Studies of phase transitions in magnetic systems

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FYS3150 - Project 4

1 Abstract

Second order phase transitions can be simulated using the widely popular Ising model. In this project the model simulates different parameters for a binary system. These values are influenced by the systems initial spin configuration, the temperature and the number of iterations in the Metropolis algorithm within the Ising model. It turns out that also the lattice size of the system very much affects the simulations, and the bigger the lattice the more accurate results.

2 Introduction

A binary system exhibits a phase transition at a critical temperature. Beneath this temperature the system is ferromagnetic, and as the temperature crosses the critical temperature the system becomes paramagnetic. The reason for this is that the net magnetization is contributed by the spin configuration in the system. How well the mean magnetization, mean energy, susceptibility and the specific heat of the system are simulated by the Ising model depends on different factors which are tested for in this project. To start with, the analytical values for a 2x2 lattice are calculated and then compared with the computed values. Then the lattice is extended to a 20x20 lattice and the equilibrium time is tested for different expectation values for separate temperatures and initial configurations. Further on the lattice is extended even more and plotted against different temperatures in order to find the critical temperature.

3 Methods

It is convenient to start with calculating the analytical values. These values are useful for comparing them to the computed results later on in this project. Calculating the analytical values, it is assumed that the spin lattice is two-dimensional. First the partition function needs to be derived. Then the expectation values to calculate are for the energy E, the mean absolute value of the

magnetic moment $|M|$ (which hereafter will be referred to as mean magnetization), the specific heat C_v and the susceptibility χ. Throughout this project the system is assumed to have periodic boundary conditions.

$$\begin{matrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{matrix} \qquad \begin{vmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{vmatrix}$$

As the "up"-spins contribute with a value of 1 and the "down"-spins contribute with a value of -1, it is quite easy to calculate the energy and the magnetization of this 2x2 system using the following equations. A two dimensional 2x2 system has 16 possible configurations. The magnetization and energy is different for some of them, but many of the energies has a degeneracy of more than one.

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l$$

$$M_i = \sum_{j=1}^{N} s_j$$

A 2x2 system with ordered spin configuration as showed in the spin matrix above has the energy:

$$\begin{aligned} E &= -J((s_{11}s_{12} + s_{12}s_{11} + s_{21}s_{22} + s_{22}s_{21}) \\ &\quad +(s_{11}s_{21} + s_{21}s_{11} + s_{12}s_{22} + s_{22}s_{12})) \\ &= -J(1+1+1+1+1+1+1+1) \\ &= -8J \end{aligned}$$

and the magnetization:

$$M = ((s_{11} + s_{12} + s_{21} + s_{22}) = 1 + 1 + 1 + 1 = 4$$

Table 1: Easily calculated energy and magnetization. Calculations in the appendix.

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

The following values are used for the analytical solution: $L = 2, T = 1.0, \beta = 1.0, J = 1.0$
The partition function is written as:

$$Z = \sum_{\imath=1}^{M} e^{\beta E_i}$$

and it uses the energies given in table 1.

$$Z_n = \sum_{S_1=\pm 1} ... \sum_{S_N=\pm 1} exp(\beta J \sum_{j=1} s_j s_{j+1})$$

Because the energy of the system can be exchanged with the surroundings, it is suitable to calculate the expectation value of the mean energy, when calculating energy:

$$\langle E \rangle = \sum_{i}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i}^{M} E_i e^{-\beta E_i}$$

The probability distribution is included in the formula:

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

To find the heat capacity it is necessary to first find the variance for energy:

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$$

Then we can use this in the equation for heat capacity:

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

The mean magnetization is given by:

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

The normal mean magnetization will sum up to become zero. Therefore it is more convenient to use the mean absolute value of the magnetization, which is solved using the formula

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

Finally, to find the susceptibility of the system, the variance of magnetization is needed. I have in this project used the mean absolute value of the magnetization in this formula :

$$\sigma_M^2 = \langle M^2 \rangle - \langle |M| \rangle^2$$

Then the susceptibility is easily calculated:

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

The energy of a binary system is defined by the contribution of each single spin. To find the resulting energy by computing it is very helpful to use the Metropolis algorithm. This concerns a Markov chain, which is a random walk that examines each single element in the spin matrix and determines if it should change its state. In the case of the binary system, the walker determines whether it is energetic favorable to flip the "spins" or not. If the spin flips, the state of the system is changed. Hence the energy, magnetization and other values will also change. When a Markov chain is run for a long enough time, the system will eventually reach its steady state. This algorithm is what I have computed to simulate the different values.

Here is an example of the program where the possible favorable energy is calculated using periodic boundary conditions:

$intdeltaE = 2 * n_matrix(x, y) * (n_matrix(x, periodic(y, L, -1)) + n_matrix(periodic(x, L, -1), y) + n_matrix(x, periodic(y, L, 1)) + n_matrix(periodic(x, L, 1), y))$

Then the most important part of the Ising model:

$$if((distribution(gen)) <= E_vector(deltaE + 8))$$

$$n_matrix(x, y) * = -1.0;$$

// If accepted: flips spin

// adding this contribution in energy and magnetization to the already existing values

$$M+ = (double)2 * n_matrix(x, y);$$

$$E+ = (double)deltaE;$$

//counting how many accepted flips

$$acc+ = 1;$$

Since the analytical values only have been solved for a system with spins in two dimensions with L=2, the first task is testing if the program returns good approximations. When the program seems to be working as it should, the project evolves towards bigger lattices.

