Phase transitions in magnetic systems

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Abstract

In this prosject we used the Ising model to study the behaviour of phase transition near critical points. We have sees that the time needed to reach equilibrium is longer for temperatures closer to critical temperature. We also noticed that with lager size of lattice, the curve for heat capacity and susceptibility will have a sharper top-point. At last we calculated that time needed to perform 40×40 lattice with 8 nodes is 8.5 minutes, and with only 1 node 22 minutes. This shows that for an even larger lattice, we must use the parallelized Ising mode.

1 Introduction

Phase transition is a change in a feature of a physical system that results in a discrete transition of that system to another state. (ref 1) We will study their behavior near critical points, the end point of a phase equilibrium curve. The model that is widely used in phase transition studies is named the Ising model and allows us to compute various thermodynamical quantities. This model was invented by the physicist Wilhelm Lenz in 1920. He solved himself the onedimensional Ising model in 1925 but it had no phase transition. Much later, in 1944 found Lars Onsager an analytical solution to the two-dimensional Ising model. (Wikipedia: Ising Model, 2020). We will employ this model in our studies of phase transitions at finite temperature for magnetic systems in two dimensions. At a given critical temperature, this model exhibits a phase transition from a magnetic phase to a phase with zero magnetization. (ref Project 4). With the Ising model we can in a simple way describe how a magnetic material responds to thermal energy and an external magnetic field. In our model each domain has a corresponding spin up or down. The model assigns a value of +1or -1 to the spins up and down respectively.

(Lecture note, s. 415)

2 Method

2.1 A simple 2×2 lattice, analytical expression

We will now assume that are only have two spins in each dimension, L=2. Since each spin takes only two values, we have $2^4=16$ possible arrangements of the two spins in two dimensions. For a two-dimensional lattice with periodic boundary conditions, each spin sees 4 neighbors. We see this illustration on the 2x2 grid in figure 1.

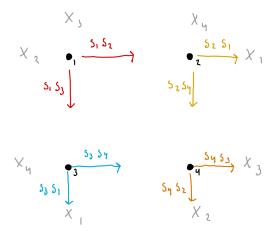


Figure 1: a nice plot

For the two-dimensional Ising model the energy is expressed as

$$E = -J \sum_{j=1}^{N-1} s_j s_{j+1} \tag{1}$$

where J is a constant expressing the strength of the interaction between neighboring spins s_j . We can rewrite the energy as

$$\frac{E}{J} = -(s_1 s_2 + s_1 s_3 + s_2 s_1 + s_2 s_4 + s_3 s_4 + s_3 s_1 + s_4 s_3 + s_1 s_2)
\frac{E}{J} = -(2s_1 s_2 + 2d_1 s_3 + 2s_3 s_4 + 2s_2 s_4)
\frac{E}{J} = -2(s_1 (s_2 + s_3) + s_4 (s_3 + s_2))$$
(2)

The energy of a two-dimensional lattice is

$$E = -2j(s_1 + s_4)(s_2 + s_3) \tag{3}$$

Magnetization is defined as

$$M = \sum_{j=1}^{N} s_j \tag{4}$$

In our case, two-dimensional lattice, the spin s_i only have 4 neighbours, s_1, s_2, s_3 and s_4 , so the magnetization is expressed as

$$M = s_1 + s_2 + s_3 + s_4 \tag{5}$$

If we sketch all sixteen possible configurations (Appendix B) and calculate the energy and magnetization for each, we can group these configurations according to their total energy and magnetization. This is shown in a table .

