Phase transitions in magnetic systems

November 2020

Contents

Abstract

In this project 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 model. When we looked at the critical temperature, we got that Tc= 2.298, while Lars Onsager got Tc= 2.269. The error is probably caused by uncertainties in our calculations.

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 the one-dimensional 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. We will study the Ising model in a binary system, which assigns a value of +1 or -1 to the spins up and down respectively. We will use the Metropolis Algorithm in our calculations, with N amount of Monte Carlo cycles. (Lecture note, s. 415)

Initially, we will use a lattice with length L = 2, and then increase the length gradually until L = 100. We will precalculate many analytical values and then check if our programme gives us good results. We will notice that when lattice size increases, the time our programme needs to simulate will increase too. Therefor we can use a technice that makes our programme much more efficient. This technice is called parallelization. That means that our programme will run many Monte Carlo cycluses simultaneously. This will reduce the simulation time considerably, which is a positive thing considering that we can get date for much less time.

2 Method

2.1 A simple 2 × 2 lattice, analytical expression

We will start by deriving the formulas for $\langle E \rangle$, $\langle |M| \rangle$, $\langle C_v \rangle$ and $\langle \chi \rangle$. We assume that there is only 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, this is shown in Appendix B. For a two-dimensional lattice with periodic boundary conditions, each spin sees 4 neighbors. We see this illustration for the 2x2 grid in figure 1.

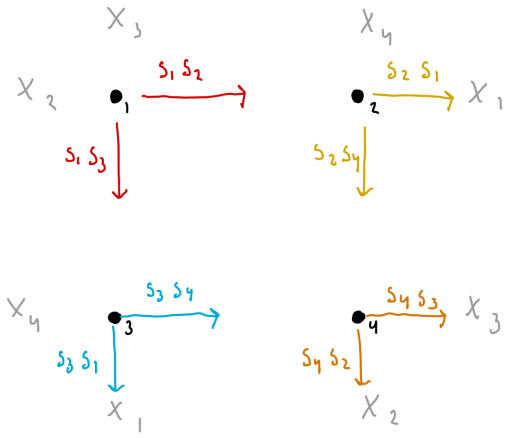


Figure 1: a nice plot

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. By using figure 1, we see that we can rewrite the energy as

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

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

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

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 for the 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 1.

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

Table 1: Lecture note, s. 424

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

$$\begin{aligned} Z &= 2e^{\beta 8j} + e^{-\beta(8j)} + 12e^{0} \\ Z &= 2e^{-\beta(-8j)} + e^{-\beta(8j)} + 12 \end{aligned} \tag{7}$$

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

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

By knowing this we can calculate the expecting values. A general equation for this value is given by

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

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

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

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

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

Quantity $e^{-\beta E}$ is called Boltzmann factor which tells us about the probability for a given state. We have that $\beta = \frac{1}{k_B T}$, k_B is Boltzmann constant, T is the temperature. The corresponding energy variance is defined as

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

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

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

Heat capacity tells us how much amount of heat has to be supplied to a given mass of a substance to produce a unit change in its temperature. In order to calculate heat capacity we also have to find $\langle E \rangle^2$ and $\langle E^2 \rangle$.

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

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

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

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

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

$$C_v = \frac{1}{k_B T^2} (\frac{16^2 cosh(8\beta j)}{Z} - \frac{-32^2 j^2 sinh^2(8\beta j)}{Z^2})$$

$$C_v = \frac{16^2 j^2}{k_B T^2 Z} (cosh(8\beta j) - \frac{4}{Z} sinh^2(8\beta j)) \tag{16}$$

Using the same method, we can also find the expected value for absolute value of the magnetization:

$$\langle M \rangle = \frac{1}{Z} \sum_i^M |M_i| e^{-\beta E_i} \tag{17}$$

Magnetization denotes the total spin of the system, i.e how many spins point up against how many spins point down. The corresponding variance is

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

The susceptibility is another quantity we will use in our calculations of the Ising model. Magnetic susceptibility of a substance describes its response to an applied field. In our case magnetic susceptibility tells us how much our substance is magnetized if it enters a magnetic field. Susceptibility 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 expected values are

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

and

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

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

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

From this we get that the susceptibility is

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

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

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 length 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

$$\begin{aligned} B[-8E + 8] = B[0] &= e^{8\beta} \\ B[-4 + 8] = B[4] &= e^{4\beta} \\ B[0 + 8] = B[8] &= e^{0\beta} = 1 \\ B[4 + 8] = B[12] &= e^{-4\beta} \\ B[8 + 8] = B[16] &= e^{-8\beta} \end{aligned}$$

Our array B then looks like $B = [e^{8\beta}, 0, 0, 0, e^{4\beta}, 0, 0, 0, 1, 0, 0, 0, e^{-4\beta}, 0, 0, 0, e^{-8\beta}]$
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 algorithm 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`.

