The Phase Transition of the 2D-Ising Model

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Contents

Abstract

In this project, the location of the phase transition in the two dimensional Ising model will be determined using Monte Carlo simulation with importance sampling. Further the evolution of the thermodynamic quantities and the correlation length near the transition and as well the relation between the J>0 and J<0 state will be examined.

1 2D-Ising Model

We wrote our program code in Java. The main code creates a lattice of randomly arranged spins at a given temperature. The spins then either flip or not by calculating the energy difference between the considered spin and its 4 nearest neighbors using the formula:

$$\Delta U = 2J \cdot spin[i][j] \cdot (spin_{left} + spin_{right} + spin_{top} + spin_{bottom}) \qquad (1)$$

The spin then directly flips if Δ U$\leq$0. If Δ U$>$0, it only flips if a randomly chosen number between 0 or 1 is smaller than the Boltzmann factor $\exp(\frac{-\Delta U}{k_B T})$.

The program starts at a certain given temperature and calculates whether the considered spin flips or not for a certain number of iterations. For each step we first performed *l* iterations to reach thermal equilibrium and then performed another *l/2* iterations to determine the physical quantities *Energy per site, Magnetization per site, Magnetic Susceptibility, Specific Heat, Correlation Function and the Correlation Length*.

1.1 Calculation of the Physical Quantities

To study the behaviour of a magnet by using Monte Carlo Simulation, the following quantities are necessary.
To determine the **Energy per site** we calculated the energy of the system after having reached thermal equilibrium E_{equ} by summing over all the energies of each spin as given by:

$$E_{spin} = -J \cdot spin[i][j] \cdot (spin_{left} + spin_{right} + spin_{top} + spin_{bottom}) \qquad (2)$$

To get the energy per site, the sum of all the energies of all the spins has to be divided by twice the amount of spins (where the factor 2 is necessary to avoid counting the spins twice. Then for all following iterations, the energies $\frac{\Delta U}{size \cdot size}$ are added up and after the last iteration they are added to E_{equ}. To then get the mean value of this energy it has to be divided by the number of iterations *l/2*.

To calculate the **Magnetization per site** we performed the same steps as for the energy per site. After having reached thermal equilibrium, we summed up all the spins but here we only divided by the amount of spins without multiplying by the factor 2. Then, for all iterations, the values $\frac{\Delta M}{size \cdot size}$ are summed up and are added to the calculated value at thermal equilibrium. After all iterations, the magnetization per site is given by dividing the final value by the number of iterations *l/2*.

To get $< E^2 >$ and $< M^2 >$, we squared the received energy in each iteration step and then proceeded in the same way as above.
With these values, we can easily calculate the **Magnetic Susceptibility** in units $[\frac{\mu}{k_B}]$ and the **Specific Heat** in units $[\frac{J}{k_B^2}]$ using the following formulas:

$$\chi = \frac{1}{T}[< M^2 > - < M >^2] \qquad C_V = \frac{1}{T^2}[< E^2 > - < E >^2] \qquad (3)$$

To calculate the Correlation Length, the Correlation Function in dependance of the distance r to the spin **spin(0)** has to be determined by using the following formula:

$$G_{spin}(r) =< spin(r)spin(0) > - < spin >^2 \quad (4)$$

where *spin* is the magnetization per site.

2 Location of the Transition

Spontaneous magnetization is called the magnetization in the absence of an external magnetic field. This means, that at low enough temperatures a given magnetic moment can influence the alignment of spins by neighbour-to-neighbour interactions, since they are separated from the given spin by a macroscopic distance. Therefore a lattice has a net magnetization even in the absence of a magnetic field.
The *Critical Temperature* denotes the highest temperature for which there can be non-zero magnetization. At this point, the system undergoes an order-to-disorder transition, called a *phase transition*.[3]
To determine the location of the transition in the 2D-Ising model, we examined the mentioned quantities between a temperature of 1.5 $[\frac{J}{k_B}]$ and 3.5 $[\frac{J}{k_B}]$ with a lattice size of 50x50 at 18'750'000 iterations.
To evaluate the critical temperature and by this the location of the transition, we fitted our plots using the corresponding formula as we will later seen in (5).
The smallest fitting error of the critical temperature showed up in the results of the magnetic susceptibility. Thus, we denoted this temperature of 2.2693 $[\frac{J}{k_B}]$ to be the critical temperature of our simulation. We then fitted again the other quantities with this value for T_c.
Another way to determine the critical temperature is the following. The most realistic value is given in the thermodynamic limit , where N is considered in the limit to infinity. Thus, we calculated the critical temperature in the same way as before, but this time with different lattice sizes. We see, that plotting 1 over N^2 versus each critical temperature results in a straight line. Its intersection with the y-axis then corresponds to the critical temperature for N going to infinity.

