FYS4150 project 4

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Abstract

We have studied the Ising model in two dimensions with periodic boundary conditions. Monte Carlo methods have been used in the development of the algorithms. For a 2×2 lattice, our algorithm needs 10^7 Monte Carlo cycles to replicate the analytic results. Applying he algorithm on a 20×20 lattice yields $10,00$ Monte Carlo cycles before equilibrium is reached with a low temperature. The temperature is increased from $T = 1.0$ to $T = 2.4$, and we now need $100,000$ Monte Carlo cycles to reach the most likely state. Based on simulations with the lattice size varying from $L = 40$ to $L = 100$, we found indication of a phase transition at $T = 2.27$, which is close to Onsager's exact result, with the critical temperature being $T_c = 2.269$

1 Introduction

A number of problems in physical science can be solved by statistical simulation methods. With today's computers getting more and more powerful, we are able to execute such simulations with satisfying precision. We can therefore expect to use such methods in later studies.

In this project we have discussed the Ising model in two dimension and developed an algorithm to study this model for a number of different sized lattices. The theory behind the model is presented followed by a thorough description of our statistical simulation method, Monte Carlo, and strategies to optimize the algorithm. Next we define the quantities we want to study in the Ising model and derive the analytic expression. In the final part of the theory section, the most interesting part of this project is presented, the critical temperature and phase transitions.

In the result part of the report, we will present results for the Ising model with a 2×2 lattice and compare them to the analytic results, then increase the size of the lattice to 20×20 and study how the quantities of this lattice changes with the number of Monte Carlo cycles. The last part of the results includes a study of phase transitions for lattices with varying size. The discussion will try to explain our results and the following conclusion will summarize the project.

2 Theory

2.1 Ising model

The Ising model is widely used in computation of phase transitions in magnetic systems. For a two dimensional system with zero external field, the Ising model can be solved exactly [1].

The system in consideration consist of a set of lattice sites, all with spins. The spin can be either $+1$ or -1. In the Ising model, the spins are arranged in a square lattice, and the interaction between them is modeled to the nearest neighbors. This gives us four neighbors per spin.

With periodic boundary conditions, we assume that the chain of spins are infinite and that it repeats itself periodically. The energy in the Ising model can be expressed as

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

where

- J denotes exchange energy which indicates the strenght of the spin-spin interaction. In our case we will look at a ferromagnetic system, e.g the spin can take two forms, and $J > 0$. The spins are aligned.
- $< kl >$ indicates the nearest neighbour. The product of $S_i S_j$ can thus be ± 1
- E is given as a Hamiltonian,

Using the concept of ensemble is common in thermodynamics, as it allows us to describe the system with expectation values and thus derive thermodynamic quantities. The probability distribution in a canonical ensemble is given as

$$P_i(\beta) = \frac{e^{\beta E_i}}{Z} \tag{2}$$

where E_i is the total energy of the microstate i, $\beta = k_B T$ is the inverse temperature with k_B being the Boltzmann constant and Z is the partition function, given as

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

which sums over all microstates M. In all calculations, we will scale the temperature so its unit it Tk_B/J but is referred to as T. For this ensemble model, the energy is an expectations value, i.e. it is a long-run average when energy is exchanged between the surroundings and the system. This expectation value is linked with the Helmholtz' free energy (F) and the entropy (S) at a given temperature (T),

$$< E >= F + TS \tag{4}$$

Inserting $F = -k_b T lnz$ and $S = k_b lnz + k_b T \frac{\partial lnz}{\partial T}$ yields

$$< E >= \frac{1}{Z}\sum_{i=1}^{m} E_i e^{-\beta E_i} \tag{5}$$

which is the mean energy of the system. This is also the partial derivative of the natural logarithm to the partition function Z. Another quantity of great import is the mean magnetization given as

$$< M >= \sum_{i}^{m} M_i P_i(\beta) = \frac{1}{Z}\sum_{i}^{m} M_i e^{-\beta E_i} \tag{6}$$

Knowing the mean energy and the mean magnetization, we can derive the specific heat capacity at a given temperature and the susceptibility χ,

$$C_v = \frac{1}{kT^2}(< E^2 > - < E >^2) \tag{7}$$

$$\chi = \frac{1}{kT}(< M^2 > - < M >^2) \tag{8}$$

The specific heat capacity is the heat capacity per unit mass and is propotional to the temperature squared. The susceptibility is a measure of how much an extensive parameter changes when an intensive parameter increases.