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8j	4
3	4	0	2
2	4	0	0
2	2	8j	0
1	4	0	-2
0	1	-8j	-4

By knowing this we can finding the partition which is given by

$$Z = \sum_{E} e^{-\beta E_i} \tag{6}$$

If use the values from table 1 vi can derive that

$$Z = 2e^{\beta 8j} + e^{-\beta(8j)} + 12e^{0}$$

$$Z = 2e^{-\beta(-8j)} + e^{-\beta(8j)} + 12$$
(7)

We can now use that $cosh(x) = \frac{e^x + e^{-x}}{2}$, which gives that the partition function for this system can be written as

$$Z = 4\cosh(8) + 12\tag{8}$$

A general equation for the expectation value is given by

$$\langle f(x) \rangle = \sum_{x} P(f(x))f(x)$$
 (9)

In our case $P(f(x)) = \frac{e^{-\beta f(x)}}{Z}$

From this we get that the corresponding expectations value for the Energy E is

$$\langle E \rangle = \frac{1}{Z} \sum E_i e^{-\beta E_i} \tag{10}$$

By using the values from table 1 we get that

$$\langle E \rangle = \frac{1}{Z} (2 \cdot (-8j)e^{8j\beta} + 12 \cdot 0 \cdot e^0 + 2 \cdot 8je^{-8j\beta})$$

$$\langle E \rangle = \frac{1}{Z} 16j(-e^{8j\beta} + e^{-8j\beta})$$

$$\langle E \rangle = \frac{-32j\sinh(8\beta j)}{Z}$$
(11)

The corresponding energy variance is defined as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i} - (\frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i})^2$$
 (12)

From equation 18 we can obtain the equation for the specific heat: The specific heat C_v is given by

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

so in order to calculate this we also have to find $\left\langle E\right\rangle ^{2}$ and $\left\langle E^{2}\right\rangle$

$$\langle E \rangle^2 = \frac{-32^2 j^2 \sinh^2(8\beta j)}{Z^2} \tag{14}$$

$$\langle E^2 \rangle = \frac{1}{Z} \sum E_i^2 e^{-\beta E_i}$$
$$\langle E^2 \rangle = \frac{1}{Z} \sum E_i^2 e^{-\beta E_i}$$

$$\langle E^2 \rangle = \frac{16^2 cosh(8\beta j)}{Z} \tag{15}$$

Then we put equation 15 and 14 into equation 13 and calculate the specific heat:

$$C_{v} = \frac{1}{k_{B}T^{2}} \left(\frac{16^{2} \cosh(8\beta j)}{Z} - \frac{-32^{2} j^{2} \sinh^{2}(8\beta j)}{Z^{2}} \right)$$

$$C_{v} = \frac{16^{2} j^{2}}{k_{B}T^{2}Z} \left(\cosh(8\beta j) - \frac{4}{Z} \sinh^{2}(8\beta j) \right)$$
(16)

Using the same method, we can also find the mean magnetization

$$\langle M \rangle = \frac{1}{Z} \sum_{i}^{M} M_{i} e^{-\beta E_{i}} \tag{17}$$

and the corresponding variance

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2 = \frac{1}{Z} \sum M_i^2 e^{-\beta E_i} - (\frac{1}{Z} \sum M_i^2 e^{-\beta E_i})^2$$
 (18)

The susceptibility is then given by

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

From tabel 1 we get that

$$\langle |M| \rangle = \frac{1}{Z} (\left| 4e^{8\beta j} \right| + \left| 4 \cdot 2e^{0} \right| + \left| 4 \cdot (-2)e^{0} \right| - \left| 4e^{8\beta j} \right|)$$

$$\langle |M| \rangle = \frac{8e^{8\beta j} + 16}{Z} \tag{19}$$

so that the expectational values are

$$\langle |M| \rangle^2 = \frac{(8e^{8\beta j} + 16)^2}{Z^2}$$
 (20)

and

$$\langle |M^2| \rangle = \left| \frac{1}{Z} \sum_{i}^{M} M_i^2 e^{-\beta E_i} \right|$$

$$\langle |M^2| \rangle = \frac{1}{Z} (|4^2 e^{8\beta j}| + |4 \cdot 2^2 e^0| + |4 \cdot (-2)^2 e^0| - |^2 e^8|)$$

$$\left\langle \left| M^2 \right| \right\rangle = \frac{32e^{8\beta j} + 32}{Z} \tag{21}$$

From this we get that the susceptibility is

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

$$\chi = \frac{1}{k_B T} (\frac{32e^{8\beta j} + 32}{Z} - \frac{(8e^{8\beta j} + 16)^2}{Z^2})$$
(22)

2.2 The Metropolis Algorithm and the Two-dimensional Ising Model

The algorithm we will use to solve the Ising problem is named Metropolis algorithm. By using a transition probability we can generate the new configurations, which only depend on the energy difference between the initial and final states.