There are some different factors that could possibly influence the equilibrium states. Among these are initial temperature and initial spin configuration. In addition the Markov chain has to be working as it should, and accept the expected changes for the system. All of these three factors needs to be taken in to consideration when estimating an equilibrium time. The system is now extended to a 20x20 spin matrix. I have plotted the mean energy and the mean magnetization, for T=1.0 and T=2.4 with both ordered and random initial spin configuration. These as functions of the number of Monte Carlo cycles, which is represented as time. I have also plotted the number of accepted configurations as a function of temperature for ordered and disordered initial configuration.

To find the probability distribution the energy for the system after each single Monte Carlo cycle can be put into a histogram, to see which is the most likely energy state for both T=1.0 and T=2.4.

The program is hereafter evolved for looping over temperatures in the interval [2.0,2.3] with small steps, for example step size = 0.01 as I used. This is to examine numerical studies of phase transitions. It should be done for a 40x40 lattice, 60x60 lattice, 80x80 lattice and 100x100 lattice. To avoid needless waiting, the code can be optimized. In this project I have used task parallelism with the MPI library. I chose this optimization because the Monte Carlo program can be divided into different problems that can be solved at the same time, independent of the other problems.

Code example of how the Metropolis algorithm is looped over different temperatures:

$$MPI_Init(argc, argv);$$

$$MPI_Comm_size(MPI_COMM_WORLD, numprocs);$$

$$MPI_Comm_rank(MPI_COMM_WORLD, my_rank);$$

$$initialize_nm_EM(L, n_matrix, E, M);$$

$$newline for(double T = 2.0; T <= 2.3; T+ = 0.01)$$

$$double beta T = 1.0/T;$$

$$cout << "T = " << T << endl;$$

$$Metropolis(L, n, n_matrix, beta T, T, E,$$

$$, ExpectationValue);$$

$$mean(ExpectationValue, n, L, T);$$
$$MPI_Finalize();$$

The example from the program also shows hos I have optimized the program with MPI commands.

The Ising model is supposed to exhibit a second order phase transition. This phase transition happens when the system crosses the critical temperature. Beneath the critical temperature, the system has a spontaneous magnetization and is ferromagnetic, but this should become zero above this critical temperature, where it becomes paramagnetic. Therefore we can find an approximation when plotting the mean magnetization against the different temperatures. The slope towards zero becomes steeper with increasing lattices. In the diagrams with the heat capacity and susceptibility as a function of the temperature, the maximal point becomes more and more visible with increasing lattices.

The Metropolis algorithm is computed using C++, which outputs the values. These values are used as input in diagrams made using python language. Here is an example of how I have found the maximum values:

M40 = np.amax(Cv_40)
    for i in range (0, k):
if ($Cv_40[i] == M40$) :
$maxT40 = T_40[i]$

4 Results

Table 2: Analytical results. I have calculated the partition function, the mean energy per spin, the mean magnetization per spin, specific heat per spin and susceptibility per spin.

Z	E	$\|M\|$	C_v	χ
5973.9166	-1.9960	0.9982	0.0318	0.0071

Table 3: Computed results. The values are respectively mean energy per spin, mean magnetization per spin, specific heat per spin and susceptibility per spin.

E	$\|M\|$	C_v	χ
-1.9960	0.9987	0.0320	0.0040

When sweeping over the lattice 100.000 times, the computed values are almost precisely equal as the analytical ones until the third decimal. I would say that

this is a very good achievement. The partition function was not needed to compute, because it contributes in the Metropolis algorithm as the values are simulated. By comparing the computed values to the analytical ones, the program of the Metropolis algorithm is "approved" and can now compute for bigger lattices.

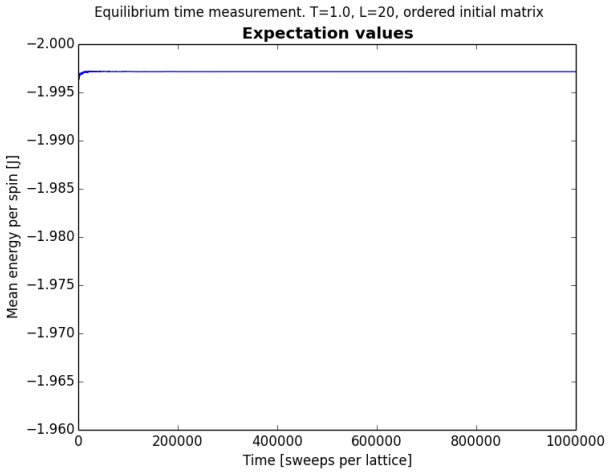

Figure 1: The expectation value of the mean energy per spin as a function of time (Monte Carlo cycles) with T = 1.0 and ordered initial spin configuration.