2.2 Monte Carlo methods

Having set the theory straight, we will now give the theory behind developing algorithms for the Ising model.

Monte Carlo methods are widely used in statistic physics. It is based on a random sampling of the probability distribution which describes the system [2]. The main principle in a Monte Carlo method is that we can calculate the variance, and thus know when we would expect the method to produce a stable solution.

2.3 Marcov chains

In order to use Monte Carlo in the Ising model, we have to make a shift to a Markov chain. This ensures that every new move in the random walk is independent of the previous one and thus will make sure that we will reach the most likely state after a large number of random simulations. In our Ising model we will need a Marcov chain in order to determine if an energy state is accepted or not. This is explained further in the next section.

2.4 Metropolis Algorithm

Now we have a random sampling method which ensures that we will reach the most likely state after a number of simulations but we still need a method which gives a suggestion to a new configuration based on the starting configuration. The Metropolis algorithm does exactly this for us. To be more specific, it is based on a probability of finding the system in a given state. The Metropolis algorithm works as follows ("recipe" credited M.Hjort [2]) :

- Set an initialize state with an energy E_b. This is done by positioning at a random configuration in the lattice.
- The initial configuration is changed by flipping, e.g one spin only, and the new energy state is computed, E_t.
- The difference in energy states is computed, $\Delta E = E_t - E_b$. If $\Delta E \leq 0$ we accept the new configuration.
- If not, we will only accept the new configuration if the probability is $e^{-\Delta E/kT}$. This will always be between 0 and 1.
- Now we have to compare this result with a random number distributed between 0 and 1. If this number is smaller than our probability, we keep the new configuration- otherwise we keep the old.
- All expectation values are updated
- We repeat the steps above until we reach a sufficient good representation of the states.
- We sweep through the lattice and divide the expectation values by the number of Monte Carlo cycles and the number of spins or temperature in order to normalize our values.

2.5 Analytic expressions using canonical ensemble

Now, by considering a 2×2 lattice we have $2^4 = 16$ configurations for the spin. Using the Ising model energy from Section 2.1 and periodic boundary conditions, we can get the expressions for partition function Z,

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 12 + 2e^{8\beta J} + 2e^{-8\beta J} \tag{9}$$

$$\rightarrow \cosh(z) = \frac{e^z + e^{-z}}{2} \tag{10}$$

$$Z = 12 + 4\cosh(8\beta J) \tag{11}$$

The expectation value E is then

$$< E > = -\frac{\partial \ln Z}{\partial \beta} \tag{12}$$

$$= -\frac{8J\sinh(8\beta J)}{\cosh(8\beta J) + 3} \tag{13}$$

$$\tag{14}$$

The specific heat capacity at constant volume is then

$$C_v = \frac{1}{kT^2}\frac{\partial^2 \ln Z}{\partial \beta^2} \tag{15}$$

$$= \frac{1}{kT^2}\frac{\partial}{\partial \beta}\Big(\frac{8J\sinh(8\beta J)}{\cosh(8\beta J)+3}\Big) \tag{16}$$

$$= \frac{1}{kT^2}\frac{64J^2(-\sinh^2(8\beta J)+\cosh^2(8\beta J)+3\cosh(8\beta J))}{(\cosh(8\beta J)+3)^2} \tag{17}$$

$$\tag{18}$$

Using Equation 6 to find the magnetization,

$$< M > = \frac{1}{Z}(4e^{8\beta J} + 8e^0 - 8e^0 - 4e^{8\beta J}) \tag{19}$$

Taking the absolute value,

$$< |M| > = \frac{1}{Z}(4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J}) \tag{20}$$

