FYS3150 - Project 4

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1 Abstract

In this project the Ising model will be used to simulate phase transitions for a binary system.

2 Introduction

3 Methods

To begin with it is sufficient to calculate 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 solve is 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.

A system with two spins in each dimension can be toughed of as a 2x2 spin matrix.

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

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 2 dimensional system has 16 possible configurations and the magnetization and energy is different for some of them, but many of the energies has a degeneracy of more than one.

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

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

Table 1 - Easily calculated energy and magnetization

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.

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

The mean energy of the system is

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

Heat capacity:

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

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

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

The mean magnetization is given by:

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

Which is 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.

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

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 convenient 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. 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 reach its steady state. This is what I have computed to simulate the different values.

Since the analytical values only have been solved for a system with spins in two dimensions, 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 dimensional systems.

There are 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 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.

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.

The Ising model is supposed to exhibit a second order phase transition because the specific heat diverges. This phase transition happens when the system crosses the critical temperature. Beneath the critical temperature, the system has a spontaneous magnetization, but this should become zero above this critical temperature.

4 Results

Table 2 - Analytical results

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

Table 3 - Computed results

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 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 for the next and more difficult simulations.

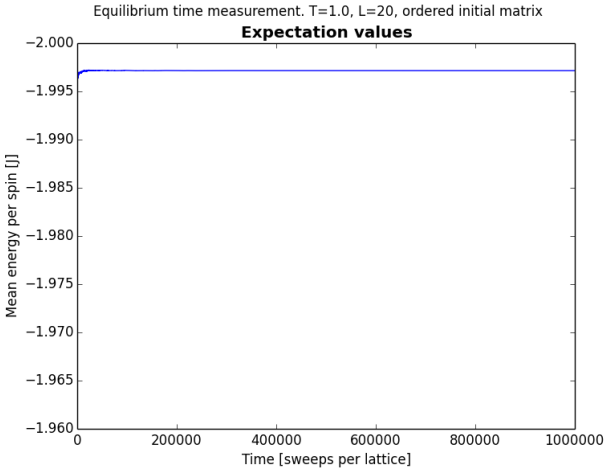

Figure 1: The expectation value of the mean energy as a function of time (Monte Carlo cycles) with T = 1.0 and ordered initial spin configuration.

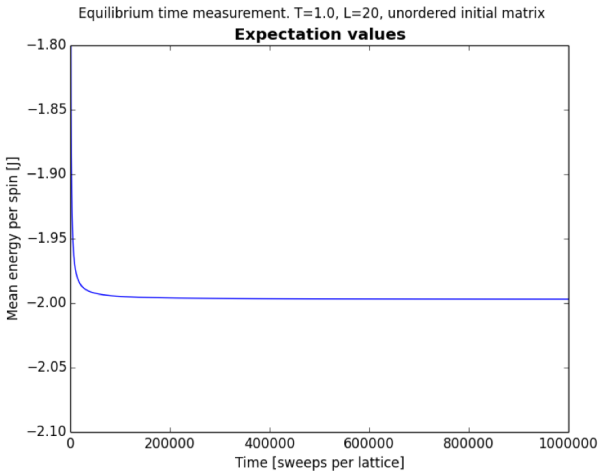

Figure 2: The expectation value of the mean energy as a function of time (Monte Carlo cycles) with T = 1.0 and random configuration initial spin matrix.

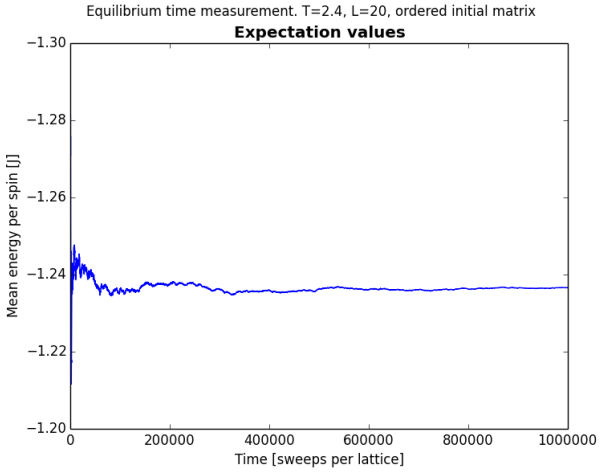

Figure 3: The expectation value of the mean energy as a function of time (Monte Carlo cycles) with T = 2.4 and ordered initial spin configuration.

