Project 4

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November 2018

Abstract

Phase transitions of a ferromagnetic system is investigated in this project. The Ising model in two dimensions is solved to obtain numerical values for expectation values for energy and magnetization when considering lattices of spins. From those values, one can calculate the associated variances and obtain the corresponding expectation values for heat capacity and susceptibility. How the magnetic system responds to heating and reaches a phase of zero magnetization is discussed in this report. The foundation of being able to solve the model is the Metropolis algorithm. This is a Monte Carlo method, in which require the calculations to be run many times in order to hopefully achieve some reasonable results. The critical temperature remarks the stage ferromagnetic materials undergo a certain sharp change in their thermal properties. In this project I will attempt to estimate this value. The estimated value was found to be $T_C = 2.27$, also for an infinite lattice based on the behavior of the variances in energy and magnetization.

1 Introduction

This project utilizes the Ising model for a ferromagnetic system with periodic boundary conditions in two dimensions to simulate phase transitions of a magnetic material, in which the magnetization is explained by a square lattice consisting of spins. Each spin exists in one of two possible states (± 1). For the Ising model, the energy of the system is computed by taken the sum over total number of spins, where the sum is taken over nearest neighbours only, see Figure 1 for an example illustration with an 8×8 lattice. At a certain critical temperature, called the Curie temperature, there exists a second-order phase transition from a magnetic phase to a phase with no magnetization. When the energy is calculated, different thermodynamic quantities can be found. In this project one are searching for expectation values for energy $\langle E \rangle$, absolute magnetization $\langle |\mathscr{M}| \rangle$, heat capacity $\langle C_v \rangle$ and susceptibility $\langle \chi \rangle$ (mean values).

To compute these quantities, so called Monte-Carlo methods in statistical physics are applied. The algorithm to be used is the algorithm of Metropolis, in which the change in energy and magnetization for the system is calculated when sweeping over the lattice and this is repeated over a certain amount of Monte Carlo cycles (MC-cycles).

The Ising model is one of the most broadly studied systems in statistical mechanics in considerations of phase transitions. In performing Monte Carlo simulations, one attempts to following the "time dependence" of a model where changes are not following predefined ways, but rather in a stochastic manner which depends on random numbers generated during the simulations [5]. My motivation for the project is to learn about how a complex system like a magnetic system and the associated

different thermodynamical quantities, respond to the Monte Carlo simulations and theirs behavior at different temperatures.

The Theory part (Section 2) explains the Ising model in two dimensions (Section 2.1), the steps contained in the Metropolis algorithm (Section 2.2) and the derivations of the analytical solutions to a 2×2 lattice. It also give a short brief of the concept of correlation length according to critical temperature.

The result and the discussion sections (Sections 3 and 4) present the behavior of energy and magnetization for a low and a higher temperature in accordance to MC-cycles for a 20×20 lattice. Among other things the probabilities for how the energy is distributed and the critical temperature are examined in these two sections. Section 5 states the conclusion.

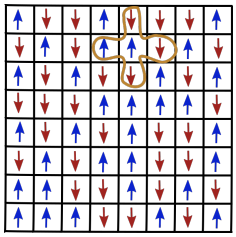

Figure 1: Example of the ising model with a 8×8 lattice, where the spins can point either up $(+1)$ or down (-1). [1]

2 Theory

2.1 The Ising model in two dimensions

The Ising model attempts to simulate phase transitions in a magnetic system consisting of N spins pointing up or down. In the year of 1944, the Norwegian chemist, Lars Onsager, obtained an analytical solution to the two dimensional Ising model, in absent of an external field [3]. The general form of the model is defined according to the total energy as follows:

$$E = -J \sum_{<kl>}^{N} s_k s_k - \mathscr{B} \sum_{k}^{N} s_k \tag{1}$$

where J defines a coupling constant indicating the strength of the interaction between neighbouring spins ($J > 0$ for ferromagnetic case), $s_k = \pm 1$ and $< kl >$ specifies that the sum is taken over nearest neighbours only. The second term including $\mathscr{B}$ concerns an external magnetic field, in which is set to zero in this project. The energy of the Ising model can then be expressed in this way:

$$E = -J \sum_{<kl>}^{N} s_k s_k \tag{2}$$

Periodic boundary conditions (PBC) in two dimensions involve that each spin's neighbour to the right takes the value left for the spin and opposite. Similar, the spin's neighbour to the north takes the value south for the spin and opposite depending on which side of the boundary of consideration.