$$= \frac{4+2e^{8\beta J}}{\cosh(8\beta J)+3} \tag{21}$$

The susceptibility χ is given as

$$\chi = \frac{1}{kT}(< M^2 > - < M >^2) \tag{22}$$

$$= \frac{1}{kT}\Big(\frac{32}{Z}(e^{8\beta J}+1)\Big) \tag{23}$$

$$= \frac{8(e^{8\beta J}+1)}{kT(\cosh(8\beta J)+3)} \tag{24}$$

2.6 Phase transitions

In this project we will study the Ising model in two dimension and for two different temperatures. When the temperature increases, we will expect our results to include a critical point where a phase transition takes place. Such a transition is marked by sudden macroscopic change in the system [2]. In our project, the Ising model undergoes a phase transition of second order, which means that below a critical temperature T_c, the model exhibit a spontaneous magnetization. As the temperature moves towards T_c, we can express the quantities listed in Section 2.1 by a power law behaviour. Rewriting Equations 6, 7, 8,

$$< M(T) > \sim (T - T_c)^\beta \tag{25}$$

$$C_v(T) \sim |T_c - T|^\alpha \tag{26}$$

$$\chi(T) \sim |T_c - T|^\gamma \tag{27}$$

where

- the critical exponent, $\beta = 1/8$
- $\alpha = 0$
- $\gamma = 7/4$

We can also define the correlation length ξ which spans over the whole system in our case. The correlation close to T_c is given as

$$\xi(T) = |T_c - T|^{\upsilon}$$

In our two-dimensional Ising model, the lattice is finite and ξ will be proportional with the size of the lattice. Using finite size scaling relations, we can relate the behaviour at finite lattices with the results for an infinitely large lattice. Scaling gives

$$T_c(L) - T_c(L = \infty) = aL^{-1/\upsilon} \tag{28}$$
$$\rightarrow T = T_c \tag{29}$$
$$< M(T) > \propto L^{-\beta/\upsilon} \tag{30}$$
$$C_v(T) \propto L^{\alpha/\upsilon} \tag{31}$$
$$\chi(T) \propto L^{\gamma/\upsilon} \tag{32}$$

when $T \leq T_c$. a is a constant.

Investigating the thermodynamic limit $L \rightarrow \infty$ with $\upsilon = 1$ we can estimate the critical temperature T_c for lattices with different size. Using Equation 28 and two lattices with different size, L_1, L_2,

$$T_c(L_1) - T_c(L = \infty) = aL_1^{-1} \tag{33}$$
$$\rightarrow a = -L_1 \cdot T_c(L = \infty) + T_c(L_1) \cdot L_1 \tag{34}$$
$$T_c(L_2) - T_c(L = \infty) = aL_2^{-1} \tag{35}$$
$$\rightarrow a = -L_2 \cdot T_c(L = \infty) + T_c(L_2) \cdot L_1 \tag{36}$$
$$\rightarrow -L_1 \cdot T_c(L = \infty) + T_c(L_1) \cdot L_1 = -L_2 \cdot T_c(L = \infty) + T_c(L_2) \cdot L_1 \tag{37}$$
$$T(L = \infty) = \frac{T_c(L_2) \cdot L_2 - T_c(L_1) \cdot L_1}{L_1 - L_2} \tag{38}$$

We will use this relation later to compare our results to the exact solution by Onsager (1944).

2.7 Parallelization and CPU

From the description of how our algorithm should work, it is safe to assume that we will need to run a large number of MC-cycles. In order to do so, we have used the Numba library with the two functions njit, a compilation mode, and prange, which specifies that a loop can be parallelized [3]. This lowers the CPU time significantly.

3 Results

3.1 Ising model 2×2 lattice

Using the theory in section 2 and implement the algorithms in Python, we can compare our analytic results from section 2.5 with numerical results, using the Metropolis algorithm to generate a Markov chain. The numerical results are presented first in Table 1 followed by the analytic results.