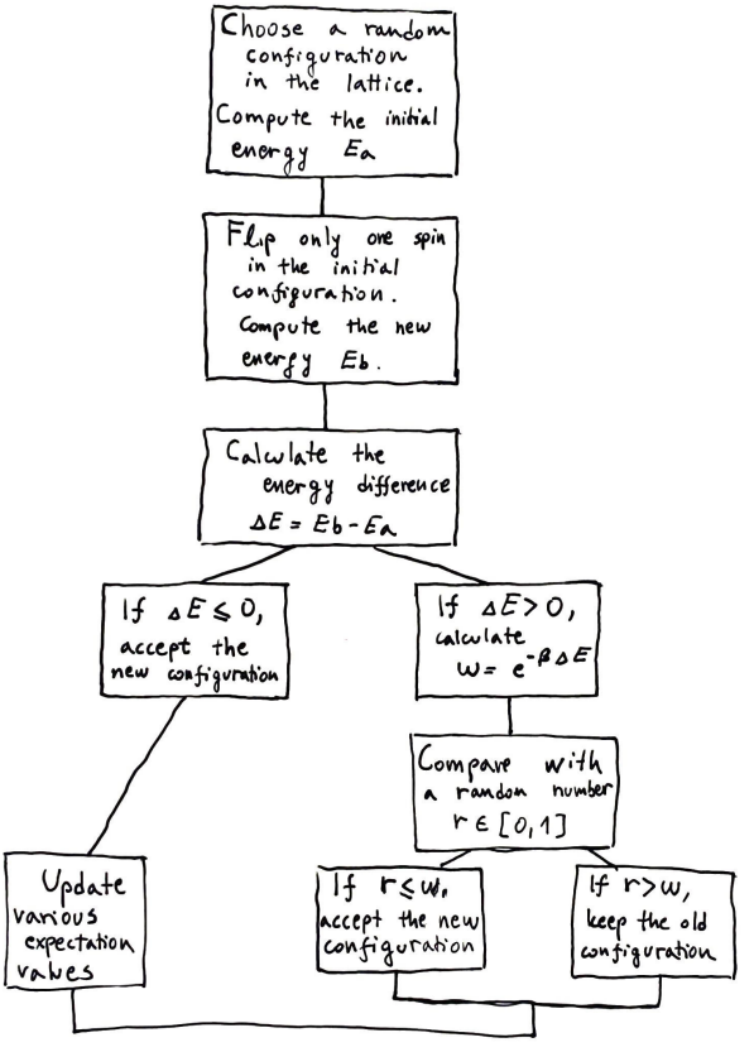


Figure 2: Steps in the Metropolis algorithm

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 Metropolis 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

$$\begin{aligned}\Delta E = E_B - E_A &= J\sum_{<kl>}^{N} s_k^A s_l^A - J\sum_{<kl>}^{N} s_k^B s_l^B \\ &= J\sum_{<kl>}^{N} s_k^B(s_l^B - s_l^A)\end{aligned} \tag{25}$$

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

$$2Js_l^A \sum_{<kl>}^{N} s_k \tag{26}$$

We can also rewrite the change in magnetisation after we flip one spin. We are only flipping the spin l, so the change is given by $s_l^A - s_l^B = \pm 2$. If we define M_1 and M_2 as the magnetizations before and after we flip a spin, we can write

$$M_2 = M_1 + 2s_l^B \tag{27}$$

Equations 26 and 27 are implemented in the Metropolis function in our code.