The different expectation values of interest for this project can be derived from a so called ensemble, an important quantity in statistical physics. An ensemble is a set of microphysics systems. There exists various types of ensembles, but in this project the canonical ensemble is emphasized.

The partition function is defined as

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{3}$$

The mean energy, mean magnetization, heat capacity and susceptibility are defined as

$$\langle E \rangle = -\frac{\partial ln Z}{\partial \beta} \tag{4}$$

$$\langle \mathscr{M} \rangle = \frac{1}{Z} \sum_{i}^{M} E_i e^{-\beta E_i} \tag{5}$$

$$\langle C_v \rangle = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

$$\langle \chi \rangle = \frac{1}{k_B T} (\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2) \tag{7}$$

in which the variances for the energy and magnetization is

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{8}$$

$$\sigma_{\mathscr{M}}^2 = \langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2 \tag{9}$$

The number of so called configurations depend on the size of the lattice and goes like $2^{L \times L}$ where L is the amount of spins in each dimensions. The concept of configurations is explained more in detail in Section 2.3 where a special case of an 2×2 lattice is examined and analytically results are derived.

2.2 Metropolis algorithm

To solve the two-dimensional Ising model and computing the desired quantities of thermodynamic, we will use the Metropolis algorithm. This algorithm is characterized as a Markov chain Monte Carlo (MCMC) method for obtaining random sampling sequences from a given probability distribution [6].

The Monte Carlo sampling function is given by

$$P_s = \frac{e^{-(\beta E_s)}}{Z} \tag{10}$$

In which P_s is the probability to find the system in a state s, E_s denotes the energy for a given state, $\beta = \frac{1}{kT}$ (k is Boltzmann constant and T is the temperature). Z is the partition function

$$Z(\beta) = \sum_{s} e^{-(\beta E_s)} \tag{11}$$

Computing the partition function when the number of spins of consideration become large, might be complicated since we need to know all the energy states. An advantage of using the Metropolis algorithm is that its not necessary to compute the partition function, there will be a limited set of energy differences ΔE in which only one spin is flipped for each configuration. The essential steps of the Metropolis algorithm is listed here:

1. Select a random spin configuration position in the lattice and then establish an initial state of energy E_b
2. Flip one spin only and compute the energy of this state E_t
3. Calculate $\Delta E = E_t - E_b$
4. In case of $\Delta E \leq 0$ one are accepting the new configuration (jump to step 7 if this is the case)
5. In case of $\Delta E \geq 0$, compute $w = e^{-(\beta \Delta E)}$
6. Compare a random number r with the w calculated in step 5. In the case of $r \leq w$, accept the new configuration, else keep the old configuration
7. Update the expectation values
8. Repeat steps 2-7 sufficiently enough times, where one sweep over the lattice corresponds to one MC-cycle

2.3 Lattice of 2×2, analytical expressions

In order to get some intuition of the behaviour of the interacting spins, consider first a two-dimensional lattice of size 2×2, in which there are L = 2 spins in each of the dimensions.
The different configurations for a lattice in this small size is $2^4 = 16$. In Figure 2, four different configurations with corresponding energies are shown. The Degeneracy for each of the energies (sums up to 16 in total) in addition to the magnetization value are displayed in Table 1. The figure and the table is taken from the lecture notes page 424 [4].

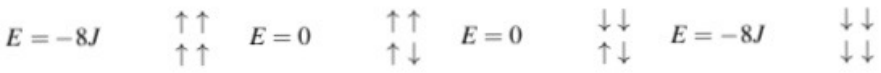

Figure 2: Examples of configurations and corresponding energies

With this in mind, we now examine the analytical solutions.

The general expression for the partition function is given by Equation 3. The exact expression for the partition function concerning a 2×2 lattice, can be derived in this way summing over all the possible energy configurations:

Number 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: Energy and magnetization for the two-dimensional Ising model with $N = 2 \times 2$ lattice with periodic boundary conditions

$$Z_{2\times 2} = \sum_{i=1}^{16} e^{-(\beta E_i)} = e^{8J\beta} + e^{-8J\beta} + e^{8J\beta} + e^{-8J\beta} + 12e^{0\beta} \tag{12}$$

$$= 2e^{8J\beta} + 2e^{-8J\beta} + 12 \tag{13}$$

$$= 4cosh(8J\beta) + 12 \tag{14}$$

Substituting for the partition function, the expectation value for the energy can then be expressed using Equation 4:

$$\langle E\rangle_{2\times 2} = -\frac{\partial ln(2e^{8J\beta} + 2e^{-8J\beta} + 12)}{\partial \beta} \tag{15}$$