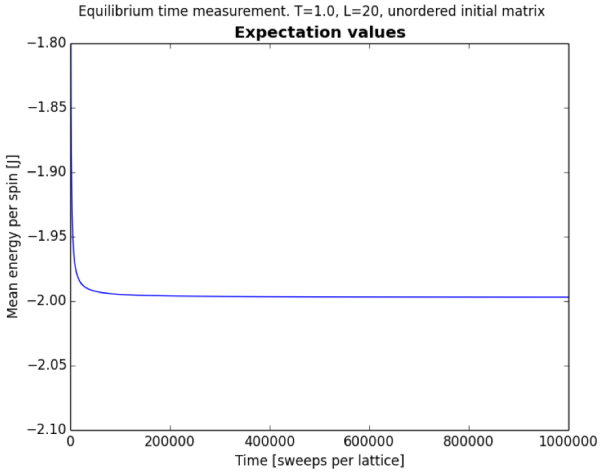

Figure 2: The expectation value of the mean energy per spin as a function of time (Monte Carlo cycles) with T = 1.0 and random configuration initial spin matrix.

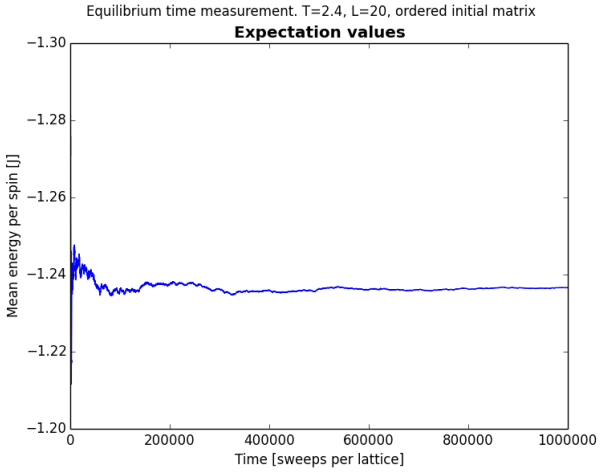

Figure 3: The expectation value of the mean energy per spin as a function of time (Monte Carlo cycles) with T = 2.4 and ordered initial spin configuration.

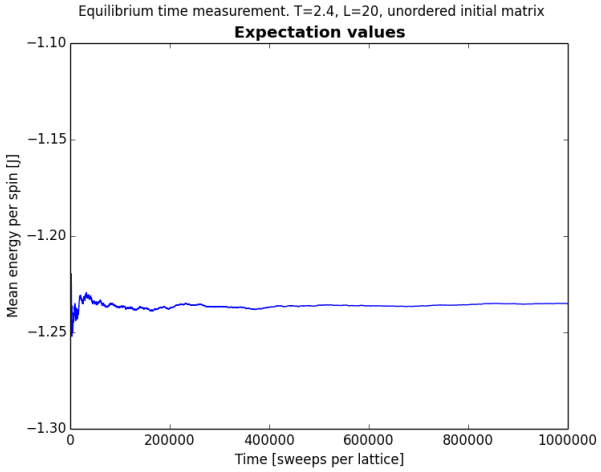

Figure 4: The expectation value of the mean energy per spin as a function of time (Monte Carlo cycles) with T = 2.4 and random configuration initial spin matrix.

The mean energy for T = 1.0 has an insignificant variance between the two simulations starting with ordered and disordered initial configurations. The energy in both diagrams converge towards approximately -1.99. For the other energy simulations, but with T=2.4, there is a slightly bigger difference to start with. In the very beginning of the diagram, before the passing of the approximate time = 100.000, there is a small difference between the two plots, but as

number of Monte Carlo cycles increase, both graphs converge towards a steady state. This steady state energy value is in both cases approximately -1.235. After many enough iterations, the initial state does not really matter as the equilibrium state is finally reached after all. For the simulations with T=1.0, the equilibrium time is much less than those with T=2.4. For T=1.0 it is somewhere around 100.000 simulations, but for T=2.4 it is approximately around 500.000 simulations.

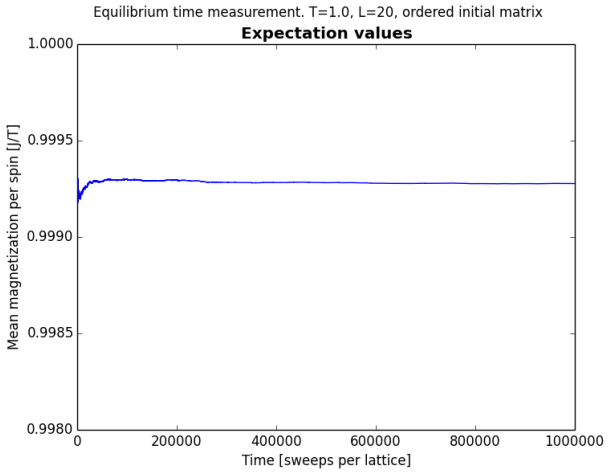

Figure 5: The expectation value of the absolute of the mean magnetization per spin, with T=1.0 and ordered initial spin matrix.

