Delta E}$. Once we have these values we can enter the metropolis algorithm.

Metropolis algorithm is as said previously the algorithm that determines whether the given spin is to be flipped or not. This is determined by the energy difference of the spin under the scope and the nearest neighbours. We then have five possible energy differences to choose from. Due to periodic boundary conditions we are able to determine the spins of the nearest neighbours in all positions in the lattice.

Listing 3: C++ Metropolis-Hasting algorithm evaluating spins in $L \times L$ -lattice

```
/*
Code snippet for Metropolis-Hasting algorithm.
*/
double Metropolis(int L, mat& SpinMatrix, double& Energy, double& Magnetization, vec
     w){
    random_device rd;
    mt19937_64 gen(rd());

    uniform_real_distribution<double> RandomNumb(0.0, 1.0);
    int Accepted = 0;

    int MaxIteration = L*L;
    for (int Iteration = 0; Iteration < MaxIteration; Iteration++){
        int Rx = (int) (RandomNumb(gen)*(double) L);
        int Ry = (int) (RandomNumb(gen)*(double) L);

        int dE = 2*SpinMatrix(Rx, Ry)*
```

```
                (SpinMatrix(Rx, PeriodicBC(Ry,L,-1))+
                 SpinMatrix(Rx, PeriodicBC(Ry,L, 1))+
                 SpinMatrix(PeriodicBC(Rx,L,-1), Ry)+
                 SpinMatrix(PeriodicBC(Rx,L,1), Ry));

        if (RandomNumb(gen) <= w(dE+8)){
            SpinMatrix(Rx,Ry) *= -1;
            Magnetization += (double) 2*SpinMatrix(Rx, Ry);
            Energy += (double) dE;
        }
    }
}
```

In order for the spin to be flipped it has to pass the if-statement: RNG $< w(\Delta E + 8)$. Where RNG is the random number generator. Initially the code-snipped chose a random spin in the lattice to be evaluated.