The probability for finding a system in a state i is expressed by the Monte Carlo sampling function

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

where E_i is the energy, Z is the partition function and $\beta = \frac{1}{kT}$. We can express the partition function as

$$Z(\beta) = \sum_{i} e^{-\beta E_i} \tag{24}$$

The number of configurations in a calculation of the Ising model is given by 2^N where N is the number of spins for a lattice of lenght L, $N = L \times L$. It would be difficult to compute the partition function since we need all E_i states, but fortunately we don't need to compute Z at all. The Metropolis algorithm considers only ratios between probabilities.

The calculation of energy difference and the change in magnetization is the difficult part. For a large number L we would need to compute the change of energy many times. Therefor we will flip one spin only in spin configuration. This means that we will end up with fewer values for ΔE . There will actually only be 5 possible values for ΔE , regardless of the size L. This can easily be shown, to see this look at the appendix A.

Since there are only 5 possible values of ΔE , we don't have to evaluate the exponential $e^{\beta \Delta E}$ for each Monte Carlo sampling. Instead, we can make an array which contains all 5 possible values of $e^{\beta \Delta E}$. As shown in Appendix A, the 5 possible values for ΔE are $\Delta E = J[-8, -4, 0, 4, 8]$. We define an array B as

$$B[\Delta E + 8] = e^{-\beta \Delta E}$$

and then calculate the array elements

$$B[-8E + 8] = B[0] = e^{8\beta}$$

$$B[-4 + 8] = B[4] = e^{4\beta}$$

$$B[0 + 8] = B[8] = e^{0\beta} = 1$$

$$B[4 + 8] = B[12] = e^{-4\beta}$$

$$B[8 + 8] = B[16] = e^{-8\beta}$$

Our array B then looks like $B=[e^{8\beta},0,0,0,e^{4\beta},0,0,0,1,0,0,e^{-4\beta},0,0,0,e^{-8\beta}]$ This way we don't need to calculate $e^{\beta\Delta E}$ each time we update the energy. (Lecture notes, s. 434-436)

2.3 Writing a code of the Ising model

To implement the Metropolis algorith you should follow steps from picture bellow. You can find all the programs for the Ising model by clicking on the link https://github.com/martelkv/Prosjekt4.

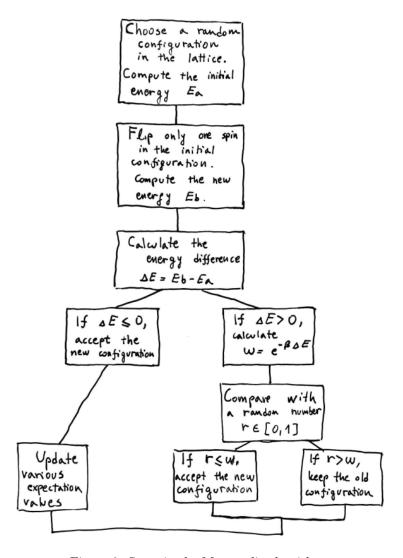


Figure 2: Steps in the Metropolis algorithm

Our program takes the initial and final temperature, as well as temperature step, number of spins in lattice in x-direction (since we have a square lattice, the x- and y-direction are the same) and number of Monte Carlo cycles as input parameters. When we perform Monte Carlo cycles we go through all the spins in the lattice and perform a Metropoli test in all the configurations after we flip one spin at a time. This is explained in a detail in a figure 2.