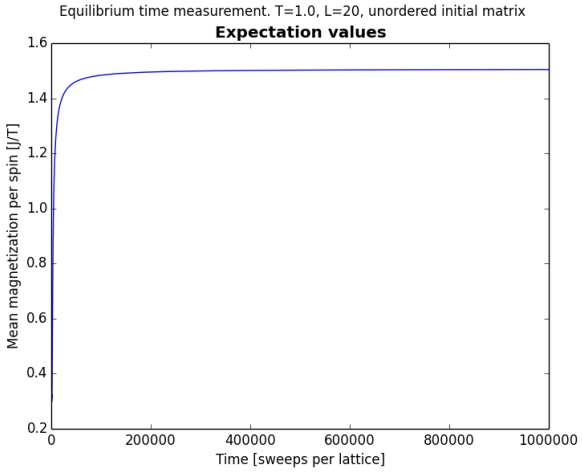

Figure 6: The expectation value of the absolute of the mean magnetization per spin, with T=1.0 and disordered initial spin matrix.

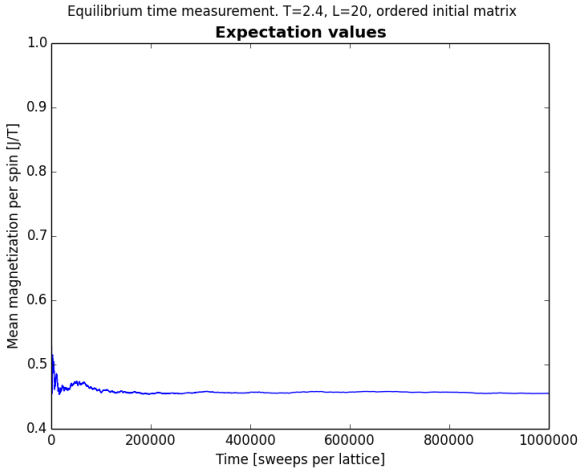

Figure 7: The expectation value of the absolute of the mean magnetization per spin, with T=2.4 and ordered initial spin matrix.

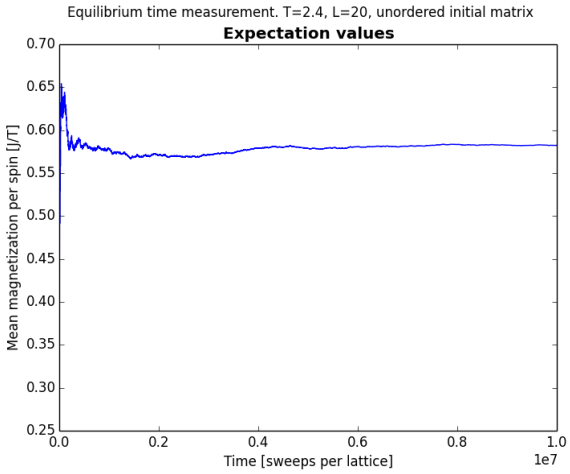

Figure 8: The expectation value of the absolute of the mean magnetization per spin, with T=2.4 and random configuration on the initial spin matrix.

Approximately the same equilibrium times can be estimated for the mean magnetization simulation. The equilibrium time is much less for T=1.0 than T=2.4. It is approximately around 100.000 for T=1.0 and 500.000 for T=2.4. The simulations for the mean magnetization differs from the energy simulations because of the difference in equilibrium states for ordered and disordered initial configuration. For both T=1.0 and T=2.4 are mean magnetization value in the

steady state higher for random configuration initial spin matrix than for the ordered spin matrix.

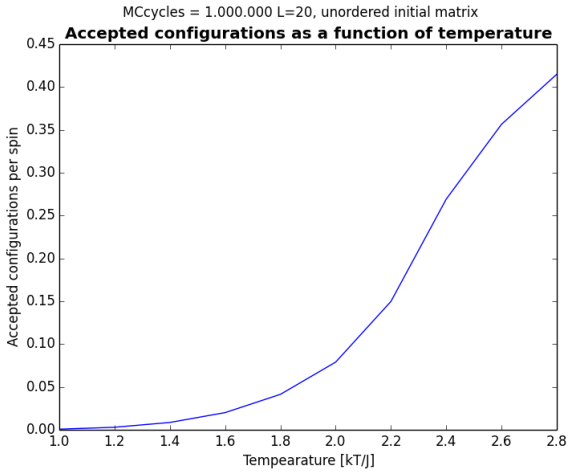

Figure 9: The accepted configurations per spin as a function of temperature and unordered/disordered initial spin configuration.

It is very obvious that the total number of accepted configurations increases parallel to increasing temperature. The temperature is therefore a very important factor influencing the expectation values of the system. As the temperature increases it becomes more energetic favorable to flip the spins, hence the accepted configurations increase with temperature. This also makes sense for the variation of equilibrium time due to different temperatures. Because there is more accepted configurations with higher temperature, it requires longer time to reach its steady state.