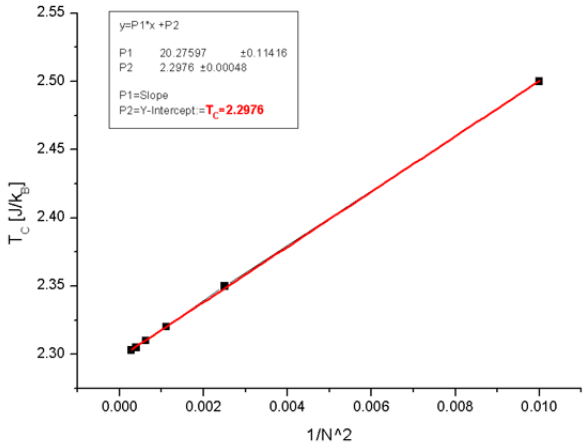

Figure 1: Critical temperature in dependance of different lattice sizes. [1]

The achieved value for the intersection with the y-axis is 2.297 which is close to the literature value of about 2.269. The inaccuracy of this value can be explained when considering that the values used to achieve this result were obtained from earlier fits.

2.1 Phase Transition in Physical Quantities

2.1.1 Magnetization

From above we know, that at the critical temperature, the spontaneous magnetization vanishes. Our model resulted in values that are plotted versus the temperature below.

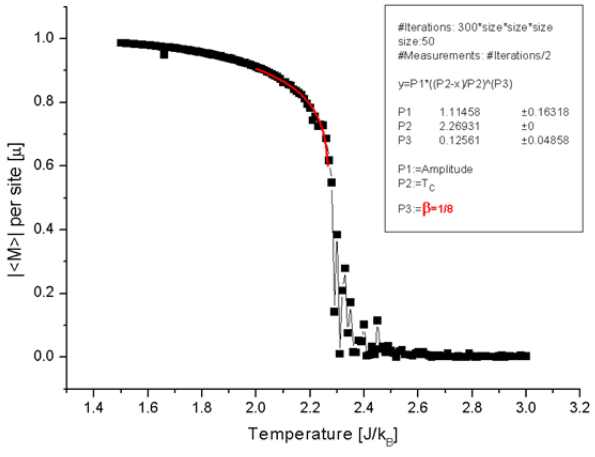

Figure 2: Magnetization per site. [1]

We clearly see, that above a certain temperature the spontaneous magnetization is zero. Where below this temperature the system is in a ferromagnetic

state, above it is in a paramagnetic state.

2.1.2 Magnetic Susceptibility

The magnetic susceptibility χ is a parameter that shows, how much an extensive parameter changes when an intensive parameter increases. Thus, the magnetic susceptibility tells us, how much the magnetization changes by increasing the temperature. From figure 2 we see, that at the transition, the magnetization rapidly decreases. Thus the magnetic susceptibility should show a fast increase to infinity. The model shows the following result for plotting the magnetic susceptibility versus the temperature by using (3).

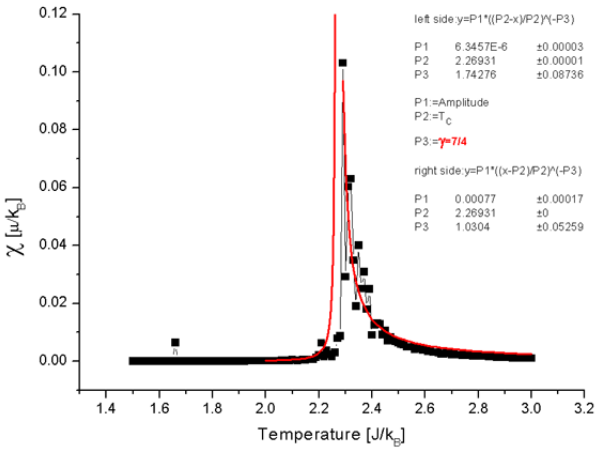

Figure 3: Magnetic Susceptibility. [1]

It can be seen, that below and above T_c the magnetic susceptibility is about zero and around T_c it goes to infinity. This shows, that below and above the transition, the change in magnetization is almost zero, where at the transition, the change is infinite. This is in good agreement with the behaviour of the magnetization as we discussed before.