After we flip a spin we will compute the energy difference. The energy difference

between an initial state A and a state B is expressed as

$$\Delta E = E_B - E_A = J \sum_{\langle kl \rangle}^{N} s_k^A s_l^A - J \sum_{\langle kl \rangle}^{N} s_k^B s_l^B$$

$$= J \sum_{\langle kl \rangle}^{N} s_k^B (s_l^B - s_l^A)$$
(25)

where k are the nearest neighbours. The spin we are flipping takes two possible values, $s_l^A = \pm 1$ and the same goes for $s_l^B = pm1$. This mean then that if $s_l^A = 1$ then $s_l^B = -1$ and opposite. So if we have $s_l^A = 1$ and $s_l^B = -1$, then $s_l^A - s_l^B = 2$, and if $s_l^A = -1$ then $s_l^A - s_l^B = -2$. Since we only flip s_l , the other spin s_k has the same value, which mean that $s_k^A = s_k^B = \pm 1$. The energy difference can then be rewritten as

$$2Js_l^A \sum_{\langle kl \rangle}^N s_k \tag{26}$$

2.4 Extracting the critical temperature

In our calculations of the two-dimensional Ising model, we are always limited to a finite lattice size. Near the critical temperature T_c we can characterize the behavior of many physical quantities by a power law behavior. Where interested in so-called finite size scaling relations. Then we could relate the behavior at finite lattices with the results for an infinitely large lattice. (Project 4 paper) The critical temperature is expressed then as

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

where a is a constant and we set $\nu=1$. In order to estimate T_c in the thermodynamic limit $L\to\infty$ we can use our simulatins with L=40, L=60, L=80 and L=100.

We can rewrite the equation 27 as

$$T_c(L) = a\frac{1}{L} + T_c(-\infty)$$

If we stare at the new equation above we can see that it looks just like a first-order function that takes form

$$y = ax + b$$

Here x is the slope and represents $\frac{1}{L}$ and b which is a crossing point between y and y-axsis represents $T_c(\infty)$ which we are interested in.

3 Results

3.1 When is the most likely state reached?

3.1.1 Results for T=1, for ordered and random start-orientations

In figure 3, 4 we see mean energy as function of the number of Monte Carlo cycles, with ordered and random start-orientation. In figure 5 and 6 we see the same for mean magnetisation. In figure 7 we see the total number of accepted configurations as function of Monte Carlo cycles. All the calculations have been performed with a 20×20 lattice for a temperature T=1.0.

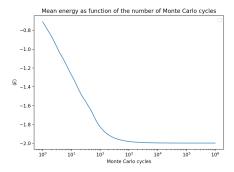


Figure 3: Mean energy as function of the number of Monte Carlo cycles when $T=1.0~\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. The start orientation used where a random orientation of spins.

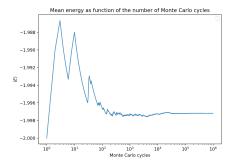


Figure 4: Mean energy as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. Ordered configuration as start configurations.

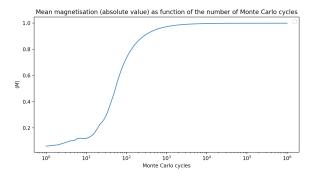


Figure 5: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. The start orientation used where a random orientation of spins.

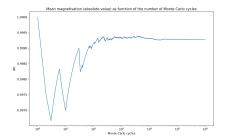


Figure 6: Mean energy as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. Ordered configuration as start configurations.

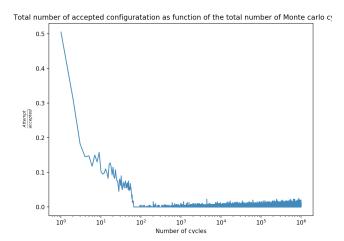


Figure 7: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice

3.1.2 Results for T=2.4, with ordered and random start-orientations

As for section 3.1.1, we can ,in figure 8, 9, see mean energy as function of the number of Monte Carlo cycles, with ordered and random start-orientation. In figure 10 and 11 we see the same for mean magnetisation. In figure 12 we see the total number of accepted configurations as function of Monte Carlo cycles. All the calculations have been performed with a 20×20 lattice for a temperature T=2.4.