2.4 Studies of 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

$$T_c(L) - T_c(L = \infty) = aL^{-1/\nu} \tag{28}$$

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 equation28 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 Analytic vs numeric

In table 2 we have presented the solutions for $\langle E \rangle$, $\langle |M| \rangle$, $\langle C_v \rangle$ and $\langle \chi \rangle$, calculated both analytical, from the equations in section 2.1, and numerical. For the numerical calculation we have listed the results, calculated with different numbers of Monte Carlo cycles. For both situations we have sett $T = 1\frac{kT}{j}$ and $k_B = 1 \to \beta = \frac{1}{KT} = 1$. To obtain the results for the analytical part, we have divided by number of elements in our lattice. Since we for now have an $2x2$ lattice, we dived by 4.

Cycles	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	$\langle C_v \rangle$	$\langle \chi \rangle$
Exact	-1.995974	0.99865	0.0382082	0.00396885
10	-2.000	1.00	0.00000	0.0000
100	-1.960	0.98000	0.31360	0.07840
1000	-1.9960	0.998500	0.031936	0.00499
10000	-1.99820	0.99930	0.014387040	0.002398040
100000	-1.995420	0.9984450	0.036556094	0.0047403279

Table 2: Analytical and numerical solution to the formulas for $\langle E \rangle$, $\langle \lvert M \rvert \rangle$, $\langle C_v \rangle$ and $\langle \chi \rangle$ at $T = 1\frac{kT}{j}$ and $L = 2x2$. We have also set $k_B = 1$.

3.2 When is the most likely state reached?

3.2.1 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.

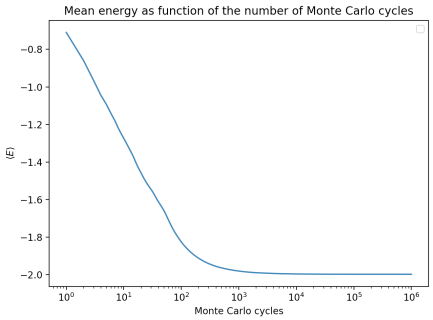


Figure 3: Mean energy as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.The start orientation used where a random orientation of spins.

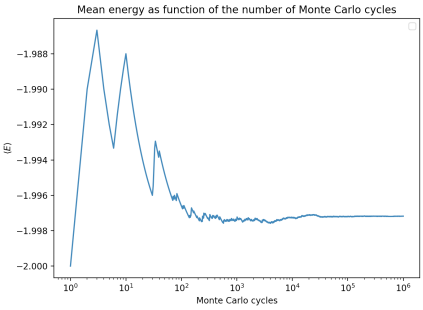


Figure 4: Mean energy as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.Ordered configuration as start configurations.

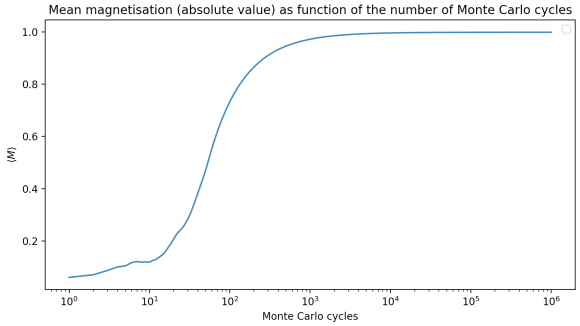


Figure 5: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice. The start orientation used where a random orientation of spins.

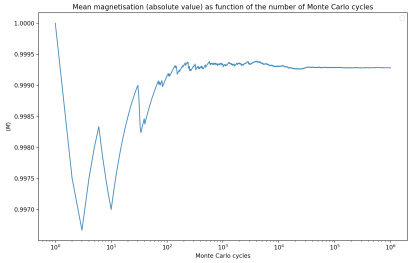


Figure 6: Absolute value of the mean magnetisation as function of the number of Monte Carlo cycles when T = 1.0 $\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.Ordered configuration as start configurations.