2.1.3 Energy per Site

If we consider the achieved values of the energy per site and plot them versus the temperature, we see that at around 2.269 $[\frac{J}{k_B}]$, the derivative $C = \left(\frac{\delta E}{\delta T}\right)$ diverges.

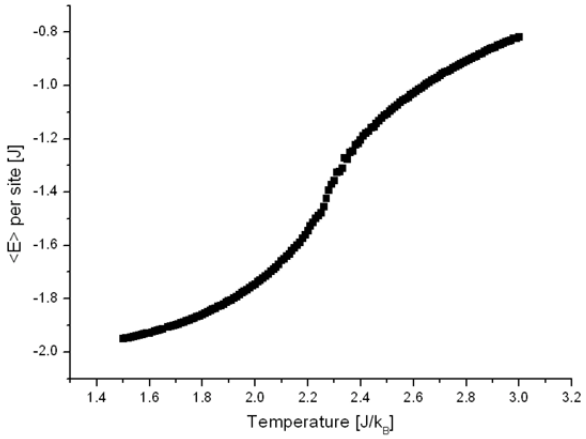

Figure 4: Energy per site. [1]

In the figure above, we see that below and above the transition the energy changes little and that it varies a lot around the transition point.

2.1.4 Specific Heat

The specific heat tells us, how much the energy changes with increasing temperature. Thus we expect to see a divergence of the specific heat at the transition. The plot of the measured specific heat versus the temperature proofs the expectation well.

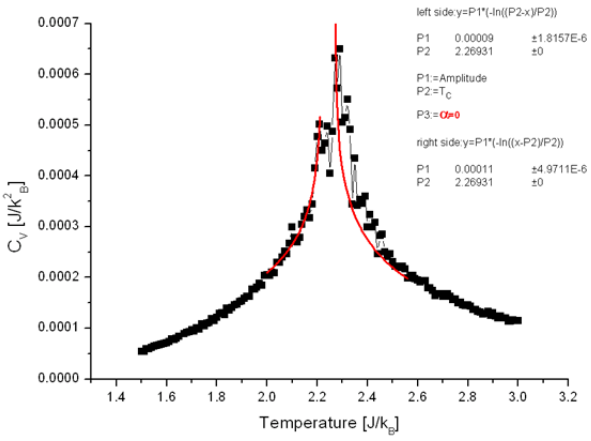

Figure 5: Specific Heat. [1]

2.1.5 Correlation Function

To calculate the correlation length, we first had to calculate the correlation function. This function shows, how much a spin is correlated with the other spins at a certain distance r and is given by (4). Because the spin correlates the most

with its nearest neighbours, we see a fast decrease of the correlation function as shown in the plot below. It shows the correlation functions around the transition. By approaching the transition, the decrease of the correlation function slows down until it reaches a maximal value at the transition.

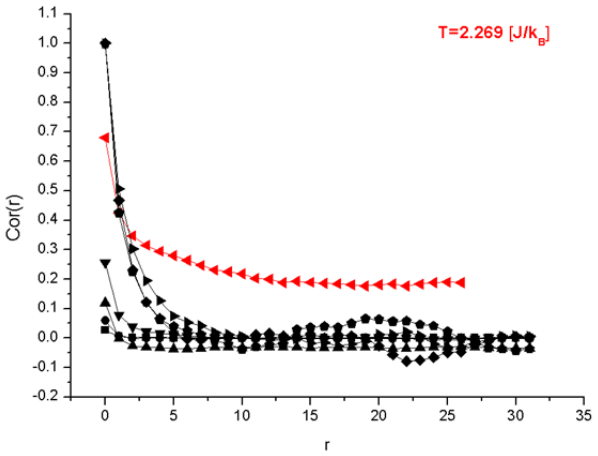

Figure 6: Correlation Functions around the transition. [1]

The next plot shows the correlation function at the critical temperature, at about 2.269 $[\frac{J}{k_B}]$. By fitting it, we can determine the critical exponent for the correlation function, which we will see later.