$$= -\frac{16e^{8J\beta} - 16e^{-8J\beta)}}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \tag{16}$$

$$= -\frac{32sinh(8J\beta)}{4(cosh(8J\beta + 3} \tag{17}$$

$$= -8J\frac{sinh(8J\beta)}{cosh(8J\beta) + 3} \tag{18}$$

The magnetization can be computed from Equation 5:

$$\langle \mathscr{M}\rangle_{2\times 2} = \frac{1}{Z}\sum_{i}^{16} \mathscr{M}_i e^{-\beta E_i} \tag{19}$$

$$= \frac{4e^{8J\beta} + 8e^0 - 8e^0 - 4e^{8J\beta}}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \tag{20}$$

$$\tag{21}$$

The absolute value of the mean magnetization is therefore:

$$\langle|\mathscr{M}|\rangle = \frac{8e^{8J\beta}+16}{2e^{8J\beta}+2e^{-8J\beta}+12} \tag{22}$$

$$= \frac{2e^{8J\beta}+4}{cosh(8J\beta)+3} \tag{23}$$

The analytically expression for the heat capacity goes like (Equation 6):

$$\langle C_v\rangle_{2\times 2} = \frac{1}{k_bT^2}\frac{\partial^2 ln(4cosh(8J\beta)+12)}{\partial\beta^2} \tag{24}$$

$$= -\frac{1}{k_bT^2}\frac{64J^2(cosh^2(8J\beta)+3cosh(8J\beta)-sinh^2(8J\beta))}{(cosh(8J\beta)+3)^2} \tag{25}$$

$$\tag{26}$$

Finally, the analytically susceptibility expression (using Equation 7):

$$\langle\chi\rangle_{2\times 2} = \frac{1}{k_bT}\sigma^2_{\mathscr{M}} \tag{27}$$

$$= \frac{1}{k_bT}\frac{16e^{8J\beta}+128+16e^{8J\beta}}{2e^{8J\beta}+2e^{-8J\beta}+12} - 0 \tag{28}$$

$$= \frac{1}{k_bT(}\frac{32e^{8J\beta}+128}{4cosh(8J\beta)+12)} \tag{29}$$

In which $k_b, T, J, \beta = 1$ and one can obtain analytical values for the quantities and then compared to the numerical values when preforming the Metropolis algorithm.

2.4 Phase transitions and critical temperature

The mean magnetization, heat capacity and the susceptibility as a function of temperature T can be approximated as

$$M(T) \approx (T-T_C)^\beta \tag{30}$$

$$C_V(T) \approx |T_C-T|^\alpha \tag{31}$$

$$\chi(T) \approx |T_C-T|^\gamma \tag{32}$$

with critical exponents $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$.

How strongly the spins are related to each other are described through the correlation length ξ. The correlation length increases when T approaching the critical temperature T_C, which means that the correlation between the spins becomes stronger. This quantity is described as

$$\xi(T)|T_C-T|^{-\nu} \tag{33}$$

ξ is proportional to the size of the lattice at the critical point. The two dimensional Ising model consider a fixed size of lattice. However, through something called finite size scaling, the critical temperature in a finite lattice might be related to the one in an infinitely large lattice as

$$T_C(L) - T_C(L = \infty) = aL^{-\frac{1}{\nu}} \tag{34}$$

a is scalar. Defining $T = T_C$, the mean magnetization, heat capacity and susceptibility as function of T can now be written

$$M(T) \approx L^{-\frac{\beta}{\nu}} \tag{35}$$

$$C_V(T) \approx L^{\frac{\alpha}{\nu}} \tag{36}$$

$$\chi(T) \approx L^{\frac{\gamma}{\nu}} \tag{37}$$

According to Lars Onsager, the exact result for the value of the critical temperature is $kT_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ [2]. Below a critical temperature (note: called the Curie temperature) T_C, the Ising model experiences a spontaneous magnetization in which $\langle \mathscr{M} \rangle \neq 0$. Above, $\langle \mathscr{M} \rangle = 0$. In other words, a phase transition undergoes a transition from a phase with finite magnetization to a paramagnetic phase with zero magnetization.