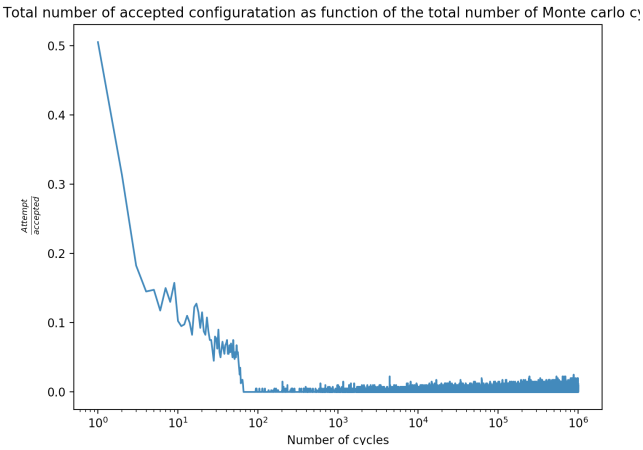


Figure 7: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0$\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice

3.2.2 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 $T = 2.4$.

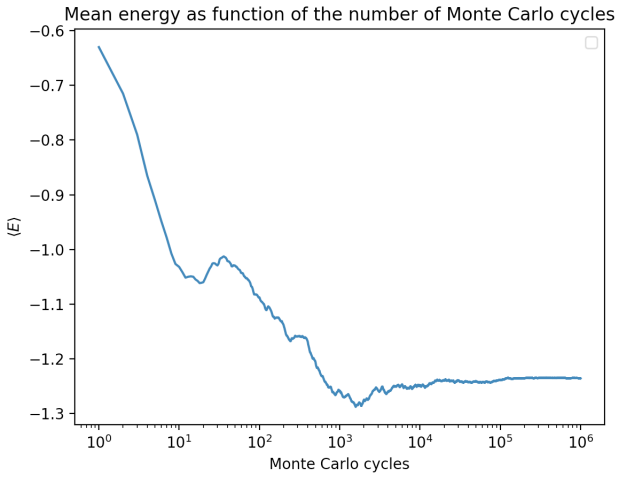


Figure 8: Mean energy as function of the number of Monte Carlo cycles when T = 2.4 $\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice.The calculations has been performed for a 20x20 lattice.The start orientation used where a random orientation of spins.

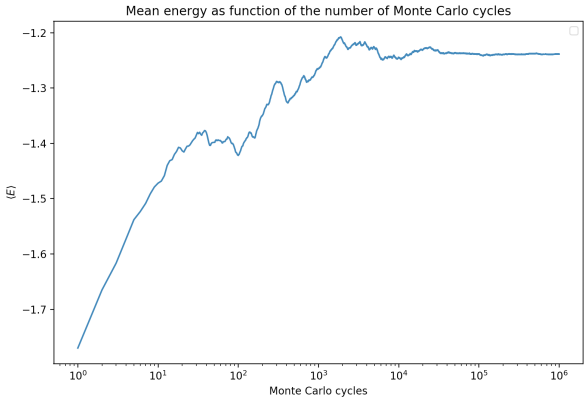


Figure 9: Mean energy as function of the number of Monte Carlo cycles when T = 2.4 $\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice.Ordered configuration as start configurations.

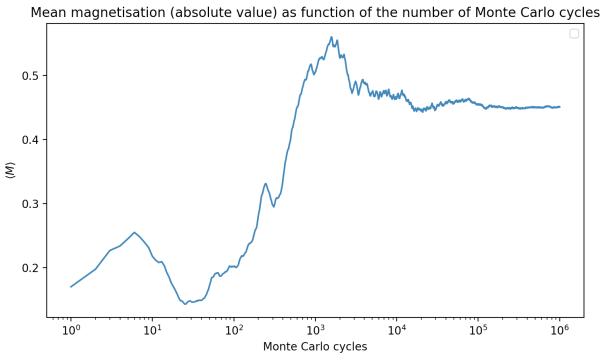


Figure 10: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = 2.4 $\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice.The calculations has been performed for a 20x20 lattice.The start orientation used where a random orientation of spins.