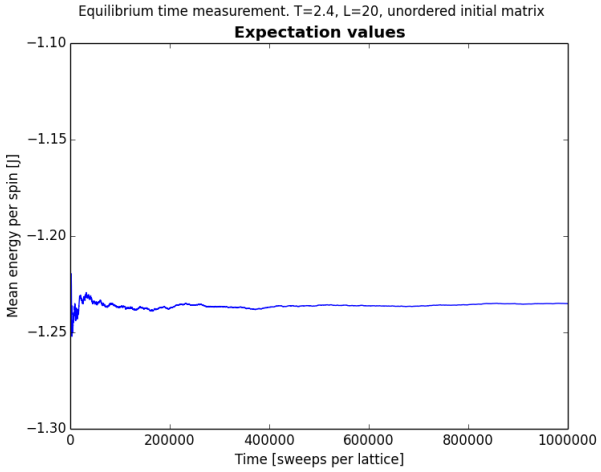

Figure 4: The expectation value of the mean energy as a function of time (Monte Carlo cycles) with T = 2.4 and random configuration initial spin matrix.

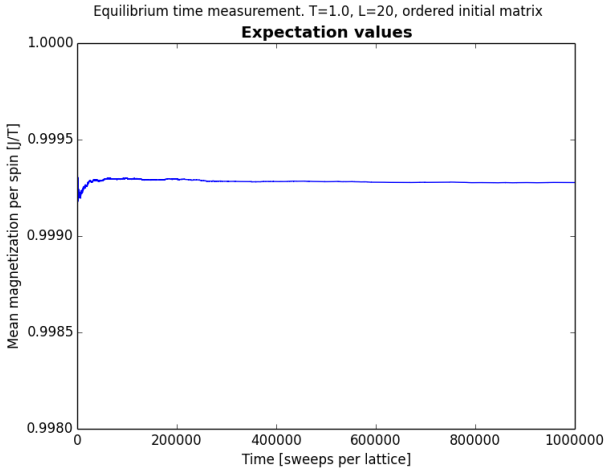

Figure 5: The expectation value of the absolute of the mean magnetization, with T=1.0 and ordered initial spin matrix.

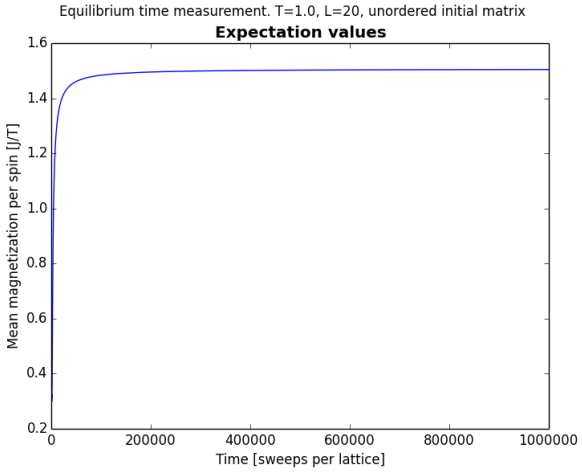

Figure 6: The expectation value of the absolute of the mean magnetization, with T=1.0 and disordered initial spin matrix.

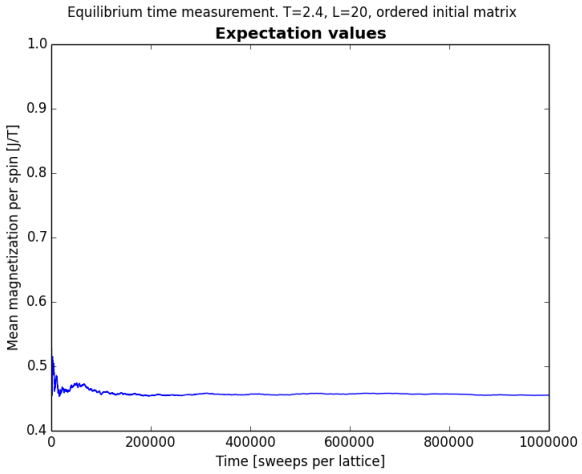

Figure 7: The expectation value of the absolute of the mean magnetization, with T=2.4 and ordered initial spin matrix.