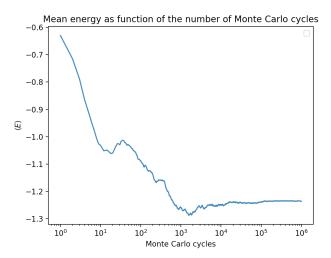


Figure 8: Mean energy as function of the number of Monte Carlo cycles when $T=2.4~\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. The calculations has been performed for a 20x20 lattice. The start orientation used where a random orientation of spins.

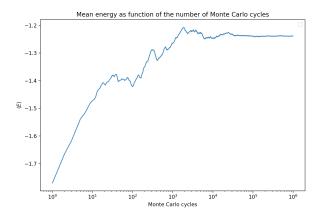


Figure 9: Mean energy as function of the number of Monte Carlo cycles when T = $2.4 \ \frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. Ordered configuration as start configurations.

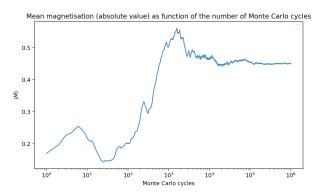


Figure 10: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = $2.4 \ \frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. The calculations has been performed for a 20x20 lattice. The start orientation used where a random orientation of spins.

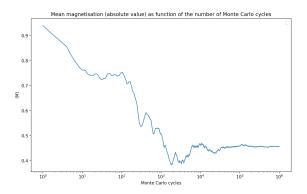


Figure 11: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = 2.4 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. Ordered configuration as start configurations

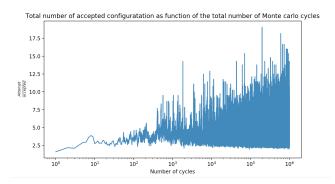


Figure 12: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=2.4 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.

3.2 Analyzing the probability distribution

Figure 13 and 14 shows the computed probability P(E) for the system with L=20 and temperatures T=1.0 and T=2.4.

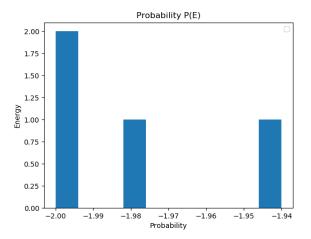


Figure 13: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.

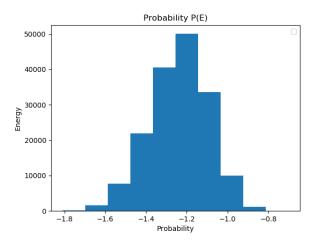


Figure 14: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.

3.3 Parallelization of the Ising Model

We performed a timing analysis of some selected runs in order to see that we get an optimal speedup when parallelizing our code. In the table below we present the time performance of runs for a different lattice size. We used 2.0 as start temperature, 2.6 as final temperature, 0.03 as temperature step and number of slot is 8.

Lattice size	Time [min]
20 x 20	4
40 x 40	15
60 x 60	32
80 x 80	57
100 x 100	87

To see how we get an optimal speedup when parallelizing our code, we performed a time analysis and 20×20 and 40×40 lattice with different number of nodes. The result are presented in the table below.

]	Lattice size	Time[s] for 8 nodes	Time[s] for 4 nodes	Time[s] for 1 nodes
	20×20	116.3	122.5	326.4
	40×40	512.3	517.1	1329.7

We wish to study the behavior of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. We calculated

and plotted the expectation values for mean energy $\langle E \rangle$ and magnetization $\langle |M| \rangle$, the specific heat C_v and the susceptibility χ as functions of T for L = 40, L = 60, L = 80 and L = 100 for T \in [2.0, 2.6] with a step temperature $\Delta T = 0.03$.

In Figures -19 we display results from the program as mentioned above.