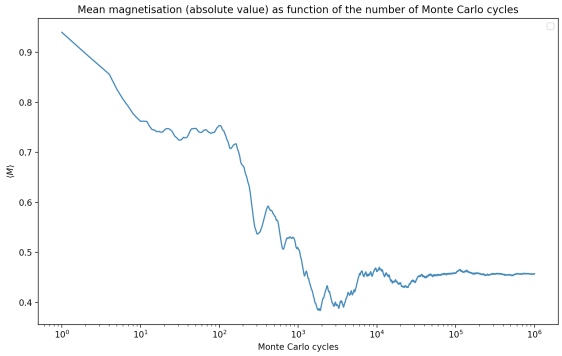


Figure 11: Absolute value of mean magnetisation as function of the number of Monte Carlo cycles when T = 2.4 $\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice. Ordered configuration as start configurations

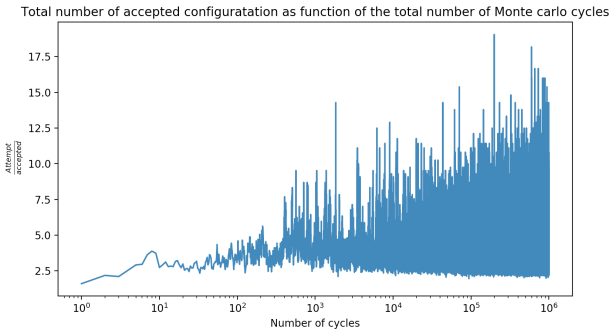


Figure 12: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=2.4$\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice.

3.3 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 $T = 2.4$.

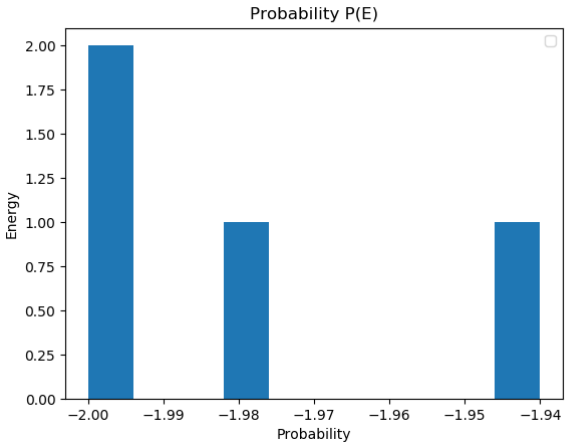


Figure 13: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0$\frac{kT}{J}$. The calculations has been performed for a 20x20 lattice.

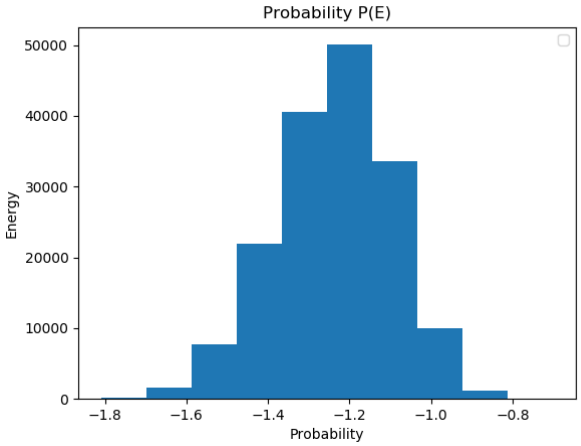


Figure 14: Total number of accepted configurations as function of the total number of Monte Carlo cycles when T=1.0$\frac{kT}{J}$.The calculations has been performed for a 20x20 lattice.

3.4 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 parellalizing 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

Table 3: Running time for different lattice size. The tempersture we used was $T_{start} = 2.0$ and $T_{final} = 2.3$. The sped size was 0.02, while the number of slots where set to 8

To see how we get an optimal speedup when parallelizating 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 x 20	116.3	122.5	326.4
40 x 40	512.3	517.1	1329.7

Table 4: Time analysis with lattice size $20x20$ and $40x40$, for 8, 4 and 1 node(s).

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 $< E >$ and magnetization $< |M| >$, 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.