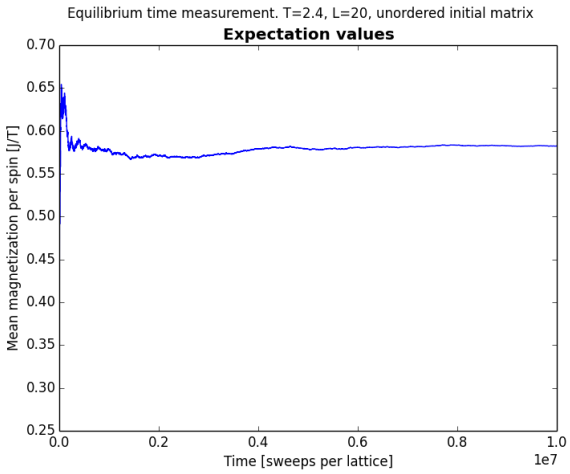

Figure 8: The expectation value of the absolute of the mean magnetization, with T=2.4 and random configuration on the initial spin matrix.

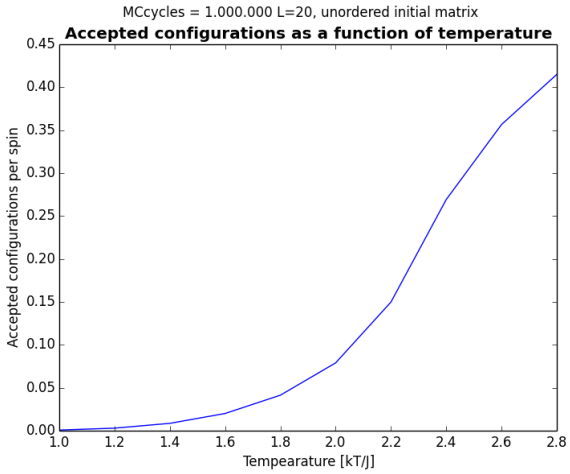

Figure 9: The accepted configurations per spin as a function of temperature and unordered/disordered initial spin configuration.

It is very obvious that the total number of accepted configurations increase parallel to increasing temperature. The temperature therefor is a very important factor influencing the parameters of the system.

The mean energy for T = 1.0 has an insignificant variance between the simulations starting for ordered and disordered initial configurations to start with. The energy in both diagrams converge towards approximately -1.99. For

the same 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 the Monte Carlo cycles increases both graphs converge towards a steady state. This energy value is in both cases approximately -1.235.

The mean magnetization is not as equal for the two initial configuration as the energy is.

All of the diagrams shows a flattening of the graph from approximately 400.000 Monte Carlo sweeps and further. I would say that the equilibrium time is around 5-600.000 sweeps, surely.

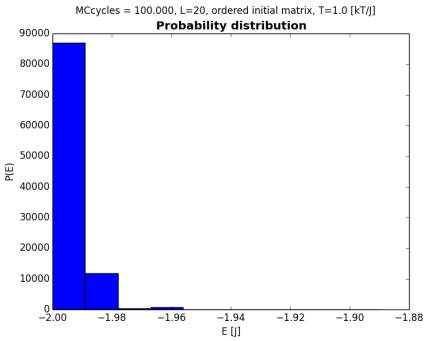

Figure 10: Probability distribution for the energy with T=1.0 and 10 bins in the histogram. The values were outputted after the equilibrium time was reached.

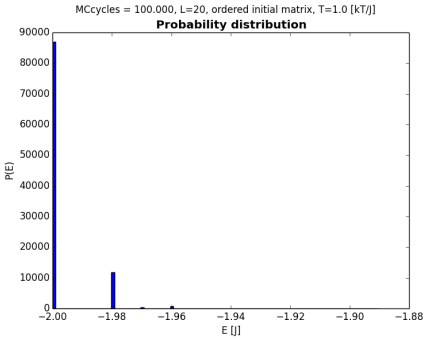

Figure 11: Probability distribution for the energy with T=1.0 and 100 bins in the histogram. The values were outputted after the equilibrium time was reached.

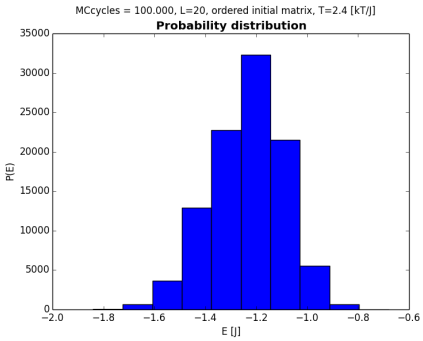

Figure 12: Probability distribution for the energy with T=2.4 and 10 bins in the histogram. The values were outputted after the equilibrium time was reached.