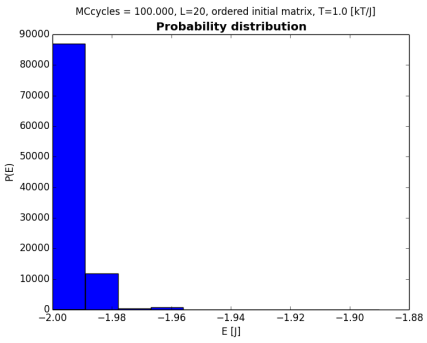

Figure 10: Probability distribution for the energy per spin with T=1.0 and 10 bins in the histogram. The values are returned after the equilibrium time is reached.

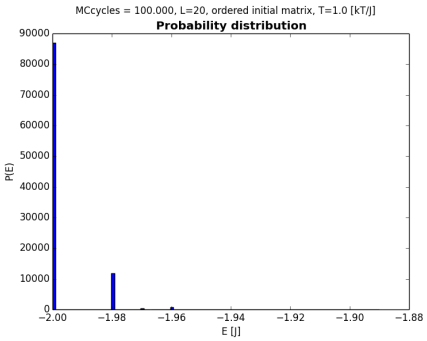

Figure 11: Probability distribution for the energy per spin with T=1.0 and 100 bins in the histogram. The values are returned after the equilibrium time is reached.

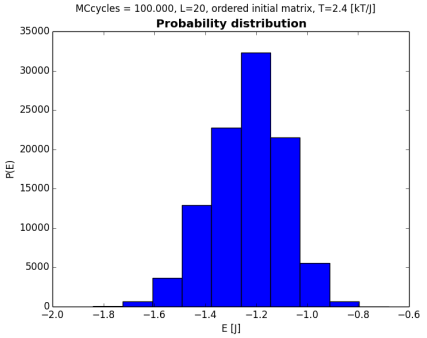

Figure 12: Probability distribution for the energy per spin with T=2.4 and 10 bins in the histogram. The values are returned after the equilibrium time is reached.

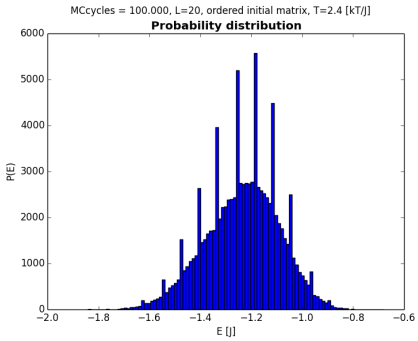

Figure 13: Probability distribution for the energy per spin with T=2.4 and 100 bins in the histogram. The values are returned after the equilibrium time is reached.

The interesting part for plotting the histograms is to examine how the energy and the magnetization oscillates around the equilibrium state. For T=1.0 the system is most likely to be find in a state with energy equal to -2.0. For T=2.4 the most likely state is with energy equal to -1.19.

In the following subplots the mean energy, the mean magnetization, the specific heat and the susceptibility is plotted as functions of temperature from 2.0 to 2.3 to examine phase transitions for different lattice sizes.

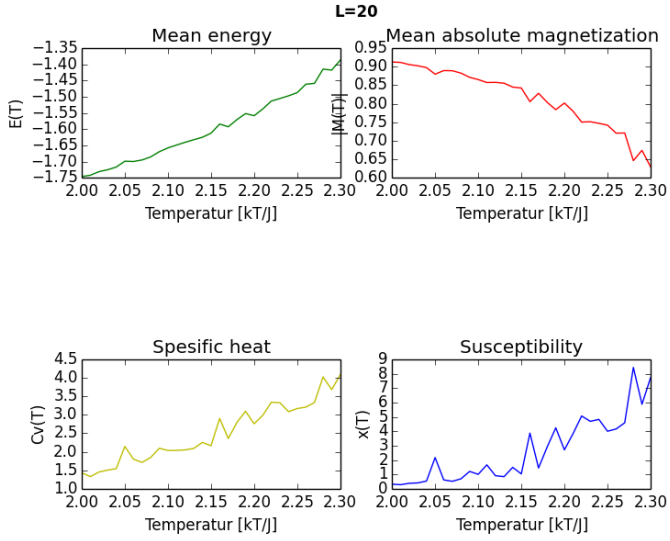

Figure 14: Lattice size: 20x20. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

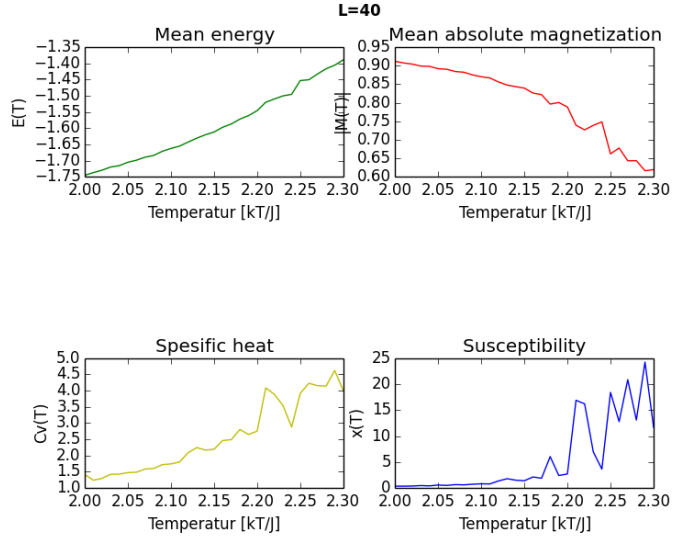

Figure 15: Lattice size: 40x40. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat per spin and the susceptibility per spin is computed as functions of the temperature.