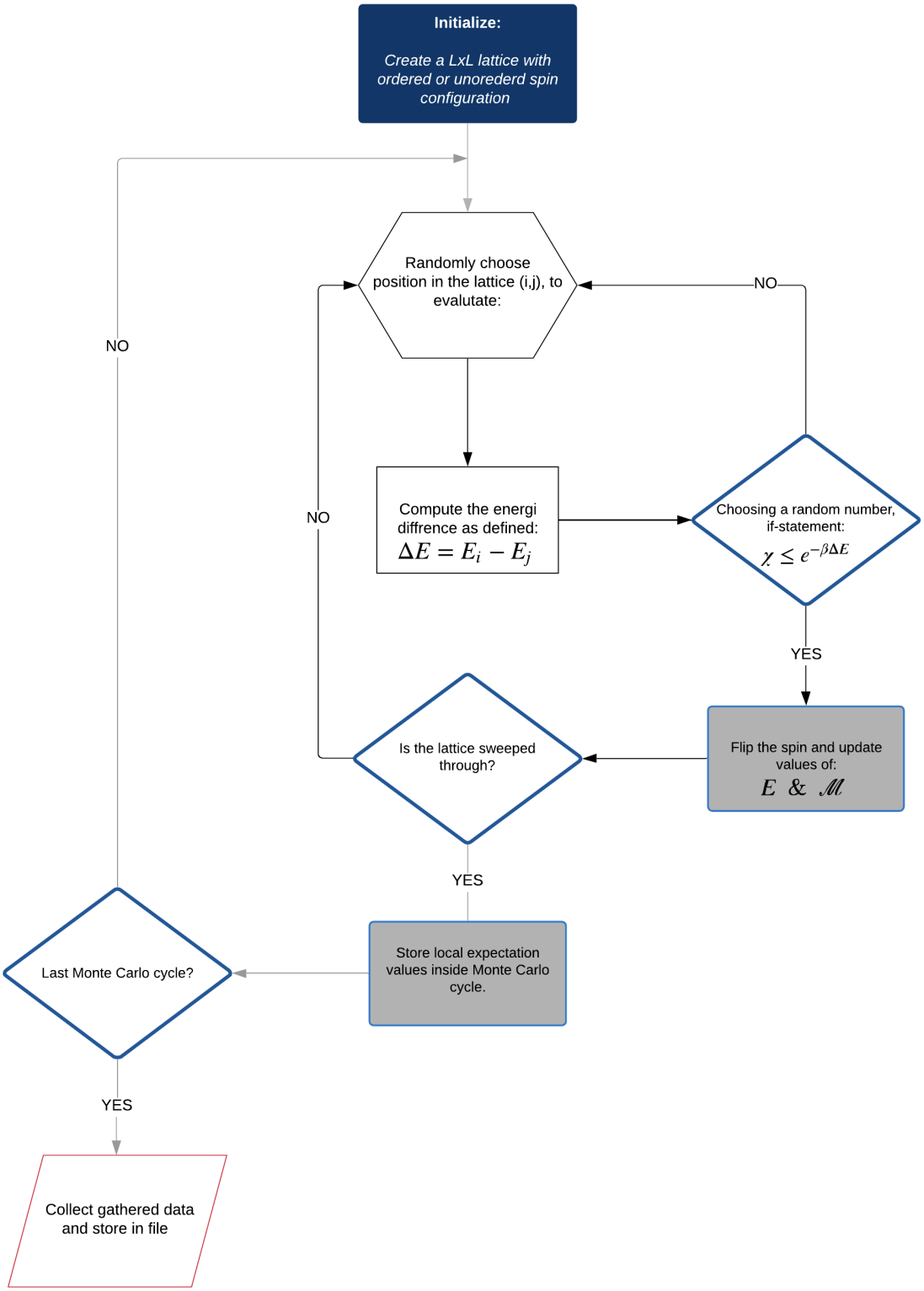


Figure 1: Flow-chart of code for Metropolis algorithm

V. Numerical results

Numerical results will be presented under this section, where we will start of with an easy comparison between our analytic solutions to the 2×2-case and numerical results. The analytic solutions is presented under A. Numerical analysis on equilibrium condition is also presented, which will act as a criterion for further analyses. Probability distribution of the system likely-hood of being in a state is also presented, as-well as phase transitions with corresponding critical temperatures. The last results presented is a comparison between parallelized code and non-parallelized code.

i. *Analytical vs. Numerical 2 x 2 Lattice*

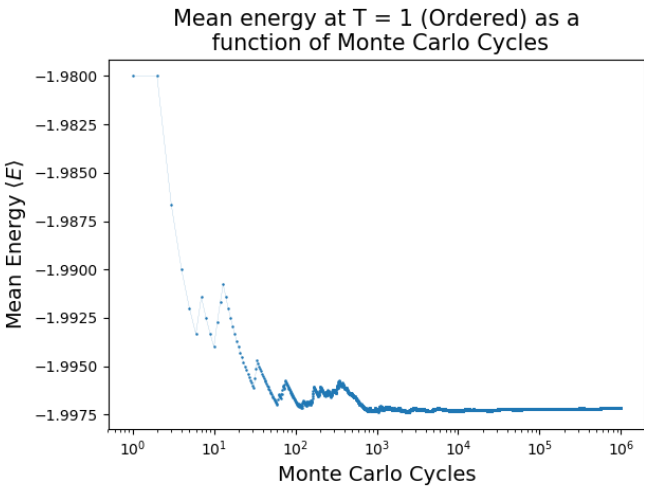
Running calculations for the 2×2 lattice and comparing the results to the analytical values is performed in Table 3 for Monte Carlo cycles ranging from 10^3 to 10^6. These values represent the output from performing the same calculation 50 times.

Table 3: $\langle E \rangle$, $\langle \mathscr{M} \rangle$, C_V and χ as a function of Monte Carlo cycles. With uncertainty as depicted in the table. Where the temperature is set to T = 1.0 and for an ordered spin configuration. (Values per spin)

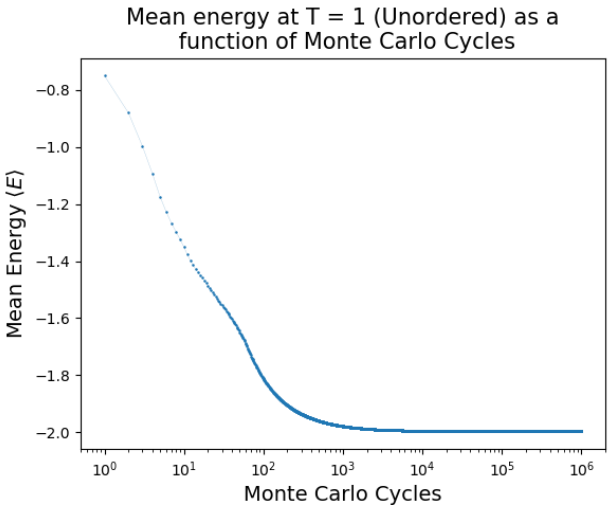
MC cycles	$\langle E \rangle$	$\langle \mathscr{M} \rangle$	C_V	χ
10^3	-1.995 ± 0.003	0.998 ± 0.001	0.03859 ± 0.02372	0.007399 ± 0.002543
10^4	-1.995 ± 0.001	0.998 ± 0.001	0.03611 ± 0.00749	0.004491 ± 0.00112
10^5	-1.996	0.999	0.03423 ± 0.00192	0.004284 ± 0.00041
10^6	-1.996	0.999	0.03204 ± 0.00011	0.004026 ± 0.00013
Analytic value:	-1.996	0.9987	0.03208	0.004011

ii. *Equilibrium condition*

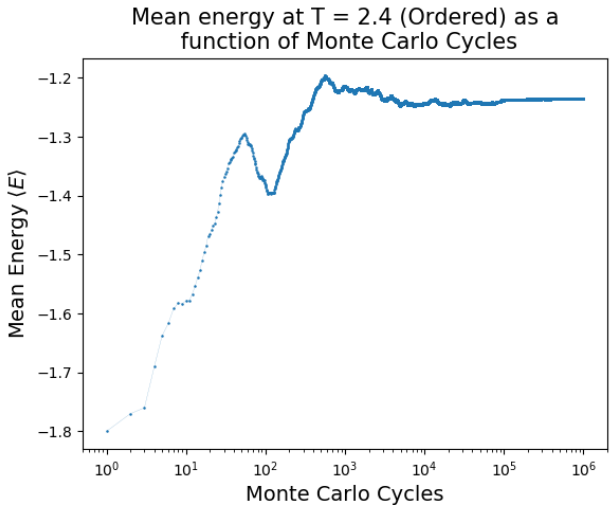
This section will present the needed number of Monte Carlo cycles required before reaching and equilibrium condition. Initial system for calculations could either be represented by all spin states ordered in one single direction or all of the spins acquiring random spin state. Thus the results presented here will show both possibilities.