3 Results

3.1 Comparison between analytical and numerical values, 2×2 lattice

Table 2 lists different mean values (expectation values) for energy, absolute magnetization, heat capacity and susceptibility in term of different choices of MC-cycles for the 2×2 lattice case. The line highlighted in blue denotes the amount of MC-cycles needed to achieve a best match as possible with the analytic values obtained from Equations 18,23,26 and 29. A million MC-cycles seem to give a quite good compliance with the analytical values.

height**Monte-Carlo cycles:**	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	$\langle C_v \rangle$	$\langle \chi \rangle$
10	-2.0000	1.0000	0.0000	0.0000
10^2	-2.0000	1.0000	0.0000	0.0000
10^3	-1.9960	0.9980	0.0319	0.0080
10^4	-1.9982	0.9995	0.0144	3.9938
10^5	-1.9959	0.9986	0.0033	3.8874
10^6	-1.9958	0.9986	0.0332	3.9798
Analytical values	-1.9950	0.9987	0.0320	3.9973

Table 2: Expectation values for energy, absolute magnetization, heat capacity and susceptibility for different MC-cycles and corresponding analytical values with $T = 1$ and a lattice $N = 2 \times 2$

3.2 Thermalization time, 20×20 lattice

Expectation values for energy as function of number of MC-cycles for a low temperature T = 1 are shown in Figure 3. Two different start configurations for the spins are considered. The red

curve is for a ordered set of spins, where all the arrows pointing up initially. The blue curve is for a random start configuration. To get a better picture of how the expectation values evolves with increasing number of MC-cycles for the two different configurations, the right hand side of the figure shows a close up where a difference can be spotted. The ordered start configuration reaches a stable equilibrium state at around -2 faster compared to a random start configuration. The needed time for stabilization to occur for a random start configuration seem to be some place after 10000 MC-cycles.

For absolute magnetization for the same temperature as considered above, is shown in Figure 4. From the close up, the random start configuration approaches the equilibrium situation around 1 before the random start configuration. The magnetization shows more or less the same behavior as for the energy case with the same number of MC-cycles needed to get stabilization.

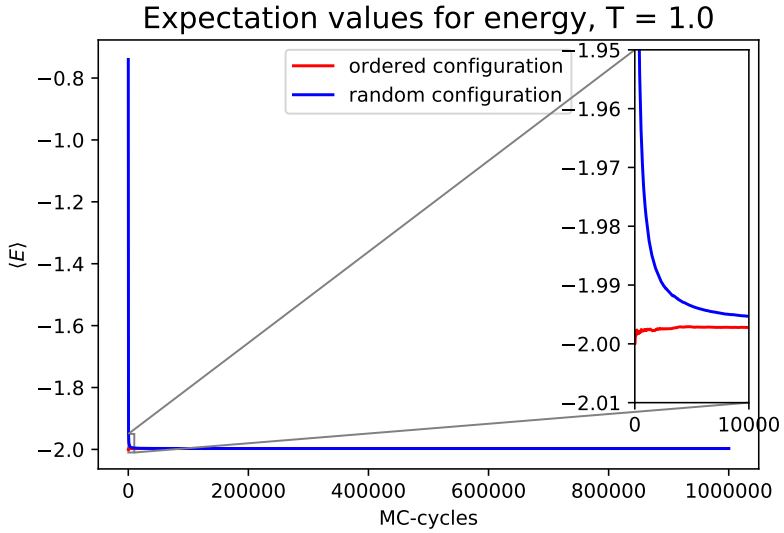

Figure 3: Mean energy per spin as a function of Monte Carlo cycles for a 2×2 lattice

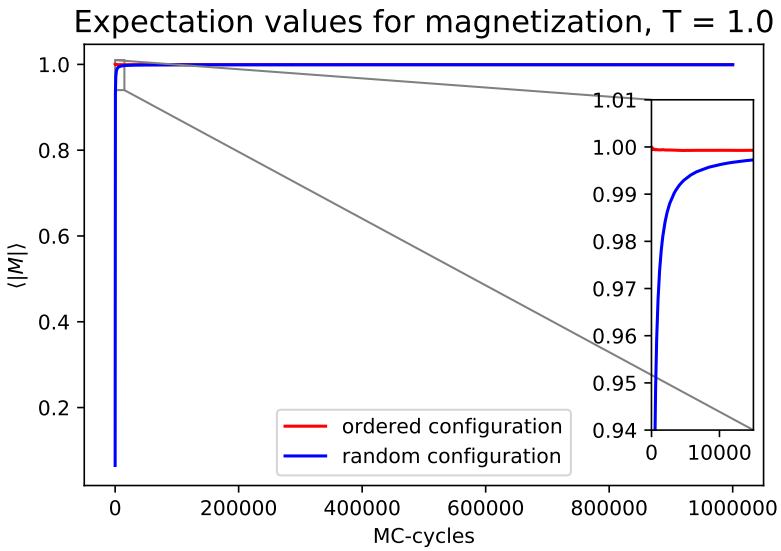

Figure 4: Mean magnetization per spin as a function of Monte Carlo cycles for a 2×2 lattice

Figure 5 displays the mean energy as function of MC-cycles for a higher temperature, namely T = 2.4. Studying the behavior for the two different start configurations in a little piece of the x and y domain (around the time 0-40000) one can observe a little different pattern compared to lower temperatures considered above. From the figure it looks like the random configuration reaches the most likely state quicker, the ordered one are oscillating more. Around a time of 40000 MC-cycles might be needed for both configurations to obtain equilibrium values.