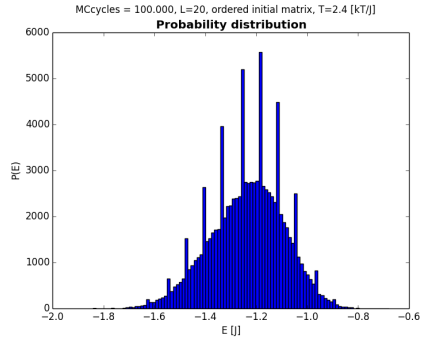

Figure 13: Probability distribution for the energy with T=2.4 and 100 bins in the histogram. The values were outputted after the equilibrium time was reached.

The interesting part for plotting the histograms is to examine how the energy and the magnetization oscillates around the equilibrium state. The equilibrium time was set to be 10000 (Monte Carlo sweeps). 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 mean energy, mean magnetization, specific heat and susceptibility is plotted as a function of temperature from 2.0 to 2.3 to examine phase transitions for different lattice dimensions.

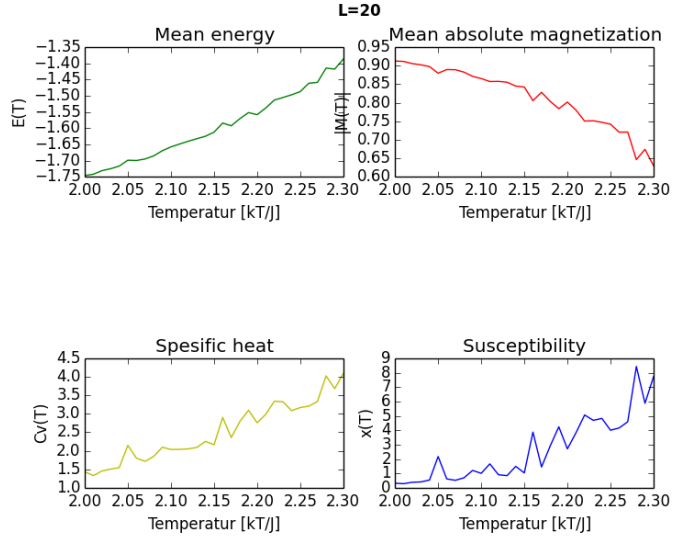

Figure 14: Lattice size: 20x20. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

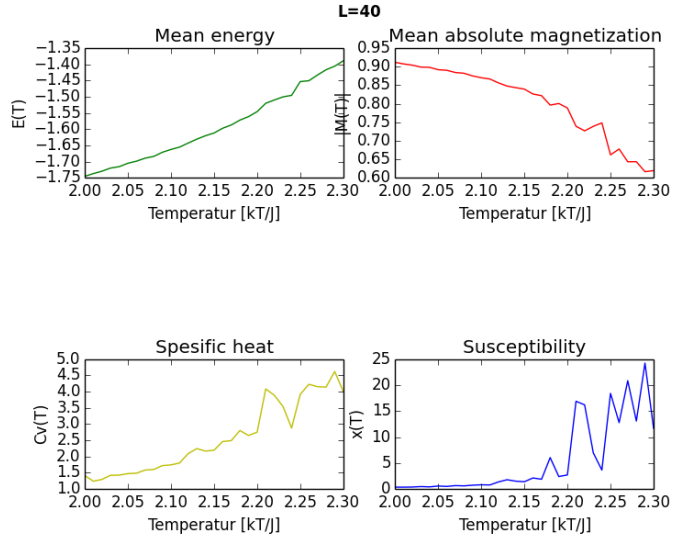

Figure 15: Lattice size: 40x40. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