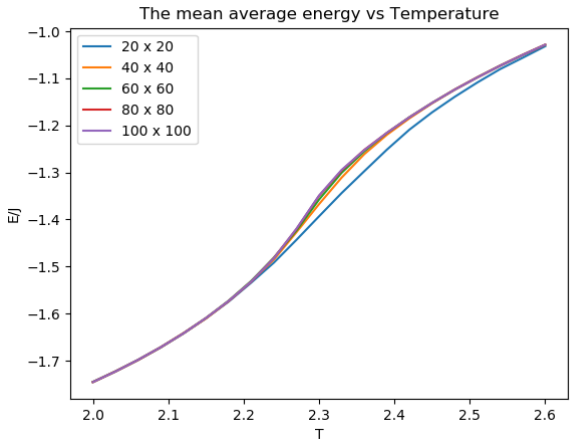


Figure 15: Average energy per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

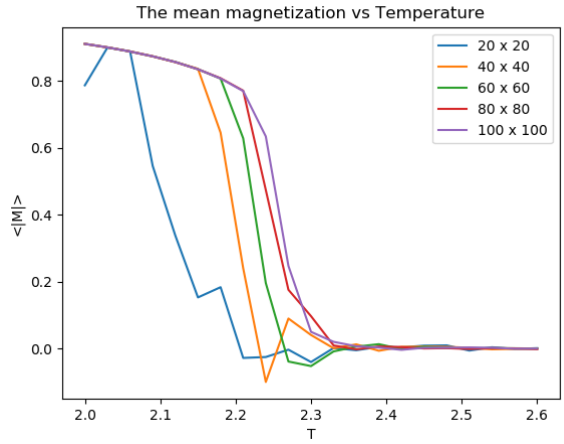


Figure 16: Absolute value of the average magnetization per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

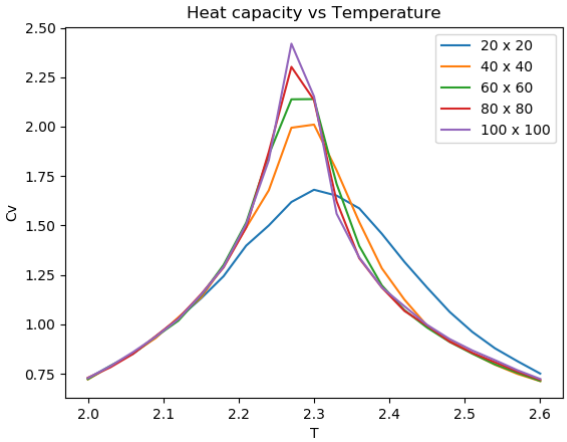


Figure 17: Heat capacity per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

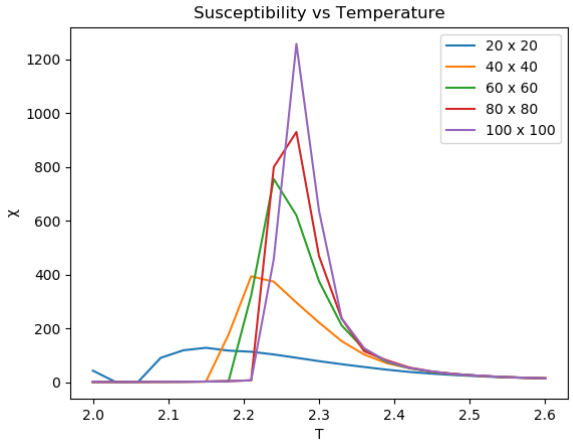


Figure 18: Susceptibility per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

3.5 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.

Lattice size	T_c
40 x 40	2.21 $\pm$0.01
60 x 60	2.24 $\pm$0.01
80 x 80	2.27 $\pm$0.01
100 x 100	2.28 $\pm$0.01

Table 5: The T_C value for different lattice sizes.

We can plot the results from table above:

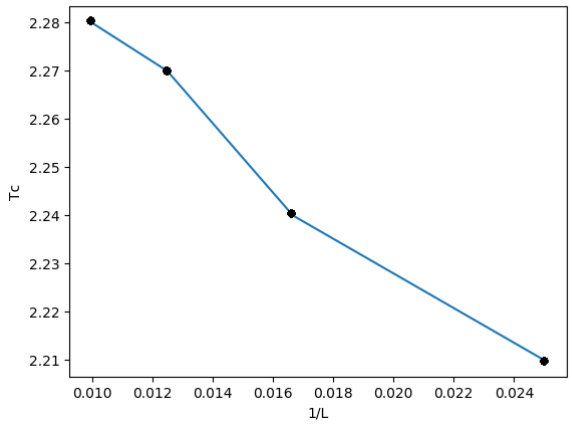


Figure 19: Susceptibility per spin as function of the lattice size for the two-dimensional Ising model, $\Delta T = 0.03$

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 $T_C(\infty) = 2.298 \pm 0.00867$.