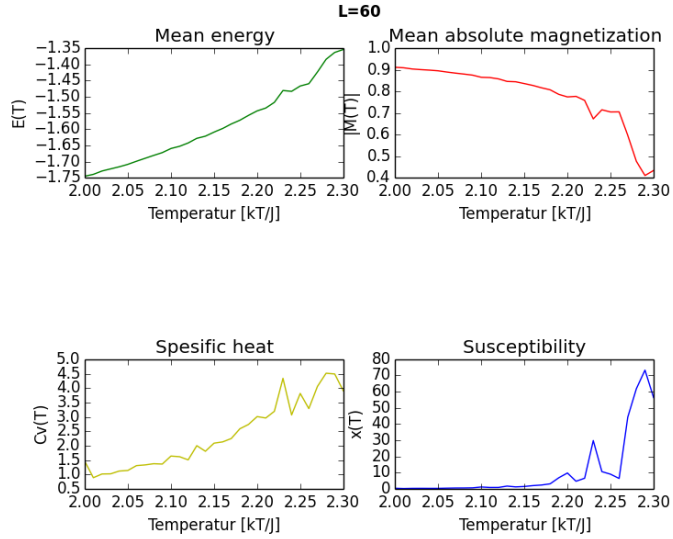

Figure 16: Lattice size: 60x60. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat per spin and the susceptibility per spin is computed as functions of the temperature.

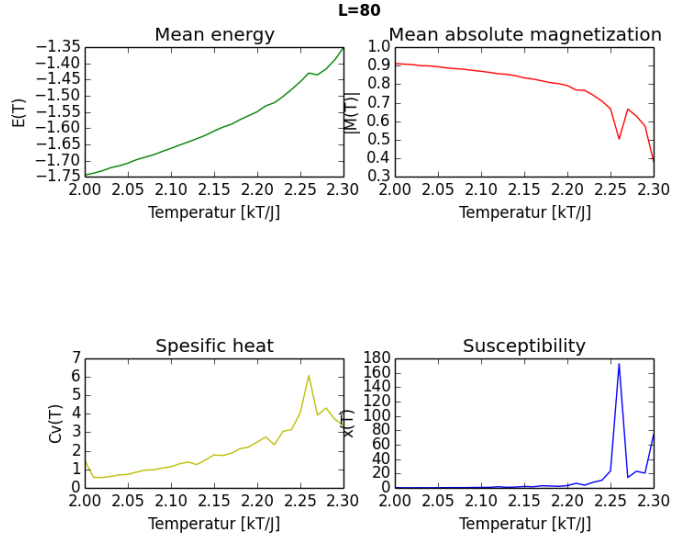

Figure 17: Lattice size: 80x80. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat per spin and the susceptibility per spin is computed as functions of the temperature.

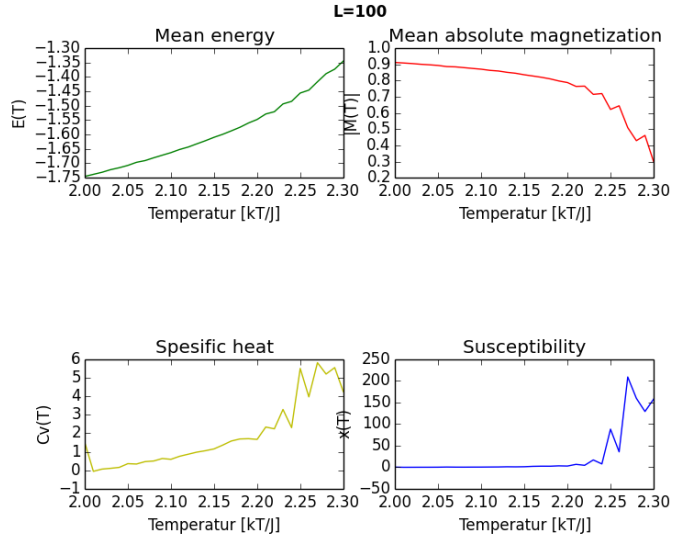

Figure 18: Lattice size: 100x100. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat per spin and the susceptibility per spin is computed as functions of the temperature.

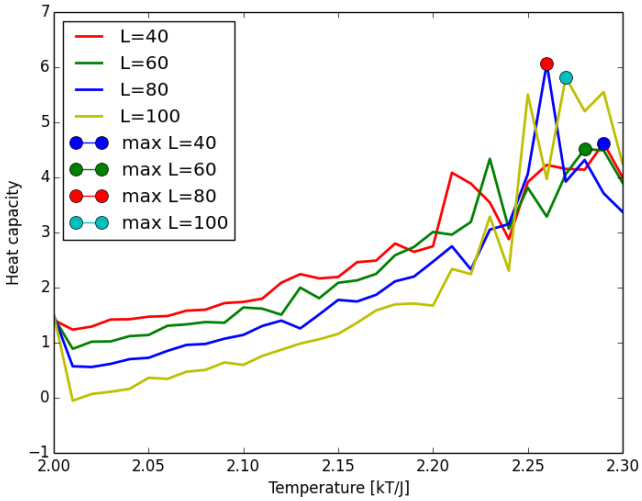

Figure 19: The heat capacity per spin simulated with 1.000.000 Monte Carlo Cycles plotted against the temperature in an interval [2.0,2.3] with step size = 0.01. The four different graphs are for L=40, L=60, L=80 and L=100. The maximum points for each graph are also marked.