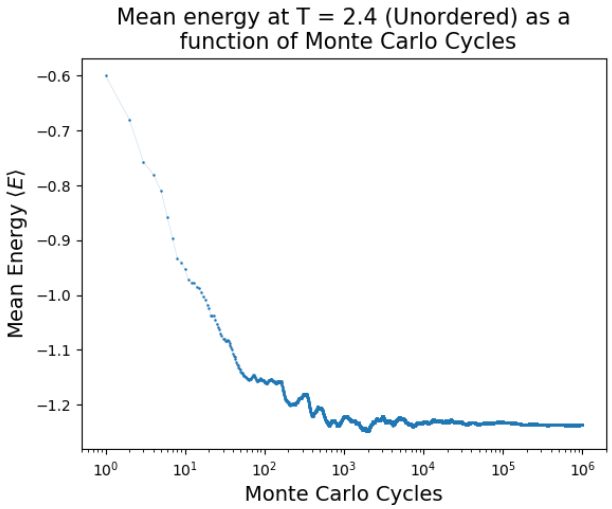
a. $\langle E \rangle$, T = 1 for ordered



b. $\langle E \rangle$, T = 1 for unordered



c. $\langle E \rangle$, T = 2.4 for ordered

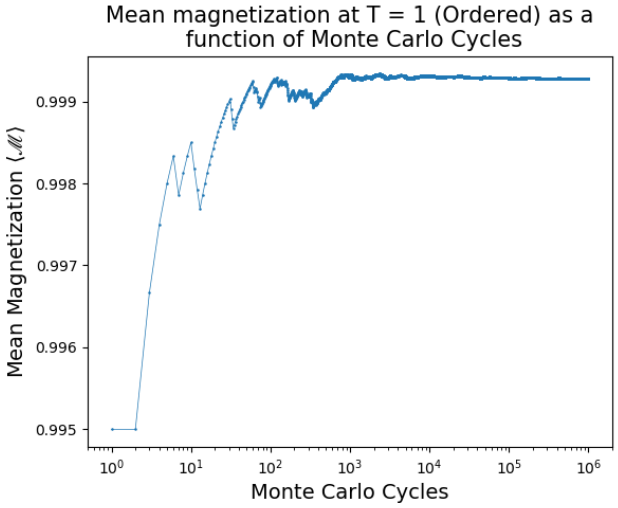


d. $\langle E \rangle$, T = 2.4 for unordered

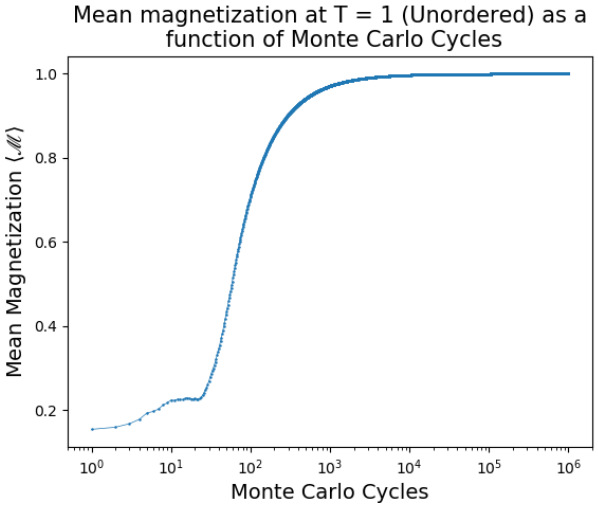
Figure 2: Mean energy for T = [1.0, 2.4], as well as for ordered and unordered configuration of spins for a 20 x 20 lattice, where it is plotted as a function of number of Monte Carlo cycles ranging $[1, 10^6]$

Figure 2 shows four plots of mean energy $\langle E \rangle$ for T = 1.0 and T = 2.4 for ordered spin configuration and unordered spin configuration. These spin configurations corresponds to ferromagnet(ordered) and paramagnet(unordered). The plots is the mean energy as a function of Monte Carlo cycles. Where a cycle refers to number of sweeps through the lattice. In this case we look at a 20×20-lattice. This gives 400 number of spins within the lattice. One Monte Carlo cycle is then when our code enters the metropolis algorithm, where it sweeps through the entire lattice.

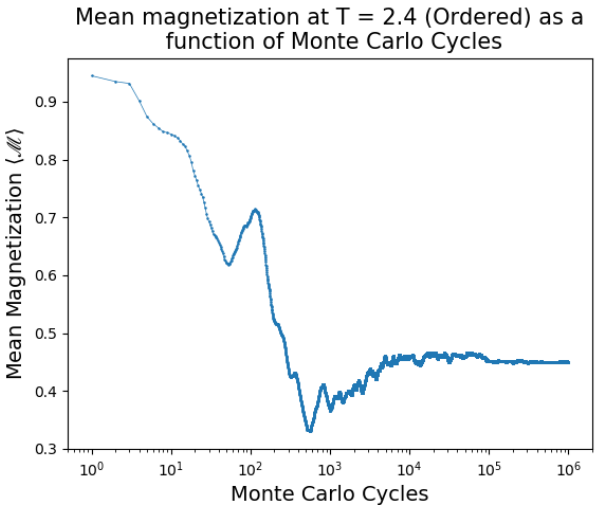
Figure 3 is the same system, except here we analyse when equilibrium is achieved when we look at mean absolute magnetic moment $\langle \mathscr{M} \rangle$.