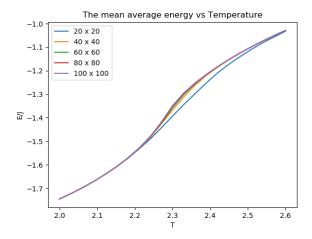


Figure 15: Average energy per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T=0.03$

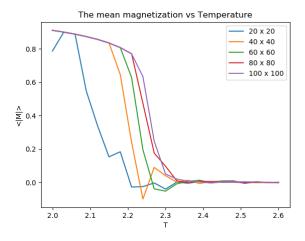


Figure 16: Absolute value of the average magnetization per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

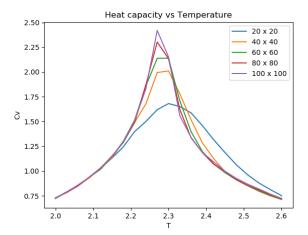


Figure 17: Heat capacity per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T=0.03$

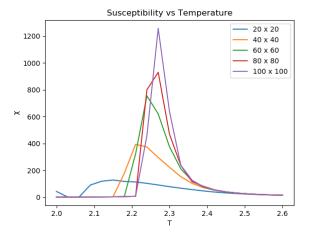


Figure 18: Susceptibility per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

3.4 Extracting the critical temperature

From figure 19 we can read the value of critical temperature T_c . T_c value corresponds to x-value of each top for each lattice size. Here we are only interested in sizes 40,60,80 and 100. In a table below you can see the T_c values we found.

We can plot the results from table above:

Lattice size	T_c
40 x 40	2.21 ± 0.01
60 x 60	2.24 ± 0.01
80 x 80	2.27 ± 0.01
100 x 100	2.28 ± 0.01

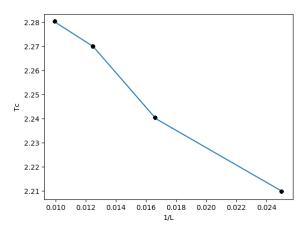


Figure 19: Susceptibility per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T=0.03$

If we now use Linear Regression in MATLAB we get the point where the function y crosses y-axis. We get that the crossing point b is 2.33 ± 0.0087 . So $T_C(\infty) = 2.33 \pm 0.00867$.

4 Discussion

4.1 When is the most likely state reached?

In our calculations we are interested in studying how many Monte Carlo cycles where need in order to reach the most likely state. Determining this is done in a brute force way, by just plotting the $\langle E \rangle$ for every cycle. For $T=1.0\frac{kT}{J}$ we see, from 3, that the most likely state for for mean energy is reached after 10^4-10^5 Monte Carlo cycles. We have the same number of cycles for the mean magnetisation. For T=2.4 we can see, from figure 8 and 10 that the stabilisation isn't reached before we have 10^6 Monte Carlo cycles, both for the mean energy and magnetisation. Thus it takes longer time for the high temperature to reach a steady state, then for lower temperatures.

If we compere the calculations from a random start-orientation (figure 3) and one with an ordered orientation (figure 4), we see that the random orientated

start-configuration brings us closer to the average value for that temperature.

We can from the to plots 7 and 12 see that the number of accepted configurations stabilises as the as we have more cycles, and when we increase the temperature we get a greater degree of variation for the the accepted configurations.

4.2 Analyzing the probability distribution

The computed probability P(E) for the two temperatures are visualized in figure 13 and 14, and are computed by just counting the number of times a given energy appears in the computation of $\langle E \rangle$. As expected we see a broader spread in the in the histogram for temperatures nearer the critical temperature. We can also see that the histograms are centered around the calculated expected values.

4.3 Writing a code of the Ising model

As we saw from the figure 8 the system reaches equilibrium state after approximate 10^5 Monte Carlo cycles. We are only interested in data afte the system reaches equilibrium, therefor we made a so-called "burn-in" function that loops over first 10^5 Monte Carlo cycles, and after that we start from the beginning and collect the data we need. This way we will get more correct data. Of course there is some uncertainty because we read from the graphs.

4.4 Parallelization of the Ising Model

The idea of parallelization of the Ising model is to make the simulation of your code much more efficient by using different nodes in your PC to run different parts of your code. From table bla we can see that for a two dimensional lattice of size 20×20 it almost takes three times as much time to run the code with one node than with 8 nodes. The same goes for 40×40 lattice. That mean that with a parallelization of the Ising model we save a lot of time to run the code, especially for very large lattice sizes.