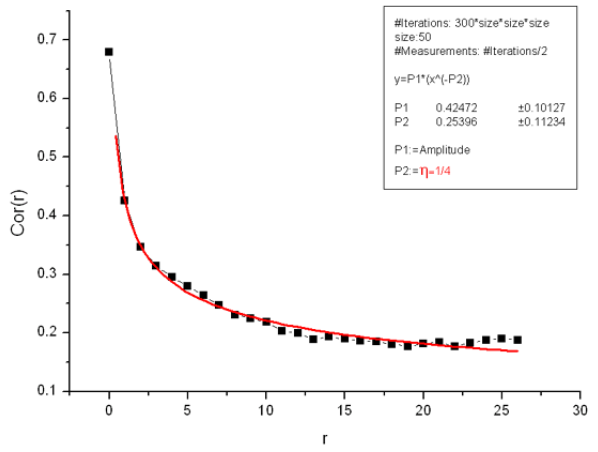

Figure 7: Correlation Function at the transition. [1]

2.1.6 Correlation Length

At absolute zero, the system can either have the values +1 or -1. At higher temperatures below T_c the state is, if we consider it as total, still magnetized. But then clusters with different prefixes occur. By again increasing the temperature, these clusters themselves are made of smaller and smaller clusters. The

typical size of these clusters is called the *correlation length*. It increases with temperature until it diverges at the transition. This means, that the whole system consists of all sizes of clusters and there is no global magnetization.

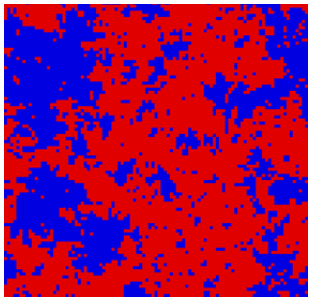

Figure 8: Graphical output of a run of the 2D-Ising model at the critical temperature of $\approx 2.269[\frac{J}{k_B}]$. [4]

Above the transition, the system has no global order, but it is made of ordered clusters, that shrink at higher temperatures. For temperatures in the limit to infinity the correlation again goes to zero and the system is not in order at all.

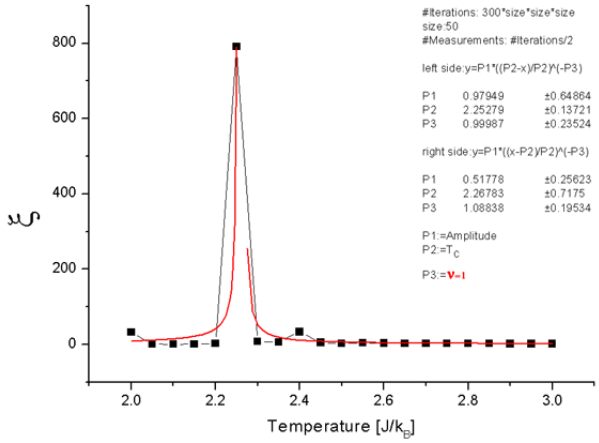

Figure 9: Correlation Length. [1]

Because of the diverging correlation length at the transition, the system interruption spreads quickly over all the small clusters and changes the system completely.
All the divergences in the thermodynamic parameters we discussed above are the consequence of the divergence of the correlation length.

2.2 Scaling Relations

By approaching the critical temperature, all the observables behave as

$$O(T) \propto \left| \frac{T - T_c}{T_c} \right|^{\alpha} \tag{5}$$

with α as an exponent. These exponents are called the critical exponents. They fulfill the so called *scaling relations*:

$$\begin{aligned} (2-\eta)\nu &= \gamma \\ \frac{\nu}{2}(\eta + d - 2) &= \beta \\ 2 - \nu \cdot d &= \alpha \end{aligned} \tag{6}$$

To determine these critical exponents, we fitted the measured values in dependance of the temperature with (5). To get the critical exponent for the correlation function, we proceeded 62'500'000 iterations at the critical temperature of about $2.269[\frac{J}{k_B}]$ and then fitted the plot with (6). And to calculate the value for the correlation length, we fitted the different correlation functions in the range of $0.2[\frac{J}{k_B}]$ around T_c with:

$$G_\phi(r) \simeq \frac{\exp(-r/\xi)}{r^{d-2+\eta}}$$

where d is the dimension, in our case 2. If we consider this formula for the correlation length in the limit ξ to infinity, so at $T = T_c$, we achieve:

$$G_\phi(r) \simeq \frac{1}{r^{d-2+\eta}} \tag{7}$$

By calculating all the critical exponents for the thermodynamic quantities above, we then achieved the following results.