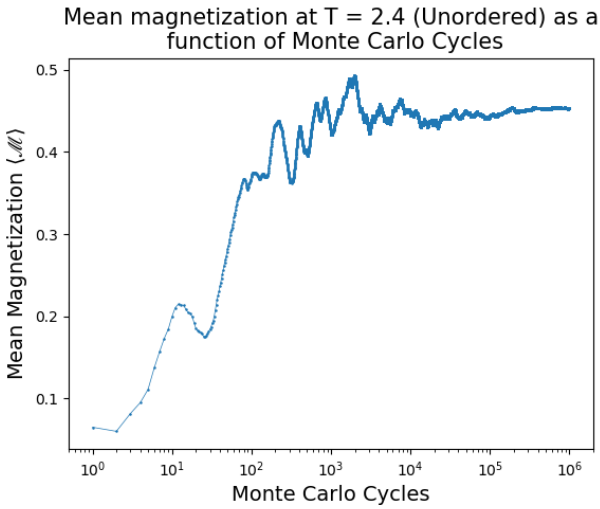
a. $\langle |\mathscr{M}| \rangle$, T = 1.0 for ordered



b. $\langle |\mathscr{M}| \rangle$, T = 1.0 for unordered

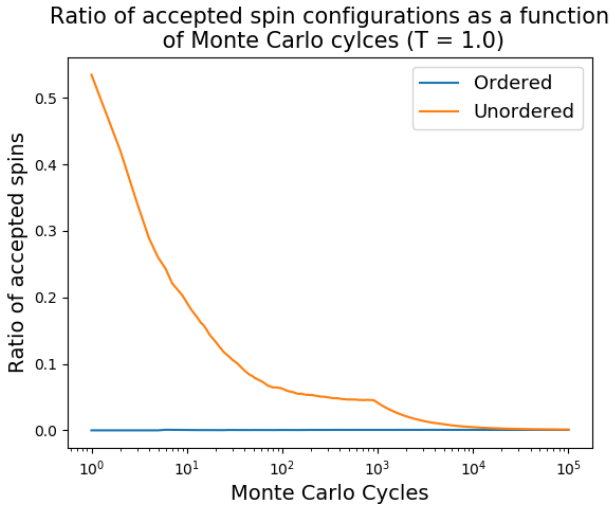


c. $\langle|\mathscr{M}|\rangle$, T = 2.4 for ordered

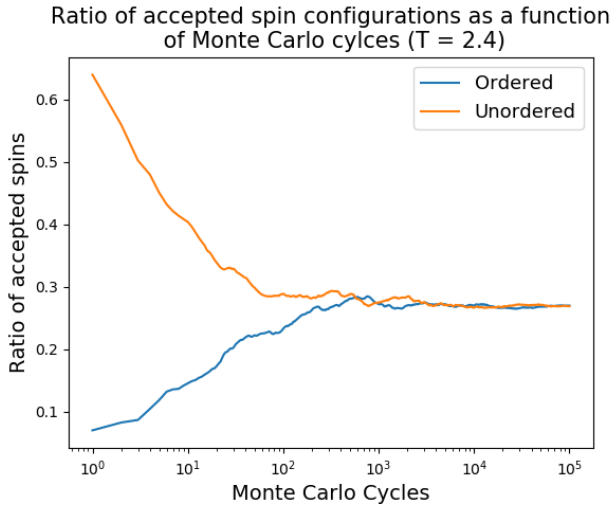


d. $\langle|\mathscr{M}|\rangle$, T = 2.4 for unordered

Figure 3: Mean magnetization for T = [1.0, 2.4], as well as for ordered and unordered configuration of spins, where it is plotted as a function of number of Monte Carlo cycles ranging $[1, 10^6]$



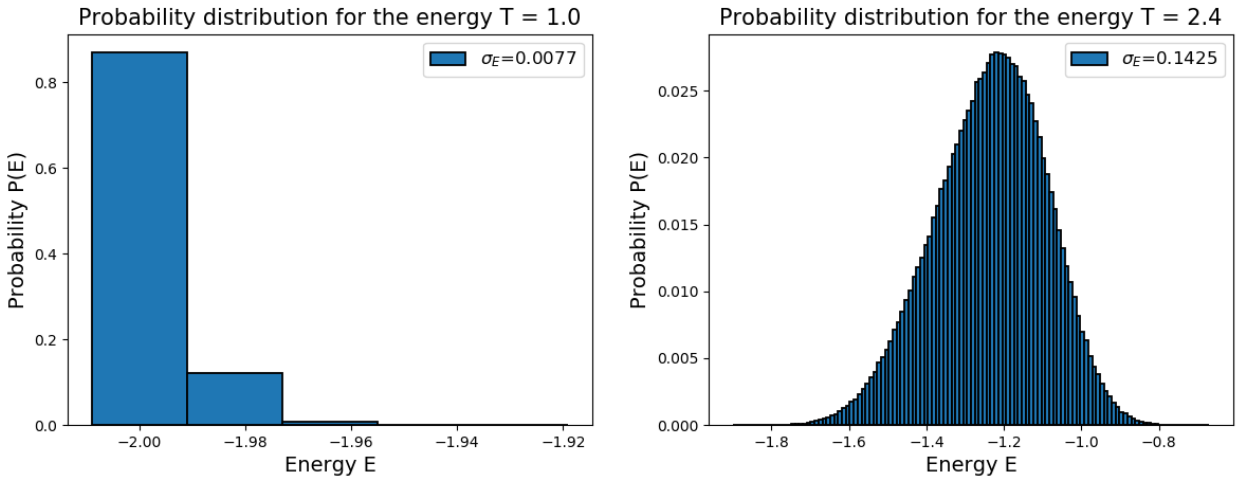
a. Ratio of accepted spins, T = 1.0



b. Ratio of accepted spins, T = 2.4

Figure 4: Plot of ratio of accepted spins as a function of Monte Carlo cycles. For T = [1.0, 2.4]. Both for ordered and unorderd configurations for a 20 x 20 lattice.