For the absolute magnetization, the time evolution is examined in Figure 6 for T = 2.4. Both the ordered and the random configuration is increasing fast in the very beginning. After approximately 50000 MC-cycles they flat more out, but there exists a gap between the two for a while until approximately 300000 MC-cycles are completed.

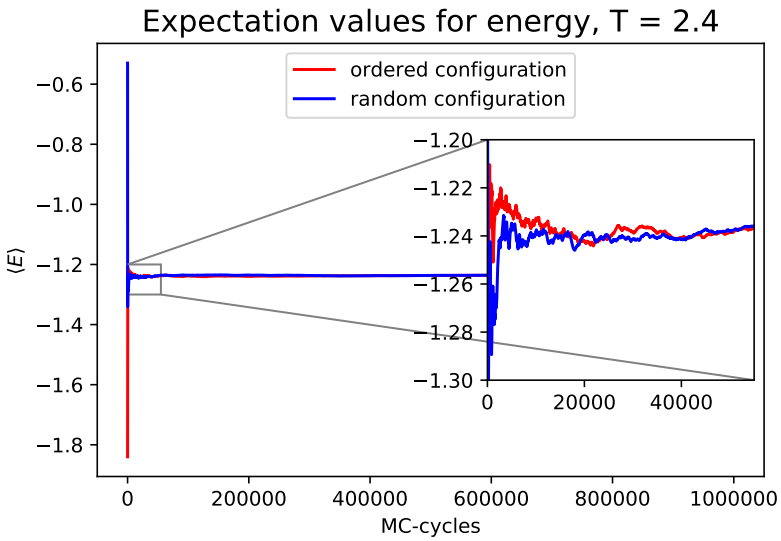

Figure 5: Mean energy per spin as a function of Monte Carlo cycles for a 2×2 lattice

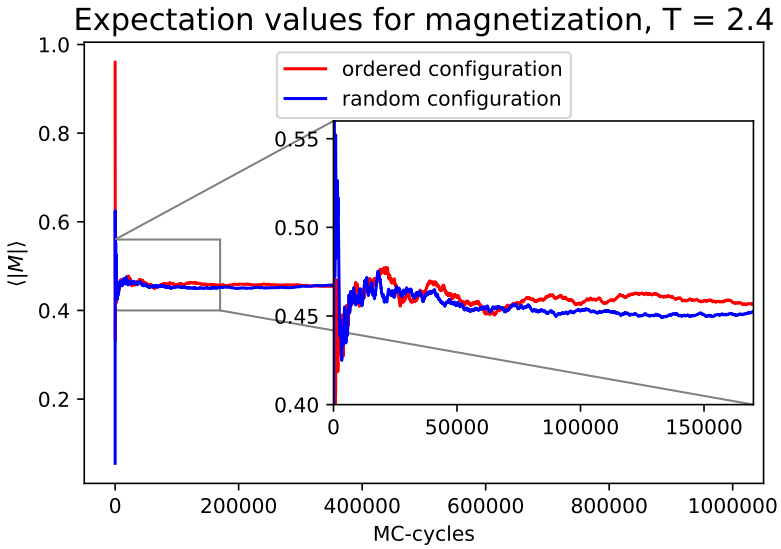

Figure 6: Mean magnetization per spin as a function of Monte Carlo cycles for a 2×2 lattice

The amount of accepted configurations are presented in Figure 7 for a time until 10 000 MC-cycles. With all the spin pointing up in the very beginning, approximately 3000 accepted configurations are found. For the random start case, a double amount, 6000 is observed for 10 000 MC-cycles.

Figure 8 shows the number of accepted configurations for a temperature T = 2.4. For this temperature, over a 1000000 number of accepted configurations are obtained for 10 000 MC-cycles. The random configuration graph lies slightly under the ordered one after 4000 MC-cycles.