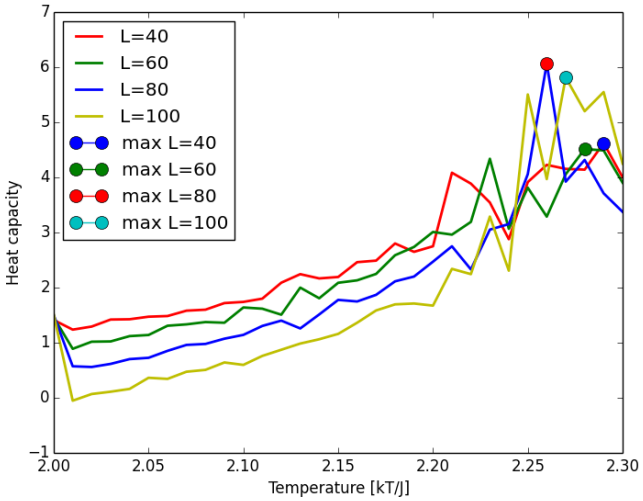

Figure 20: The susceptibility per spin simulated with 1.000.000 Monte Carlo Cycles plotted against the temperature in an interval [2.0,2.3] with step size = 0.01. The four different graphs are for L=40, L=60, L=80 and L=100. The maximum points for each graph are also marked.

Table 4: The critical temperature approximation from plotting the specific heat and the susceptibility as functions of the temperature, for different size lattices. The critical temperatures are found by locating the maximum value for both the specific heat and the susceptibility.

L	Tc (C_v)	Tc(χ)
40	2.29	2.29
60	2.28	2.29
80	2.26	2.26
100	2.27	2.27

The exact result for the critical temperature is: 2.269. Solved by Lars Onsagers formula [4]:

$$kT_c/J = 2/ln(1+\sqrt{2}) \approx 2.269$$

Both maximums points for the susceptibility show good approximations to the critical temperature for L=100. When running the program as a function of temperature, I chose to have a step size equal to 0.01 and therefore my computed temperature results only have two decimals. To get more precisely results it is convenient to have a narrower domain for the temperature.

5 Conclusion

First the equilibrium time was tested for different temperatures and the results shows that the equilibrium time is less during lower temperatures. The reason for this is that the accepted spin configurations increase with increasing temperature. Hence the longer time for the system to reach its equilibrium state.

The initial spin configuration has an insignificant effect on the energy. The mean magnetization value on the other hand is quite affected by the initial configuration. However, this does not really affect the equilibrium time.

It is possible to find an approximately value of the critical temperature where the system exhibits phase transitions by finding the maximum values for the susceptibility and the heat capacity of the system as functions of temperature. These maximums peaks becomes sharper and more obvious as the lattice becomes bigger.

A possible improvement for a better simulation would be to compute the mean energy, mean magnetization, specific heat and susceptibility with even smaller step size than 0.01. Another improvement could be to expand the temperature interval from [2.0,2.5] so that the critical temperature would be more visible and the mean magnetization would be even closer to zero.

The Ising model surely makes good approximations and I can understand why it is so popular for studying phase transitions.

6 Appendix

Some of the calculations for table 1:

$$\begin{matrix}\uparrow & \uparrow \\ \downarrow & \downarrow\end{matrix}\begin{vmatrix} s_{11} & s_{12} \\ s_{21} & s_{22}\end{vmatrix}$$

$$\begin{aligned} E = -J((&s_{11}s_{12} + s_{12}s_{11} + s_{21}s_{22} + s_{22}s_{21}) \\ &+(s_{11}s_{21} + s_{21}s_{11} + s_{12}s_{22} + s_{22}s_{12})) \\ &= -J(1+1+1+1-1-1-1-1) \\ &= 0 \end{aligned}$$

$$\begin{matrix}\downarrow & \uparrow \\ \downarrow & \downarrow\end{matrix}\begin{vmatrix} s_{11} & s_{12} \\ s_{21} & s_{22}\end{vmatrix}$$

$$\begin{aligned} E = -J((&s_{11}s_{12} + s_{12}s_{11} + s_{21}s_{22} + s_{22}s_{21}) \\ &+(s_{11}s_{21} + s_{21}s_{11} + s_{12}s_{22} + s_{22}s_{12})) \end{aligned}$$

$$= -J(-1-1+1+1+1+1-1-1)$$
$$= 0$$

$$\begin{matrix}\uparrow & \downarrow \\ \downarrow & \uparrow\end{matrix}\begin{vmatrix} s_{11} & s_{12} \\ s_{21} & s_{22}\end{vmatrix}$$

$$E = -J((s_{11}s_{12} + s_{12}s_{11} + s_{21}s_{22} + s_{22}s_{21})$$
$$+(s_{11}s_{21} + s_{21}s_{11} + s_{12}s_{22} + s_{22}s_{12}))$$
$$= -J(-1-1-1-1-1-1-1-1)$$
$$= 8J$$