Numerical results vs Analytic, L = 2				
Monte Carlo cycles	$< E >$	$< M >$	C_v	χ
100	-2.0000	1.0000	0.0000	0.0000
1000	-2.0000	1.0000	0.0000	0.0000
10000	-1.9968	0.9990	0.0256	3.8835
100000	-1.9956	0.9986	0.0348	3.9846
1000000	-1.9960	0.9987	0.0322	3.9915
10000000	-1.9961	0.9987	0.0314	3.9922
Analytic	-1.9960	0.9987	0.0321	3.9933

Table 1: Analytical results vs Numeric for $L = 2$

We can see that we need more than 10^7 cycles of Monte Carlo in order to obtain results which are almost identical to the fourth decimal. Increasing the number of Monte Carlo cycles to 10^8 will not improve our results - on the contrary it will for most quantities make them less accurate.

3.2 Ising model 20×20 lattice

After running our algorithm for a 2×2 lattice and made sure that the results are what we expect, we can now run the model for bigger square lattice. In this section we will look at the results from a 20×20 lattice.

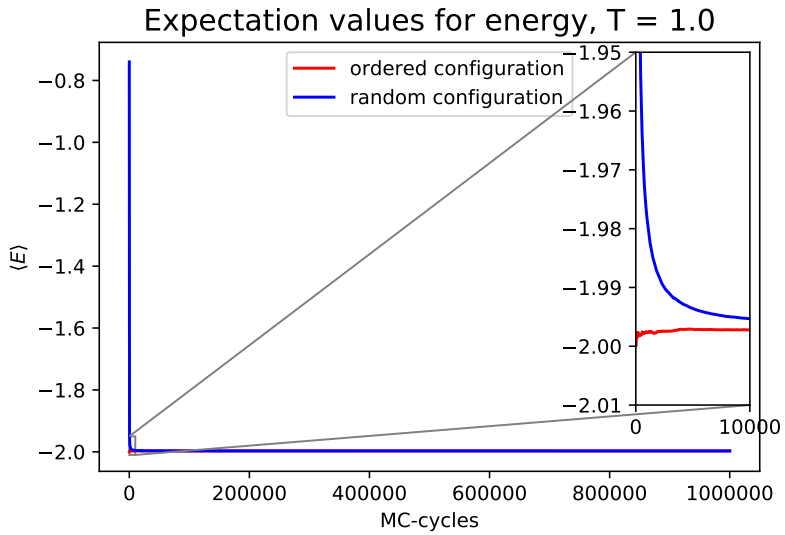

Figure 1: Expectation value for the energy as a function of Monte Carlo cycles (1e6 cycles), T = 1.0

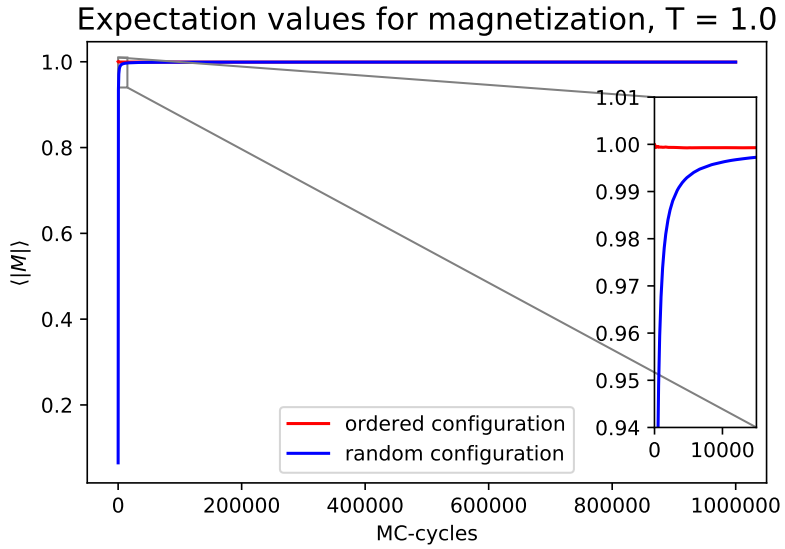

Figure 2: Expectation value for the magnetization as a function of Monte Carlo cycles (1e6 cycles), T = 1.0