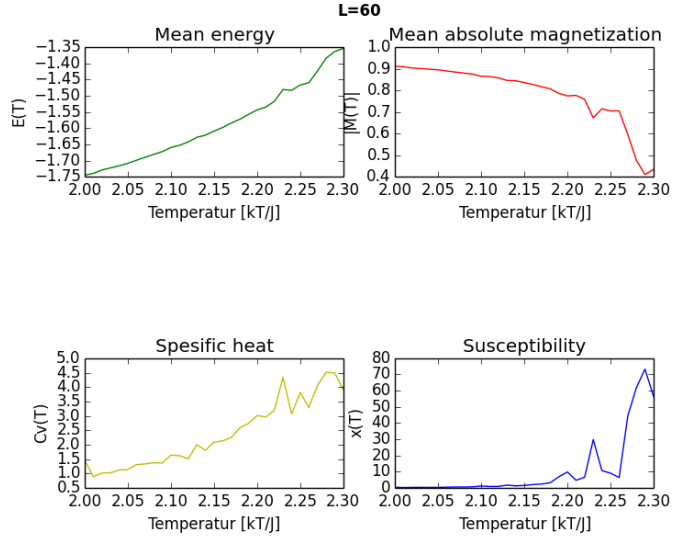

Figure 16: Lattice size: 60x60. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

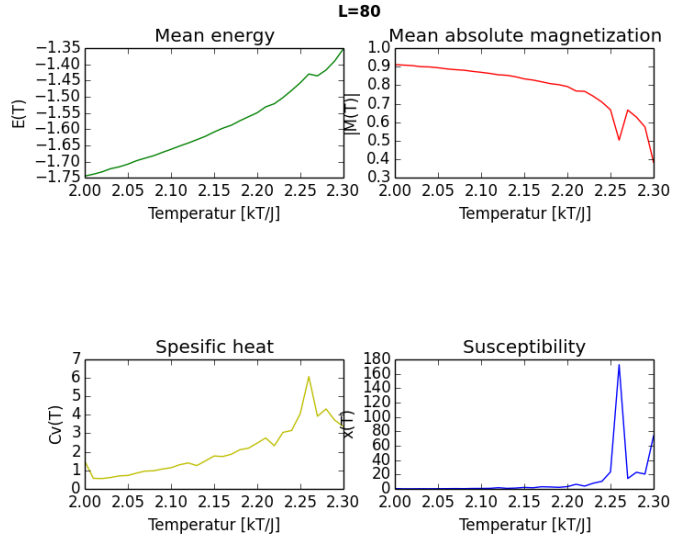

Figure 17: Lattice size: 80x80. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

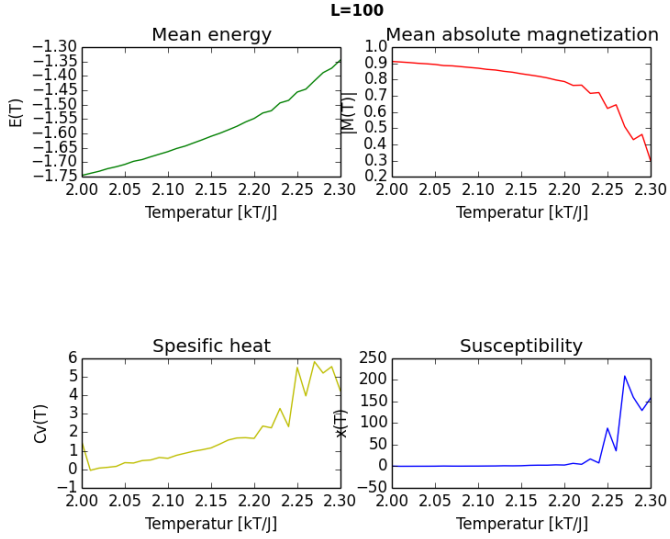

Figure 18: Lattice size: 100x100. The expectation values for the mean energy per spin and the mean magnetization per spin, as well as the specific heat and the susceptibility is computed as functions of the temperature.

5 Appendix

Calculations of analytical values in table 1. Partition function:

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

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

$$\begin{aligned} Z(1) &= e^{8J} + 4e^0 + 4e^0 + 2e^{-8J} + 4e^0 + e^{8J} \\ &= 2e^{8J} + 2e^{-8J} + 12 \end{aligned}$$

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:

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

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

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 $\mathrm{n}_E 2.txt ... T = 1 Monte Carlo cycles = 10000000 Spin matrix dimension = 2 Mean energy = -1.99599 Mean abs magn = 0.998671 The heat capasity of the system = 0.0320045 The susceptibility of the system = 0.00395893 Time used = 12.15031900 seconds.

List of Figures