Figure 5 shows two plots of the probability distribution as a function of energy. The system is a 20×20-lattice with temperatures set to T = 1.0 and T = 2.4. The standard deviation is calculated to be $\sigma_E = 0.0077$ for T = 1.0 and $\sigma_E = 0.1425$ for T = 2.4. Where the number of Monte Carlo cycles set to value where equilibrium situation is achieved, see figure 2 and 3.

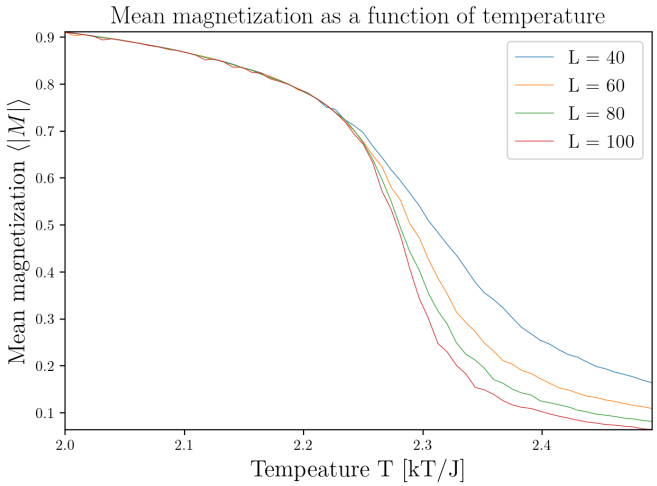


a. Histogram for energy after equilibrium, T = 1.0

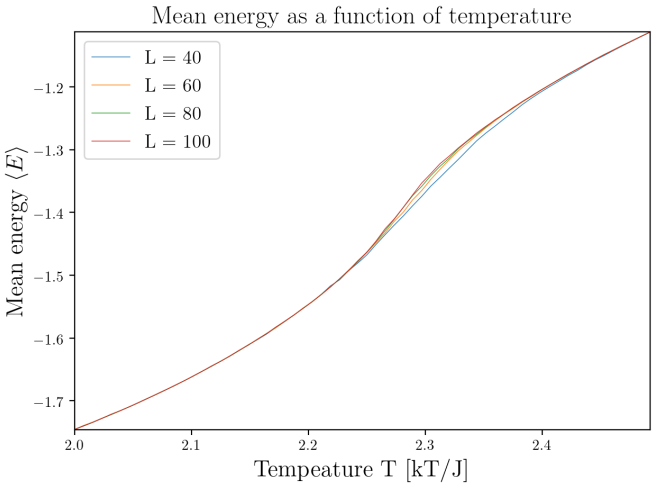
b. Histogram for energy after equilibrium, T = 2.4

Figure 5

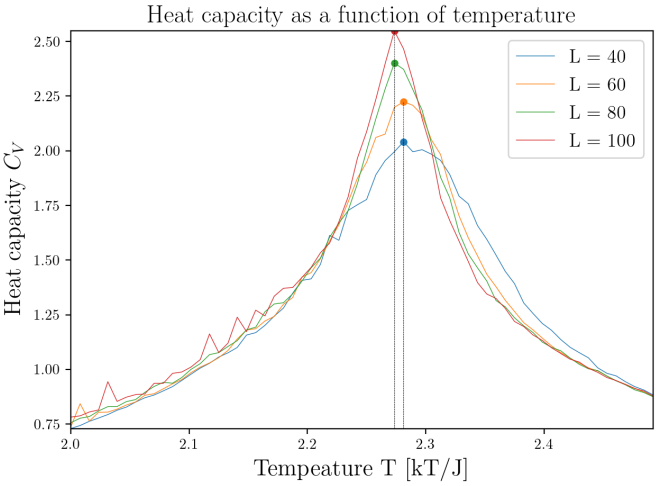
iii. *Phase transition and critical temperature*



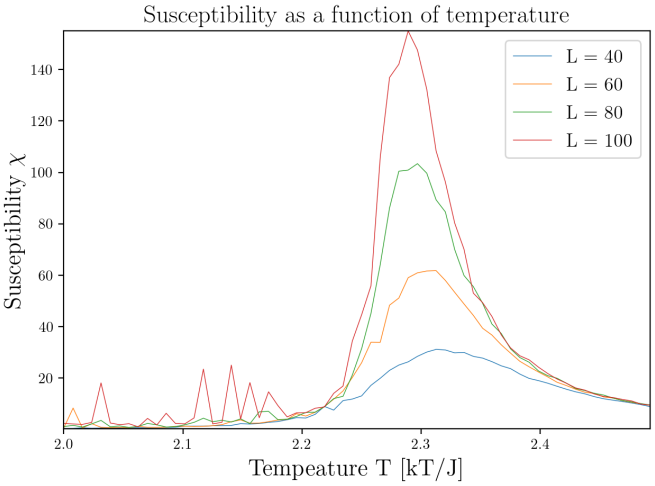
a. $\langle |\mathscr{M}| \rangle$, for L = [40,60,80,100] and unorderd



b. $\langle E \rangle$, for L = [40,60,80,100] and unorderd



c. C_V, for L = [40,60,80,100] and unorderd



d. χ, for L = [40,60,80,100] and unorderd

Figure 6: Plot of $\langle E \rangle, \langle |\mathscr{M}| \rangle, C_V, \chi$, for a temperature intevall T= [2.0,2.5]. Temperature step is set to 0.0078125 for a 64 points distribution. The number of Monte Carlo cycles for these plot where set to 10^6.