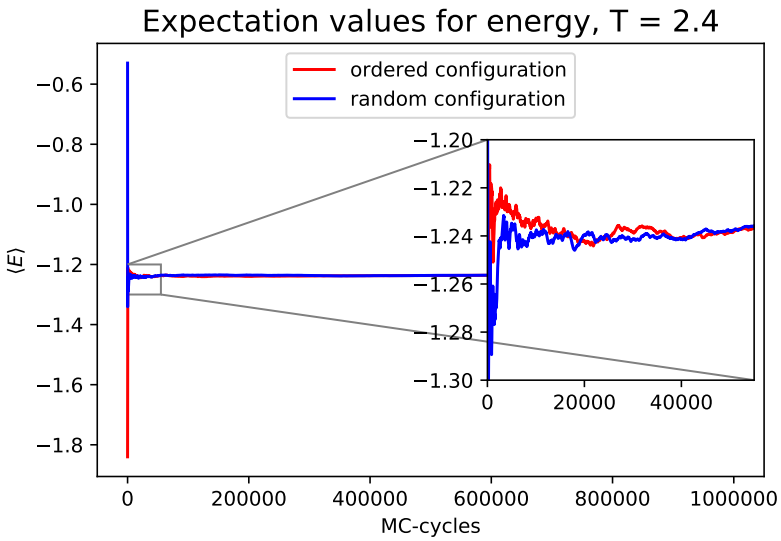

Figure 3: Expectation value for the energy as a function of Monte Carlo cycles (1e6), T = 2.4

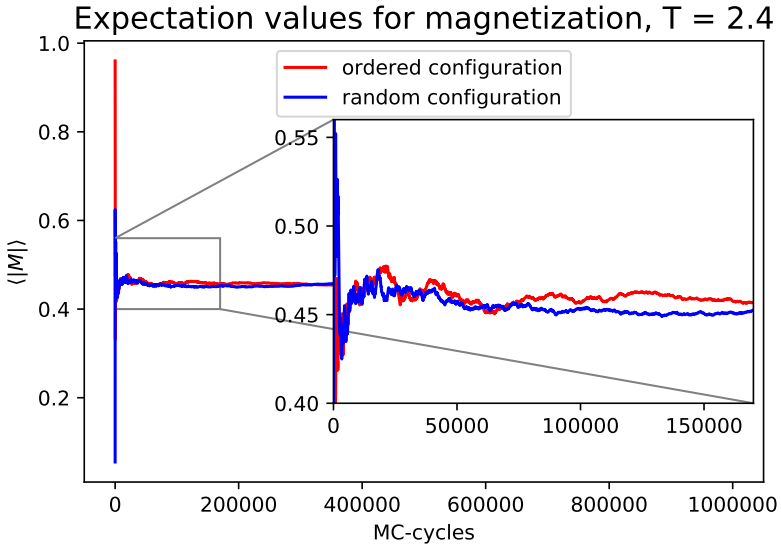

Figure 4: Expectation value for the magnetization as a function of Monte Carlo cycles (1e6), T = 2.4

In Figures 1 to 4, the mean energy and magnetization is displayed as a function of number of Monte Carlo cycles. Both the a random and the ordered (e.g all spins pointing in one direction) configurations are used. In Figure 1 we can see that the random configuration starts at a significant

higher energy value than the ordered configuration. After about $10,000$ MC-cycles it is clear that the random configuration stabilizes and both configuration reaches its most likely state. Similar results are obtained for the magnetization in Figure 2, with the random configuration starting at a much lower energy than the ordered before it stabilizes.

The temperature is set to $T = 2.4$ and the results are displayed in Figure 3 and Figure 4. Now both configurations need a number of cycles to reach the most likely state. It also uses an increased number of cycles - from our zoomed plot we can estimate it to be about $100,000$ cycles.