From figure we can see that with larger lattice size we get a steeper line. The transition from law magnetization to higher one becomes sharper. We can say that this is a sign of a phase transition. We go from a place where the most spins point in in the spesific direction, to a phase where there is equal possibillity for both spins. We call the "ordered" phase at low temperatures a farromagnetic phase, while the disordered phase is called the paramagnetic phase.

From figure 17 and 19 we can see that when the lattice size increases, the spesific heat becomes sharper and sharper around the critical temperature. We can see the similar behavior for susceptibility as well, but with a sharper form.

4.5 Extracting the critical temperature

Since we read the values for T_c from graphs, there will be curtain uncertainty in the measurements. For better results we could have ran our program with smaller temperature steps and higher number of Monte Carlo cycles.

5 Conclusion

We have studied behaviour of phase transitions near critical points. The model that we used in our research is called the Ising model. We have worked with two-dimensional lattice with increasing sizes. We started with seeing how long time the system need before it reaches the equilibrium, and concluded that the time needed to reach the equilibrium is longer for temperatures closer to critical temperature.

We wanted also to show how average energy per spin, the mean magnetization, and other physical quantities like heat capacity and susceptibility behave with different amount of spins in our lattice. We noticed that with larger size of lattice the curve for heat capacity and susceptibility will have sharper top-point.

We have modified our program so that we let different nodes perform a given set of Monte Carlo samples. This way we made the program more efficient. The time needed to perform 40×40 lattice with 8 nodes is 8.5 minutes, and with only 1 node 22 minutes. This shows that for an even larger lattice, we must use the parallelized Ising model.

Appendix A: Five possible values for Δ E

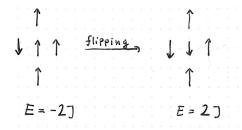
We start with a random sping x,y position where all spins are pointing up. We calculate the energy for this configuration with equation $1 E = -J(1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1) = -4J$. Then we flip a spin (as shown below) and calculate the new energy $E = -J(-1 \cdot 1 + (-1) \cdot 1 + (-1) \cdot 1 + (-1) \cdot 1) = 4J$.

$$\uparrow \uparrow \uparrow \frac{\text{flifting}}{\uparrow} \uparrow \downarrow \uparrow$$

$$\uparrow E = -47$$

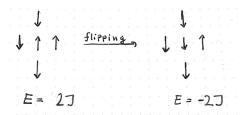
$$E = 47$$

The energy difference ΔE after flipping one spin is $\Delta E = 4J - (-4J) = 8J$. The new configuration is:

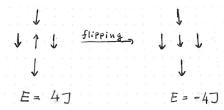


The new energy difference is $\Delta E = 2J - (-2J) = 4J$. Next configuration is

with the new energy difference $\Delta E = 0 - 0 = 0$. Next configuration is shown below

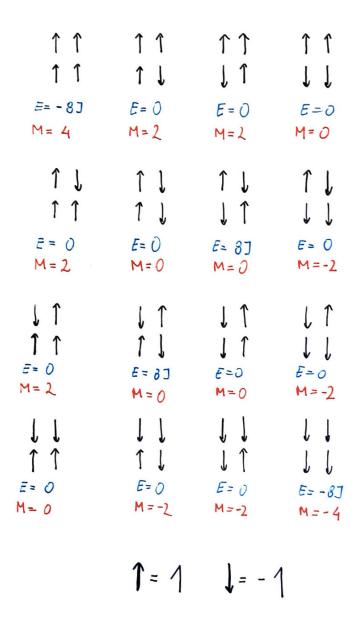


and the new energy difference is $\Delta E = -2J - 2J = -4J$. And the last possible configuration is



with the energy difference is $\Delta E = -4J - 4J = -8J$.

Appendix B: Sixteen possible configurations for two spins in two-dimensions



6 Sources

- \bullet ref 1 https://www.yourdictionary.com/phase-transition
- $\bullet\,$ Hjorth-Jensen M. (2015). $Computational\,Physics$. Department of Physics, University of Oslo.
- Wikipedia (2020, 26.
november). Ising Model. https://en.wikipedia.org/wiki/Ising
 $_model$