In figure 6 it we look at the phase transition in the system as the lattice size is increased. L = [40,60,80,100], where used, with 10^6 number of Monte Carlo cycles. The initial spin configuration of the system was unordered, however, the equilibrium situation has occurred. The temperature domain was set to T = [2.0,2.5] with a temperature step-size of 0.0078125, which corresponds to 64 points. The plots describes behaviours of mean absolute magnetization $\langle |\mathscr{M}| \rangle$, mean energy $\langle E \rangle$, heat capacity C_V and susceptibility χ.

Table 4: Values taken from figure 6c, where maximum of the plot is the critical temperature for a given lattice. With the exact value of T_C as given by Lars Onsager [1]

Lattice size	T_C **[kT/J]**
40	2.281
60	2.281
80	2.273
100	2.273
Exact T_C**:**	2.269

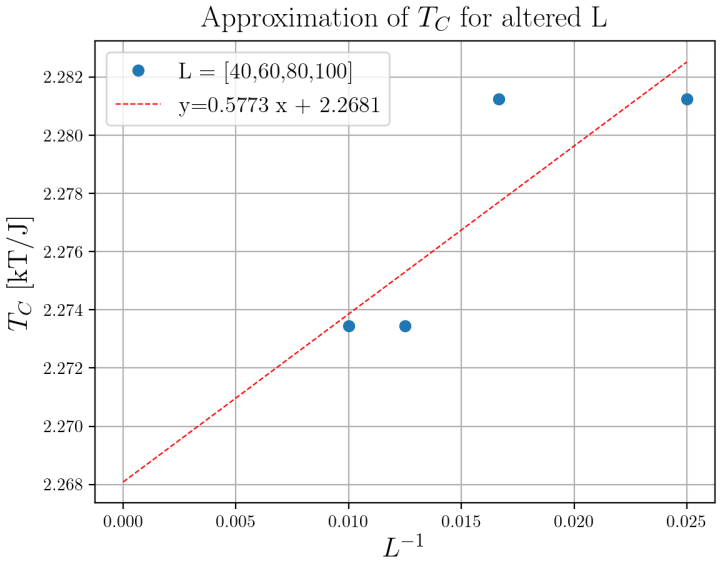


Figure 7: Linear regression of estimated T_C for lattices with dimension [40,60,80,100]. Where the red line is the linear equation containing information about the constant a from subsection Phase transition. The blue circles is the values taken from table 4

iv. *Parallel computing*

Table 5: For lattice size of 20 x 20. Comparing parallelized code vs non-parallelized code. For Monte Carlo cycles [10 000, 50 000, 100 000], with temperature points $\#T$ =[4, 8, 16].

Monte Carlo cycles	**#Temperatures**	**Time [s]**	**Parallelized [s]**
10 000	4	1.016	0.2966
	8	1.9661	0.5868
	16	3.9219	1.2187
50 000	4	4.875	1.5354
	8	9.7031	2.9452
	16	19.4121	5.8653
100 000	4	9.6718	2.9268
	8	19.3906	5.7752
	16	38.7430	11.8491

VI. Discussion

i. *Comparison of Analytical vs Numerical values for 2 x 2 lattice*

First approach for simulating the model was comparing the numerical values to the know analytical ones from Appendix A for a simple case of a 2 x 2 lattice at T = 1.0. Results given in Table 3 show that the obtained expectation values are close to the analytical and that higher number of Monte Carlo cycles leads to a better approximation for values of heat capacity C_V and susceptibility χ. Explanation for such an improvement for these values could be due to heat capacity C_V and susceptibility χ being represented as variance of the energy and magnetization. For low temperature and a 2 x 2 lattice there would be fluctuations at the start contributing to a larger deviation from the mean in results, which has less significance when the amount of contributions becomes big. Deviations from the equilibrium once and then represent a larger portion of all the contributions for so few Monte Carlo cycles and that affects the output. This can be seen from Table 3 where the standard deviation is a lot higher for fewer Monte Carlo cycles.

ii. *Equilibrium condition*

Behaviour of the system at the start of calculations changes drastically, thus acquiring the steady state condition where the values stabilize before extracting any of the expectation values was needed. In order to achieve this the mean energy $\langle E \rangle$ and mean magnetization $\langle M \rangle$ was plotted as a function of Monte Carlo cycles as shown in Figure 2 and 3. Monte Carlo cycles represented time, where the goal was to find out when the system achieved an equilibrium state.