Analyzing this further, we plot the number of configurations accepted as a function of the temperature. This is presented in Figure 9 and Figure 10. The figures are displayed in Appendix A. At $T = 1.0$, the random spin configuration is clearly the preferred configuration, as it will always have a higher number of accepted states compared to the ordered configuration, not depending on the amount of MC cycles. When we plot the same relation for $T = 2.4$, we see that there is not a notable difference between the two configurations. Plotting the energy distribution for the random configuration with the two temperatures, it is clear that with $T = 1.0$, the variance in energy is relatively small and most configurations have energy $< E >= 2$. Also this changes for an increased temperature. Figure 12 shows a Gaussian distribution for the energy, with configurations having a more uniform distribution. The variance of energy increases as a result. The computed probability distribution is started after the steady state situation has been reach in order to avoid noise and misleading results, based on the results presented earlier in Section 3.2.

3.3 Phase transition with lattices of larger size

We will now study the same quantities as in Section 3.2 but we will increase the lattice size, computing for $L = 40, 60, 80, 100$, and compare our results.

In Figure 5, the expectation values of the energy for the different lattices are presented. We observe that the energies follows the same line up to $T = 2.25$, where the lines split up for a short period before they meet at $T = 2.35$. When plotting the magnetization with the same settings, we observe a similar trend - at $T = 2.26$ the magnetization for the various lattices starts to differ as $T \to 2.40$.

Two more interesting quantities to study are the heat capacity C_v and the susceptibility χ. Figure 7 shows a clear peak in C_v when $T = 2.26$, with $L = 100$ expecting the highest heat capacity, and a clear indication of a phase transition. The form on the plot of all lattices before and after the critical temperature is very uniform and consistent with Section 2.6.

Studying the susceptibility in Figure 8, this shows larger contrasts than the other plots. It is safe to assume that we see a phase transition where we have a peak in the susceptibility. Reading off T_c in Figure 8 we can make a table for the critical temperature, and the analytic values for the magnetization and susceptibility. This is seen in Table 2. Comparing the analytic values with Figure 6 and 8, the heat capacity is quite consistent whereas the susceptibility is close to two times the analytical values.
The temperature closes to the exact result (from Onsager) $T_c \approx 2.269$ is the $L = 100 \times 100$ lattice. These results are consistent with Section 2.6 and applying Equation 38, we can see that our results for the critical temperature is close Onsager's exact solution.

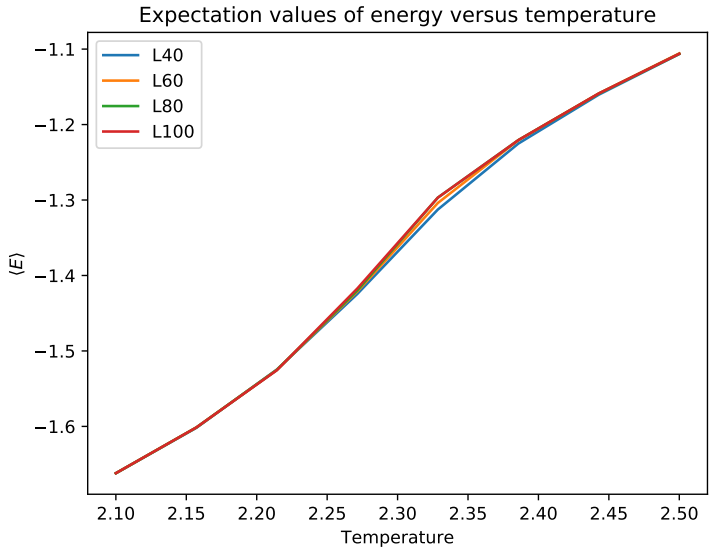

Figure 5: Expectation values of energy as a function of T, with varying lattice size