4 Discussion

4.1 Analytic vs. Numeric

In this section we have looked at how expected values for L=2 varies based by the amount of Monte Carlo cycles. From table 2, we can see that with a larger number of Monte Carlo cycles we get a more exact value. Expected values for heat capacity and susceptibility are not as exact as the others. This is most likely because the two quantities are calculated based by the other quantities, so the error depends on these. When we have 10 cycles we see that heat capacity and susceptibility are zero, and that is because the error is bigger than the exact value. It looks like for 100 000 Monte Carlo cycles we get values close to the analytical values. We assume that for 1 000 000 MC-cycles we would get values that match exact values completely.

4.2 When is the most likely state reached?

In our calculations we are interested in studying how many Monte Carlo cycles where needed in order to reach the most likely state. Determining this is done

in a brute force way, by just plotting the $< E >$ for every cycle. For $T = 1.0\frac{kT}{J}$ we see, from figure 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 two plots in figure 7 and 12 see that the number of accepted configurations stabilises as we have more cycles, and when we increase the temperature we get a greater degree of variation for the accepted configurations.

4.3 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 $< E >$. 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.

For low temperatures, figure 13, probabilities varies only to right for the expected value. The reason for this is that the steady state will correspond to all the spins pointing in the same direction, since this gives the low energy. From our progamme we get that the variance in energy for T=1 is 0.3, so we expect a small spread in distribution, as we can see in the figure 13.

For T=2.4 we get from our programme that the variance in energy is 1.4, which is bigger than for lawer temperatures. So we expect a wider distribution. This matches with the figure 14. Here we can also see that probability varies both on left and right side of expected value, and this is because equilibrium is in a state where we have a mixture of spins up and down, and then our energy can both increase and decrease.

4.4 Writing a code of the Ising model

As we saw from the figure 8 the system reaches equilibrium state after approx-

imate 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.

4.5 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.

4.6 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. When we looked at the critical temperature, we got that Tc= 2.298. Lars Onsager calculated critical temperature too and got Tc= 2.269. Because of errors which we will discuss in next subsection we didn't get the exact value as Lars, but it was close.

4.7 Sources of error

In our research we made several assumptions which will have an impact on our calculations. For example we have assumed that quantities $k_B = J = 1$.

As mentioned in the previous subsection, we have might have imprecise reading of the graphs, which might give raise to an error.

Another part of the that might had an impact on the result, was the choice of time-step for the temperature. We could have gotten an more accurate result if we decreased the time-step. This would on the other hand made our run-time even slower.

When we used our program for the calculation we also used an function called "burn in", which got rid of the first part of the calculations before it had stabilized. When choosing how long this would run, we used the number of Monte Carlo steps that needed to stabilize from the section called "When is the most likely state?" . Error in this calculation for the number of Monte Carlo step, would therefor might also impact the further calculation.

J=k=1

5 Conclusion

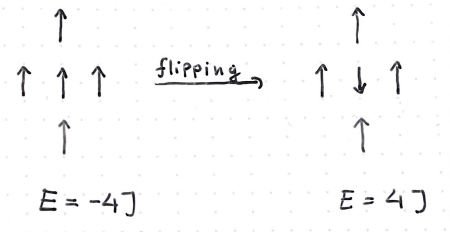
We have studied the behaviour of phase transitions near critical points. The model we used in our research is called the Ising model. We have worked with two-dimensional lattice with increasing sizes. We started by seeing how much time the system need before it reaches the equilibrium, and concluded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

We also wanted 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 a sharper top-point.

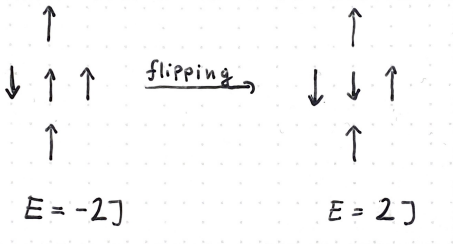
We have modified our program so that we let different nodes perform a given set of Monte Carlo samples. This way we made the program more efficient. The time needed to perform 40×40 lattice with 8 nodes is 8.5 minutes, and with only 1 node 22 minutes. This shows that for an even larger lattice, we must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