Calculations of analytical values in table 2. Partition function:

$$Z(\beta) = \sum_s e^{-\beta E_s}$$

With $\beta = 1$ the partition function is:

$$Z(1) = e^{8J} + 4e^0 + 4e^0 + 2e^{-8J} + 4e^0 + e^{8J}$$
$$= 2e^{8J} + 2e^{-8J} + 12$$

The J-value is set to 1, so the exact partition function is:

$$Z(1) = 2e^8 + 2e^{-8} + 12 = 5973.9166$$

Expectation value for mean energy:

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

$$\langle E \rangle = \frac{1}{5973.9166}(-8 * e^8 + 2 * 8 * e^{-8} - 8 * e^8) = \frac{1}{5973.9166} - 47695 = -7.9840J$$

Mean energy per spin:

$$\langle E \rangle / L / L = \frac{-7.9840}{2^2} = -1.9960$$

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

$$\langle E^2 \rangle = \frac{1}{5973.9166}(64 * e^8 + 2 * 64 * e^{-8} + 64 * e^8) = \frac{1}{5973.9166}381562 = 63.8714$$

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = 63.8714 - (-7.9840)^2 = 0.1272$$

The heat capacity is then:

$$C_V = \frac{1}{k_B T^2} \langle E^2 \rangle - \langle E \rangle^2 = 0.1272$$

Specific heat per spin:

$$C_V/L/L = \frac{0.1272}{2^2} = 0.0318$$

Mean magnetization:

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

$$\langle M \rangle = \frac{1}{5973.9166} \quad 4e^8 + \mid 2e^0 - 2e^0 - 4e^8 = 0$$

The absolute value of the mean magnetization is solved as:

$$\langle |M| \rangle = \frac{1}{5973.9166} \quad (\mid 4e^8 \mid + \mid 2e^0 \mid + \mid -2e^0 \mid + \mid -4e^8 \mid) = 3.9926$$

The absolute value of the mean magnetization per spin:

$$\langle |M| \rangle /L/L = \frac{3.9926}{2^2} = 0.9982$$

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

$$= \frac{1}{5973.9166} (\mid 16e^8 \mid + \mid 4e^0 \mid + \mid 4e^0 \mid + \mid 16e^{-8} \mid) = \frac{95398.6556}{5973.9166} = 15.9691$$

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2 = 15.9691 - 0^2 = 15.9691$$

Using the absolute value:

$$\sigma_M^2 = \langle M^2 \rangle - \langle M_a bs \rangle^2 = 15.9691 - 3.9926^2 = 0.0283$$

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

In this project the values are resolved in terms of

$$k_B$$

being equal to 1. For T = 1, the susceptibility is equal to the magnetic variance:

$$\chi = 0.0283$$

Susceptibility per spin:

$$\chi/L/L = \frac{0.0283}{2^2} = 0.0071$$

Code example for table 3:

17:58:49: Starting /Users/marielauliehinderaker/Documents/FYS3150/Project4/build-Project4-Debug/output/T1/Project4 2 10000000 1.0 $n_E 2.txt$...
$T = 1$
$MonteCarlocycles = 10000000$
$Spinmatrixlattice = 2$
$Meanenergy = -1.99599$
$Meanabsmagn = 0.998671$
$Theheatcapasityofthesystem = 0.0320045$
$Thesusceptibilityofthesystem = 0.00395893$
$Timeused = 12.15031900seconds.$

Code examples for table 4:

Mariels-MacBook-Air:python marielauliehinderaker python project4e.py $4e_L = 40.txt 4e_L = 60.txt 4e_L = 80.txt 4e_L = 100.txt$
$('ForL = 40themaximumvalueofSusceptibilityis24.25821',' andthecriticaltemperatureis2.29')$
$('ForL = 60themaximumvalueofSusceptibilityis73.277791',' andthecriticaltemperatureis2.29')$
$('ForL = 80themaximumvalueofSusceptibilityis172.43373',' andthecriticaltemperatureis2.26')$
$('ForL = 100themaximumvalueofSusceptibilityis208.99476',' andthecriticaltemperatureis2.27')$

Mariels-MacBook-Air:python marielauliehinderaker python project4e.py $4e_L = 40.txt 4e_L = 60.txt 4e_L = 80.txt 4e_L = 100.txt$
$('ForL = 40themaximumvalueofheatcapacityis4.6224992',' andthecriticaltemperatureis2.29')$
$('ForL = 60themaximumvalueofheatcapacityis4.5148549',' andthecriticaltemperatureis2.28')$
$('ForL = 80themaximumvalueofheatcapacityis6.0663332',' andthecriticaltemperatureis2.26')$
$('ForL = 100themaximumvalueofheatcapacityis5.8144627',' andthecriticaltemperatureis2.27')$

List of Figures

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