Performing these calculations on different systems, consisting of ordered and unordered spins and temperature at T = 1 and T = 2.4, gave some interesting results for the 20 x 20 lattice. For the system initialized with all spins oriented in one direction at T = 1, the energy seems to start close to the equilibrium mean energy of $\langle E \rangle \approx$ -1.996 (Figure 2a). Meanwhile for the case of all spins having random orientation the mean energy is off-set a lot more at the start (Figure 2b) and equilibrates after around 10^3 Monte Carlo cycles. A similar case is present for the absolute mean magnetization at T = 1 (Figure 3ab), where the ordered system starts close to the equilibrium of $\langle |\mathscr{M}| \rangle \approx 0.9987$ while the unordered system approaches this value after approximately 10^3 Monte Carlo cycles. Reasoning behind those values can be explained by the fact that at a low temperature such as T = 1, the system is at the most stable state when all spins are oriented in the same direction known as being ferromagnetic. Looking at the Figure 4 showing the amount of accepted spins strengthens this claim.

When comparing this to the system when temperature is set to T = 2.4 this is no longer the case. Neither the ordered or the unordered system start near the most likely state. Acquiring a more stable state at higher temperature requires more Monte Carlo cycles and fluctuates a lot more as seen from 2cd and 3cd as the system now requires 10^4 Monte Carlo cycles to achieve equilibrium condition of $\langle E \rangle \approx$ -1.23 and $\langle M \rangle \approx 0.45$. Analysing the acceptance ratio for this case seems to show that at higher temperature there is a higher likelyhood for flipping a state and thus more fluctuations occuring for a statistical system like the one being investigated here. Ratio of accepted spins for this temperature flattens out at around 30%, which tells us that at this temperature the system continues flipping the spins even when at equilibrium leading to fluctuations of the mean values.

Acceptance ratio is temperature dependent, as the threshold for flipping will be lower for a higher temperature and thus the system will fluctuate around the most stable state.

iii. *Phase transition*

Phase transition and critical temperature is presented under results, subsection *phase transition and critical temperature*. Figure 6, provides a clear description of when phase transition occurs. Figure 6a,b describes the mean absolute magnetization and the mean energy of the system. As we can see by Figure 6a, the mean absolute magnetization approaches zero as L is increased. This is a fundamental part, where where at the paramagnetic phase it should loose its ability to self magnetize. As discussed under the theoretical part under subsection *Phase transition*, the system is in a ferromagnetic stage before undergoing the phase transition. One can see that by figure 6a, that as one increases the dimension of the lattice, it slowly converges to a critical temperature. This temperature was established by the Lars Onsager [1], as mentioned previously. And the magnetic moment goes towards zero for $T >> T_C$.

By figure 6b, it is clear that the mean energy of the system increased as the temperature increases. As the magnetic moment goes towards zero, the energy increases. The reason is because the system has stabilized it spins such that the mean magnetic moment is zero.

The heat capacity and susceptibility has discontinuous shape at the critical temperature. This discontinuity describes the phase transition. As we can see by figure 6c,d both plots has a discontinuity at a certain temperature. Values from figure 6c is depicted in table 4. Where all peaks is given by lattice size and numerical result of the critical temperature T_C. As we saw by equation 17.

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{26}$$

Which can be rewritten as:

$$T_C(L) = aL^{-1/\nu} + T_C(L = \infty) \tag{27}$$

This is an linear equation. We have values of L and T_C. We may then approximate $T_C(L = \infty)$ as well as the constant a. This is done by figure 7. Where the equation in the figure corresponds to the equation 27. By this we see that the constant $a = 0.058$, and the approximation of $T_C(L = \infty) = 2.268$.

$$\epsilon_{rel} = \frac{|2.269 - 2.268|}{2.269} \times 100\% \approx 0.040\% \tag{28}$$

Which is a good estimate of $L = \infty$. The reason for a good agreement of the critical temperature, is due to high value of L, as well as small step-lengths in the temperature interval. As mentioned the temperature step-length was set to 0.0078125. A smaller value would most likely give a better agreement with the exact value of $T_C = 2.269$. As we can see by table 5, the time consumption increased as the number of points increases. By this we used an parallelized code when running for temperature interval.

VII. Conclusion

References

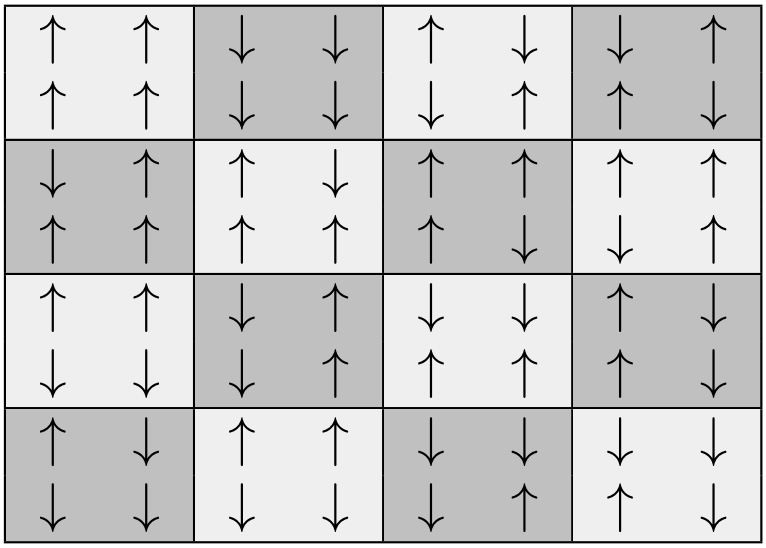
[1] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117, 1944.

[2] Daniel V Schroeder. An introduction to thermal physics, 2014.

[3] M. Hjorth-Jensen. Computational Physics. *University of Oslo*, `https://github.com/CompPhysics/ComputationalPhysics`, 2013.