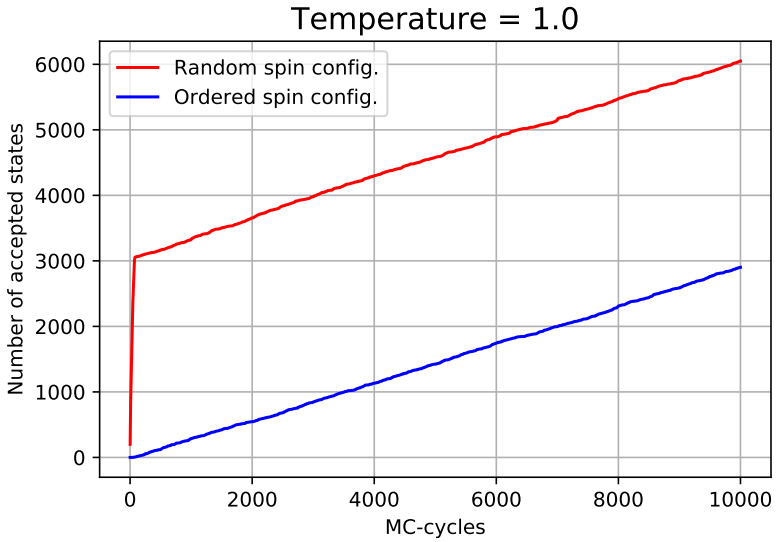

Figure 7: Amount of accepted configurations as a function of MC-cycles for random and ordered spin configurations with T = 2.4

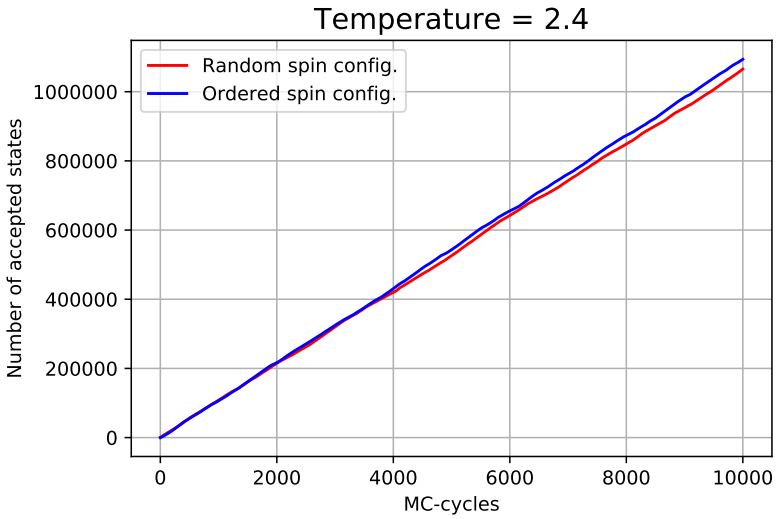

Figure 8: Amount of accepted configurations as a function of MC-cycles for random and ordered spin configurations with T = 2.4

3.3 Probability distribution

Figure 9 shows the energy probability distribution when T = 1. The obtained result is based on how many times a given energy shows up during the calculations. From the figure its quite clear that the energy is concentrated around two values, namely -2 and -1.98 (in values of per spin).

The distribution for a higher temperature can be seen in Figure 10. Here, T = 2.4, and it can be observed from the figure that the energy takes a widely larger range/spectre of values. The distribution tends to take a Boltzmann distribution with its characterized bell shape.

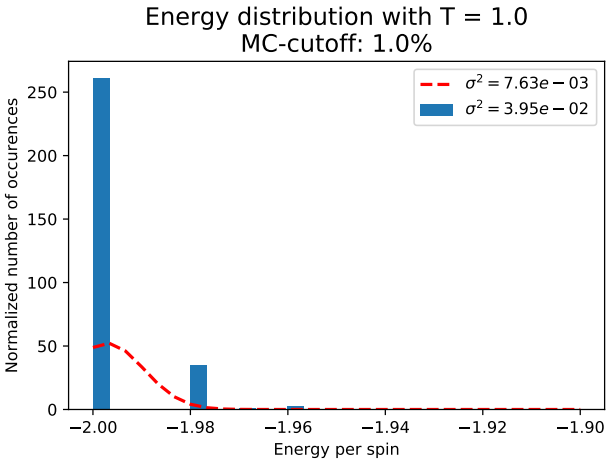

Figure 9: Probability distribution and variances for T = 1 with a $N = 20 \times 20$ lattice