Quantity	Critical Exponent	Literature Value	2D-Ising model
Magnetization	β	1/8	0.125 $\pm$0.008
Magnetic Susceptibility	γ	7/4	1.7 $\pm$0.1
Specific Heat	α	0	0
Correlation Function	η	1/4	0.3 $\pm$0.1
Correlation Length	ν	1	1.0 $\pm$0.2

By inserting the achieved values in (6), we see that they well fulfill these scaling relations.

3 Relation between the $J > 0$ and $J < 0$ State

Ferromagnetism and antiferromagnetism are exchange interactions that are caused by *Pauli's Principle* and *Coulomb interactions*. If we consider two spins S_1 and S_2, the exchange interaction is in the form of $\pm J \cdot S_1 S_2$, where J is a positive and distance-dependent coupling constant. This coupling constant is determined by the overlap that consists of Coulomb interactions.[2]
Now, all the values we calculated, base on the fact, that we used a positive coupling constant. In this case the exchange energy, $-J \cdot S1S2$, is negative and thus the spins prefer to be parallel, which leads to ferromagnetism and as we have seen before, below the transition, spontaneous magnetization. If we chose J to be negative, the exchange energy, $-J \cdot S1S2$, is positive and the spins then

prefer to be antiparallel which can lead to antiferromagnetism. In this case, the spins show alternating magnetic order below the transition.

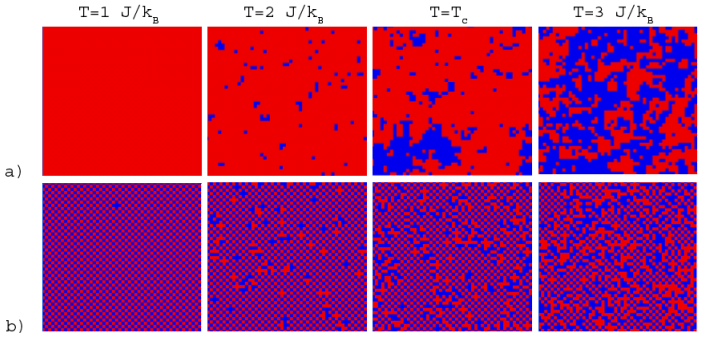

Figure 10: Graphical Output of several runs of the 2D-Ising model. Each red square represents an up dipole and each blue square represents a down dipole. *a)* ferromagnetism, $J > 0$; *b)* antiferromagnetism, $J < 0$. [4]

Without an applied magnetic field, both cases result in the same behaviour of the thermodynamic quantities. If we would apply a magnetic field, the situation would be different. The ferromagnetic system can either have +1 or -1 values and thus, the magnetic field would choose only one favourite value, whereas the antiferromagnetic system remains the same, because of the alternating spins.

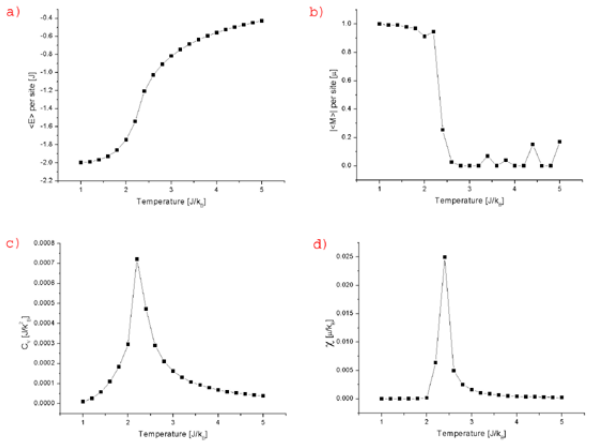

Figure 11: Graphical output of the thermodynamic quantities: a) Energy per site, b) Magnetization per site, c) Specific Heat, d) Magnetic Susceptibility. [1]

References

[1] Graphs created with OriginPro 7.5

[2] Franz Schwabl, Statistische Mechanik, dritte, aktualisierte Auflage, Springer Verlag

[3] David Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987

[4] Graphical Outputs of the 2D-Ising model, written in Java