Appendix A: Five possible values for Δ E

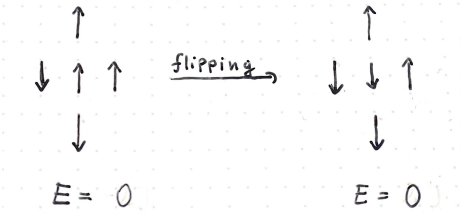
We start with a random sping x,y position where all spins are pointing up. We calculate the energy for this configuration with equation 1 $E = -J(1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1) = -4J$. Then we flip a spin (as shown below) and calculate the new energy $E = -J(-1 \cdot 1 + (-1) \cdot 1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



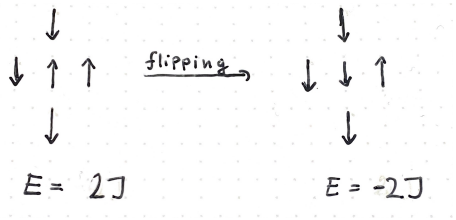
The energy difference ΔE after flipping one spin is $\Delta E = 4J - (-4J) = 8J$. The new configuration is:



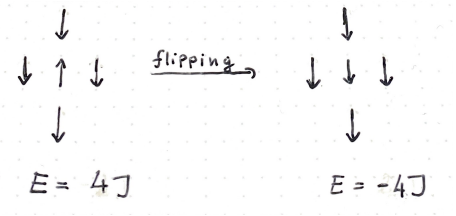
The new energy difference is $\Delta E = 2J - (-2J) = 4J$. Next configuration is



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

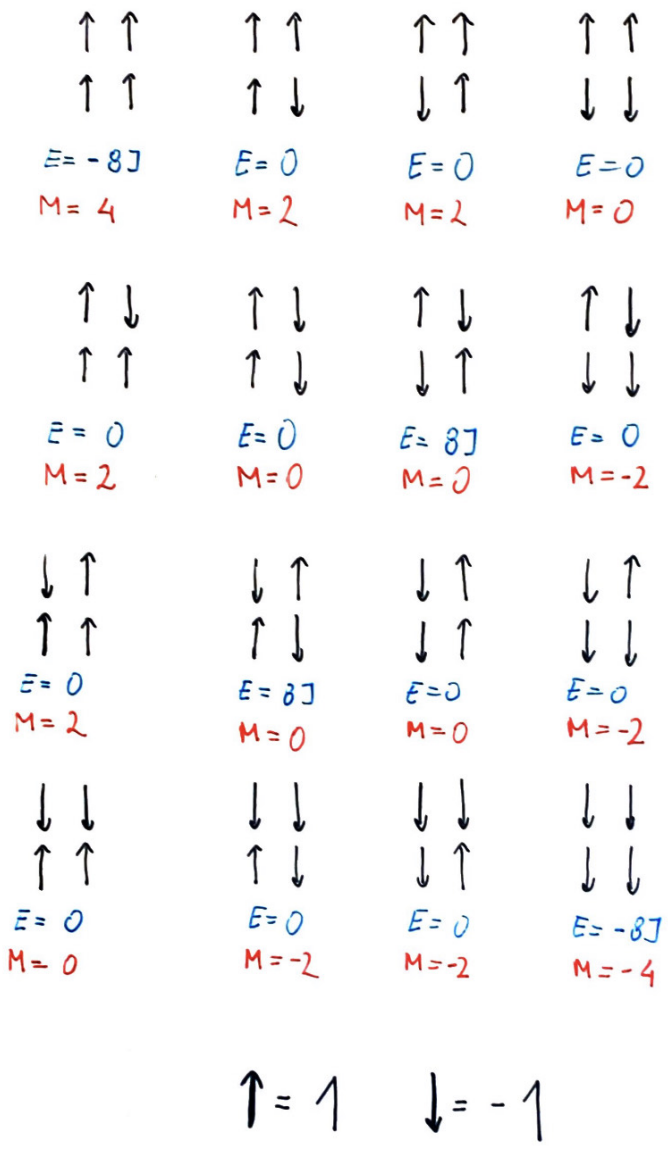


and the new energy difference is $\Delta E = -2J - 2J = -4J$. And the last possible configuraton is



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

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



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