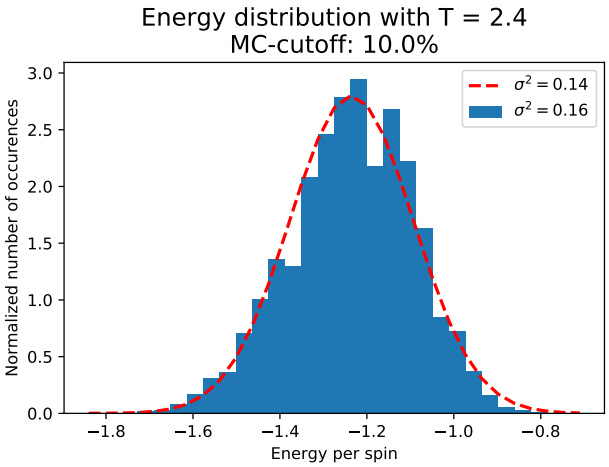

Figure 10: Probability distribution and variances for T = 2.5 with a $N = 20 \times 20$ lattice

3.4 Phase transitions and critical temperature

The expectation value $\langle E \rangle, \langle |\mathscr{M}| \rangle, C_v$ and susceptibility $\langle \chi \rangle$ are displayed in he Figures 11 -14 as functions of T for the lattice sizes L = 40, L = 60, L = 80 and L = 100 in the temperature interval [2.10 2.50]. It can be observed that the energy increases before it splits a little bit among the different lattice sizes. The magnetization tends more towards zero for larger lattices and the heat capacity C_V and susceptibility χ reaching a higher maximum value as the size of the lattice is increased.

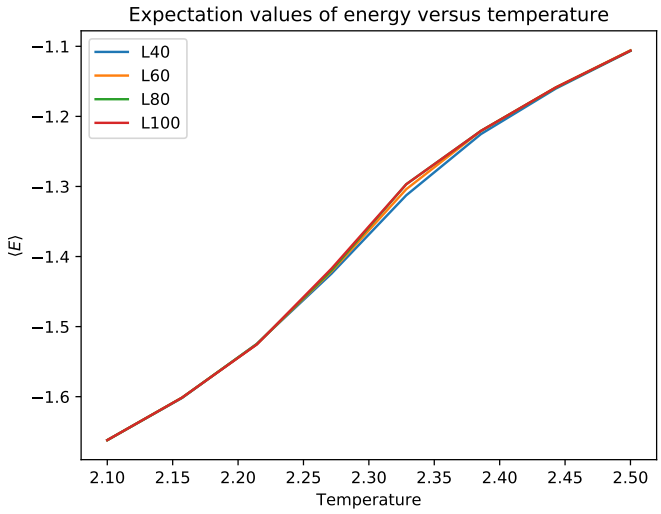

Figure 11: Mean energy for different lattice sizes as a function of temperature

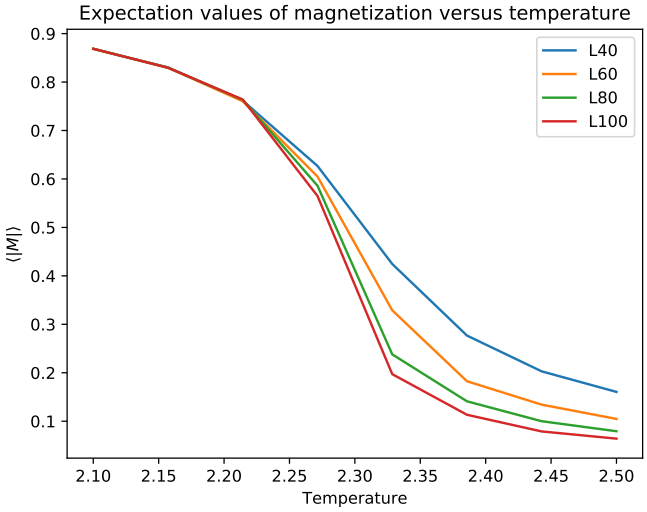

Figure 12: Mean magnetization for different lattice sizes as a function of temperature

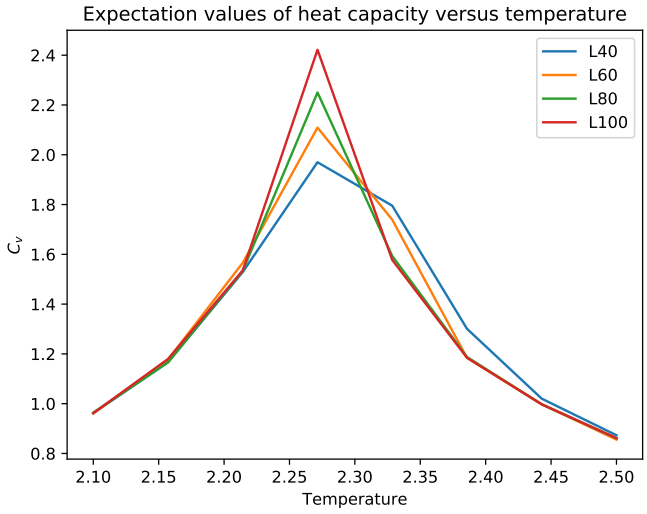

Figure 13: Specific heat for different lattice sizes as a function of temperature