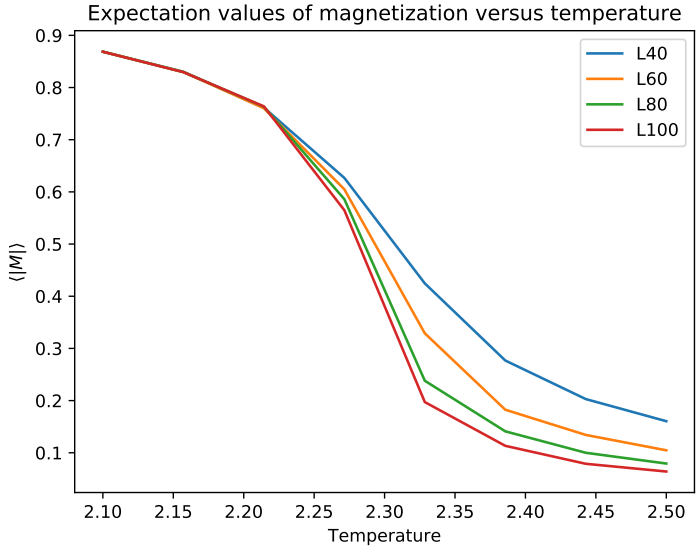

Figure 6: Expectation value of magnetization as a function of T, with varying lattice size

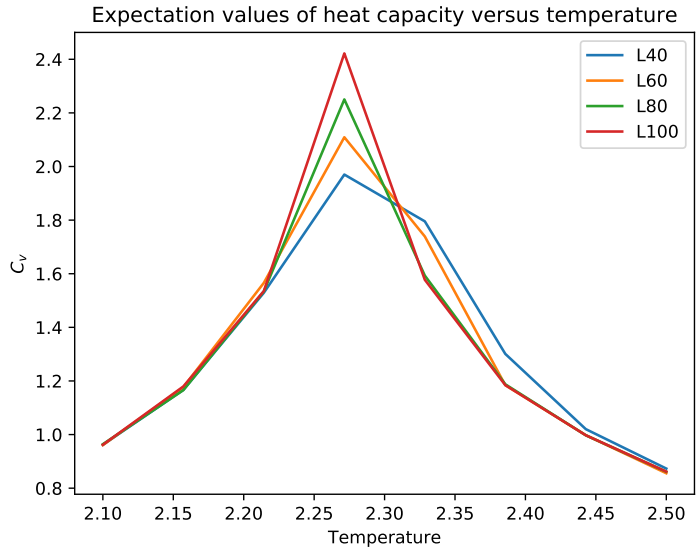

Figure 7: Spesific heat C_v a function of T, with varying lattice size

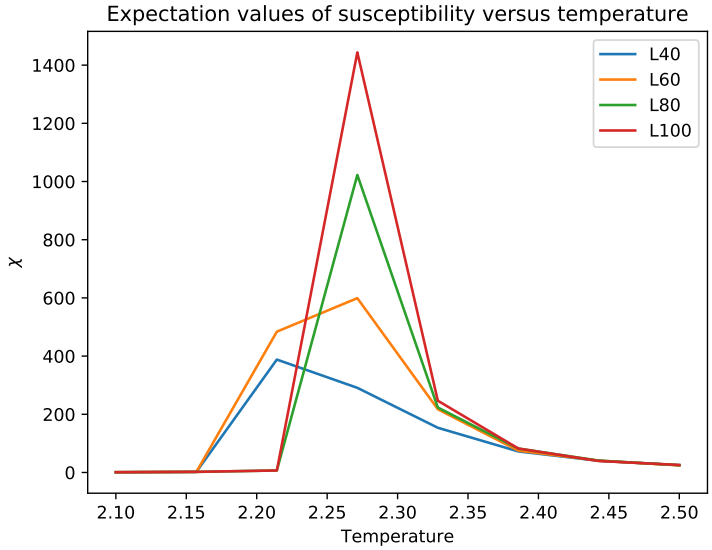

Figure 8: Susceptibility as a function of T, with varying lattice size

4 Discussion

In the results from Section 3.1 we can clearly see that our numerical results for a 2×2 lattices gets closer to the analytic results as the number of Monte Carlo cycles increases but even with the

Critical temperatures for various L				
L	40	60	80	100
T_c	2.21	2.26	2.27	2.27
$< M(T) >$	0.631	0.599	0.578	0.562
χ (T)	636.217	1293.495	2139.969	3162.278

Table 2: Critical temperature from Figure 8

number of MC- cycles = 10^8 we still do not get an exact result. However, we obtain a satisfying result for 10^7 number of Monte Carlo methods.