Appendices

A. Analytical solution 2×2 case.



# Spins up	*# Spin configurations*	*Energy*	*Magnetization*
4	1	-8J	4
3	4	0	2
2	2	8J	0
2	4	0	0
1	4	0	-2
0	1	-8J	-4

The energy and magnetization can be written as:

$$E = -J \sum_{<kl>} s_k s_l \qquad M = \sum_l s_l$$

The mean energy is calculated with the help of the partition function which is for 2×2-lattice case:

$$Z = \sum_i e^{-E_i \beta} = 2 \cdot e^{8J\beta} + 2 \cdot e^{-8J\beta} + 12 = 4\big(\cosh(8J\beta) + 3\big)$$

We can now calculate the mean energy $\langle E \rangle$:

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-E_i \beta} = \frac{2 \cdot 8Je^{-8J\beta} - 2 \cdot 8Je^{8J\beta}}{4\big(\cosh(8J\beta) + 3\big)} = -\frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3}$$

The exact solution to the mean energy per spin is $\langle E \rangle = -1.99598208594$. To be able to calculate the heat capacity we first find the mean energy squared:

$$\langle E^2 \rangle = \frac{1}{Z} \sum_i {E_i}^2 e^{-E_i \beta} = \frac{2 \cdot (-8J)^2 e^{8J\beta} + 2 \cdot (8J)^2 e^{-8J\beta}}{4\big(\cosh(8J\beta) + 3\big)} = \frac{64J^2 \cosh(8J\beta)}{\cosh(8J\beta) + 3}$$

The heat capacity is the formulated as such:

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} = \frac{1}{k_B T^2} \left(\frac{64J^2 \cosh(8J\beta)}{\cosh(8J\beta) + 3} - \left(- \frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3} \right)^2 \right)$$

$$= \frac{1}{k_B T^2} \left(\frac{64J^2 \cosh(8J\beta)\big(\cosh(8J\beta) + 3\big)}{\big(\cosh(8J\beta) + 3\big)^2} - \frac{64J^2 \sinh^2(8J\beta)}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{1}{k_B T^2} \left(\frac{64J^2 \cosh^2(8J\beta) + 3 \cdot 64J^2 \cosh(8J\beta) - 64J^2 \sinh^2(8J\beta)}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{64J^2}{k_B T^2} \left(\frac{\cosh^2(8J\beta) - \sinh^2(8J\beta) + 3\cosh(8J\beta)}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{64J^2}{k_B T^2} \left(\frac{1 + 3\cosh(8J\beta)}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

The exact solution to the heat capacity per spin is then $C_V = 0.03208233186$. Further on we calculate the mean absolute magnetic moment $\langle |\mathscr{M}| \rangle$. Which can be done in the same way as for energy, reasons showed under the subsection Boltzmann statistic. We then have the mean absolute magnetic moment written as:

$$\langle |M| \rangle = \frac{1}{Z} \sum_i |M_i| e^{-E_i \beta} = \frac{2 \cdot 4e^{8J\beta} + 8 \cdot 2}{4\big(\cosh(8J\beta) + 3\big)} = \frac{2e^{8J\beta} + 4}{\cosh(8J\beta) + 3}$$

The exact solution to the mean absolute magnetic moment per spin is $\langle |\mathscr{M}| \rangle = 0.99866073274$. Further on we do as before, and find the mean absolute magnetic moment squared. in order to find the susceptibility.

$$\langle M^2 \rangle = \frac{1}{Z} \sum_i {M_i}^2 e^{-E_i \beta} = \frac{2 \cdot 4^2 e^{8J\beta} + 8 \cdot 2^2}{4\big(\cosh(8J\beta) + 3\big)} = \frac{8e^{8J\beta} + 8}{\cosh(8J\beta) + 3}$$

The susceptibility is the formulated as:

$$\chi = \frac{\langle M^2 \rangle - \langle |M| \rangle^2}{k_B T} = \frac{1}{k_B T}\left(\frac{8e^{8J\beta} + 8}{\cosh(8J\beta) + 3} - \left(\frac{2e^{8J\beta} + 4}{\cosh(8J\beta) + 3} \right)^2 \right)$$

$$= \frac{1}{k_B T}\left(\frac{\big(8e^{8J\beta} + 8\big)\big(\cosh(8J\beta) + 3\big)}{\big(\cosh(8J\beta) + 3\big)^2} - \frac{4e^{16J\beta} + 16e^{8J\beta} + 16}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{1}{k_B T}\left(\frac{8e^{8J\beta}\cosh(8J\beta) + 24e^{8J\beta} + 8\cosh(8J\beta) + 24 - 4e^{16J\beta} - 16e^{8J\beta} - 16}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{1}{k_B T}\left(\frac{4e^{8J\beta}\big(e^{-8J\beta} + e^{8J\beta}\big) + 24e^{8J\beta} + 4\big(e^{-8J\beta} + e^{8J\beta}\big) + 24 - 4e^{16J\beta} - 16e^{8J\beta} - 16}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{1}{k_B T}\left(\frac{4 + 4e^{16J\beta} + 24e^{8J\beta} + 4e^{-8J\beta} + 4e^{8J\beta} + 24 - 4e^{16J\beta} - 16e^{8J\beta} - 16}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

$$= \frac{4}{k_B T}\left(\frac{6\cosh(8J\beta) + 3 - 2e^{-8J\beta}}{\big(\cosh(8J\beta) + 3\big)^2} \right)$$

Where the exact value of the suscpetibility per spin is $\chi = 0.00401073951$