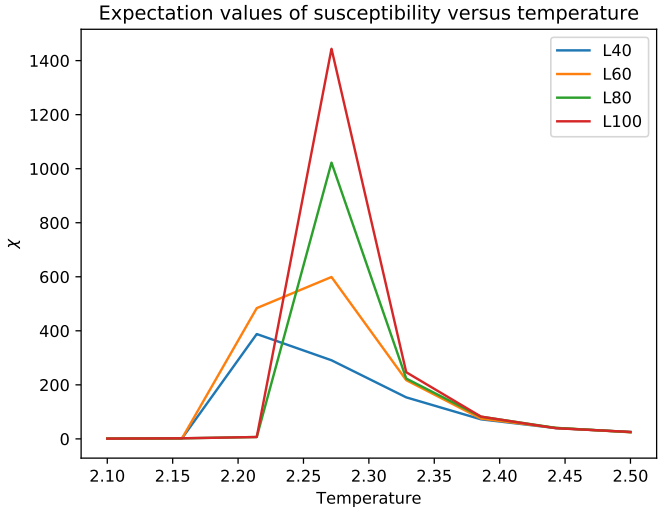

Figure 14: Susceptibility for different lattice sizes as a function of temperature

4 Discussion

According to the thermalization time, the time needed to stabilize the expectation values, it seems that for higher temperatures, the amount of needed MC-cycles increases in order to obtain stabilization. There is also a much greater variety of energy states at higher temperatures, something to expect as higher temperature gives more available energy.

From Equation 34, the critical temperature for an infinite large lattice with $\nu = 1$ can be computed by setting the first term on the right hand side of the equation:

$$T_C(L = \infty) = T_C(L) - aL^{-\frac{1}{\nu}} \tag{38}$$

The result from the Figures 11 - 14 shows some interesting behaviour. It is of interest to have a closer look into the different quantities, and see if there is any indication of spotting the curie temperature T_C. Lars Onsager found the critical temperature to be ≈ 2.269 (see Section 2.4). A peak that becomes sharper and higher when increasing the lattice size is evident from both the heat capacity and susceptibility plots. It reaches a maximum value before it starts to decrease. This might indicate the mark of the position of the curie temperature. Roughly, the peak seem to be positioned at $T \approx 2.27$ for $L = 100$. Using Equation 38 and solving for the constant a, one can estimate the critical temperature for an infinite lattice by using the critical temperatures between two lattices. The same estimate of$T_C \approx 2.27$ is obtained for $T_C(L = \infty)$. This value coincide quite well with what Onsager found.

The indication of the curie temperature is not as clear for the expectation value for the energy $\langle E \rangle$ and magnetization $\langle \mathscr{M} \rangle$. Nevertheless, an indication of an existing turning point is likewise to observe. As L increases, the magnetization gets closer to paramagnetic phase with a suddenly

drop. Its a little difficult to state exacly where this turning point occur, but not very far from the temperature estimated from Equation 38 is likely.

5 Conclusion

The Ising model and its features have been studied through this project. Against one million Monte Carlo cycles were preformed in the computations of energy $\langle E \rangle$, magnetization, $\langle \mathscr{M} \rangle$, heat capacity $\langle C_v \rangle$ and susceptibility $\langle \chi \rangle$ by using the algorithm of Metropolis. The heat capacity and susceptibility showed some indication of spotting the critical temperature, when lattice sizes up to $L = 100$ were treated as function of T. The peaks grew proportional to the size of L. The critical temperature was found to be $T_C \approx 2.27$, not a bad estimate compared to what Onsanger found.

5.1 Documentation

The material used in this project can be found in the group member's repository in GitHub:

`https://github.com/marikoll/FYS4150_projects/tree/master/project_4/python_code`

The numerical values for the thermodynical variables obtained in 3.1 are extracted from the example Ising program for python language found at the github course homepage:

https://github.com/CompPhysics/ComputationalPhysics/tree/master/doc/Programs/PythonCodesLectureNotes

References

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