In Section 3.2, we can draw a conclusion from the results that the random configuration needs a higher number of Monte Carlo cycles to stabilize and reach the most likely state when the temperature is low, $T = 1.0$. The ordered configuration is expected to not oscillate as much as the random because it will start in the lowest energy state possible and will from there stabilize. This is also consistent with our results. When the temperature increases to $T = 2.4$, both configurations needs about $100,000$ MC-cycles to reach equilibrium, which is now close to -1.24.

These results are applied when plotting the the number of configurations accepted as a function of temperature. We now know we should omit about 1.0% of the 10^6 MC-cycles for lower temperatures, and about 10% for the higher ones in order to only include configurations in equilibrium. We get a higher number of accepted states for the random configuration than the ordered when the temperature is low. When the temperature increases, both cycles produces similar results, as expected when looking at Figure 3. The histograms plotting the energy distribution reflects the fact that for higher temperatures we access more energy states and we see a clear Boltzmann distribution. The variance from the linear fit and the data are comparable, and the small difference can be explained by the fact that as the temperature becomes higher than T_c, the system is likely to be in disorder and the energies are expected to be spread the equilibrium point [2].

We have looked at how we should see a phase transition in our result and how good our results are compared to Onsager's exact result for the critical temperature, T_c. From Figure 8 and Figure 7 we can clearly see a phase transition, with an abrupt change in both the susceptibility and the heat capacity. Comparing our T_c from Table 2, we see that with a lattice size $L = 100$ we are very close to Onsagers $T_c \approx 2.269$.
In Figure 6 we can see that the magnetization starts to diverge as the temperature increases. This can be explained by the fact that the system becomes more chaotic.
Our result for the specific heat (Figure 7 have the same shape as [1] which also uses the two dimensional Ising model.
We compare the analytic values of the magnetization and susceptibility to values from the figures, and find that they match quite well with the magnetization but not at all with the susceptibility. This is something we should look into further.

5 Conclusion

For a small lattice, $L = 2$, we achieve a good agreement between our implemented Ising model and the analytic results when the number of MC- cycles are 10^7.

For a larger lattice, $L = 20$, we need close to $10,000$ MC-cycles before the random spin configuration reaches equilibrium for $< E >$ and $< M >$ when the temperature is $T = 1$. The ordered configuration does not. When $T = 2.4$, we need close to $100,000$ for both configurations. The variance in energy distribution is larger when the temperature is high, whereas the energies takes more or less the same value when the temperature is low.

We see a clear indication of a phase transition when $T \to 2.7$. Our results are therefor a good approximation to Onsager's exact result for the critical temperature.

For further work, we would have to investigate Figure 8 and see if we have made a mistake or if our algorithm is not working. What would be interesting is to use what we have learned in this project and apply it for our field of study, geophysics.

6 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`

The Python 3.6 scripts and figures can be found at:
`https://github.com/marikoll/FYS4150_projects/tree/master/project_4/python_code` *Note: The codes have been developed in cooperation with Marit Kollstuen and Stine Sagen*

References

[1] Markus Deserno. Microcanonical and canonical two-dimensional ising model: An example. *Department of Chemistry and Biochemistry UCLA, USA*, 2004.

[2] Morten Hjorth-Jensen. *Computational Physics*. Department of Physics, University of Oslo, 2015.

[3] Wikipedia. Numba — accelerate python functions. `http://numba.pydata.org/`, [Online; accessed 18-November-2018].

A Appendix: Figures for 20×20 lattice

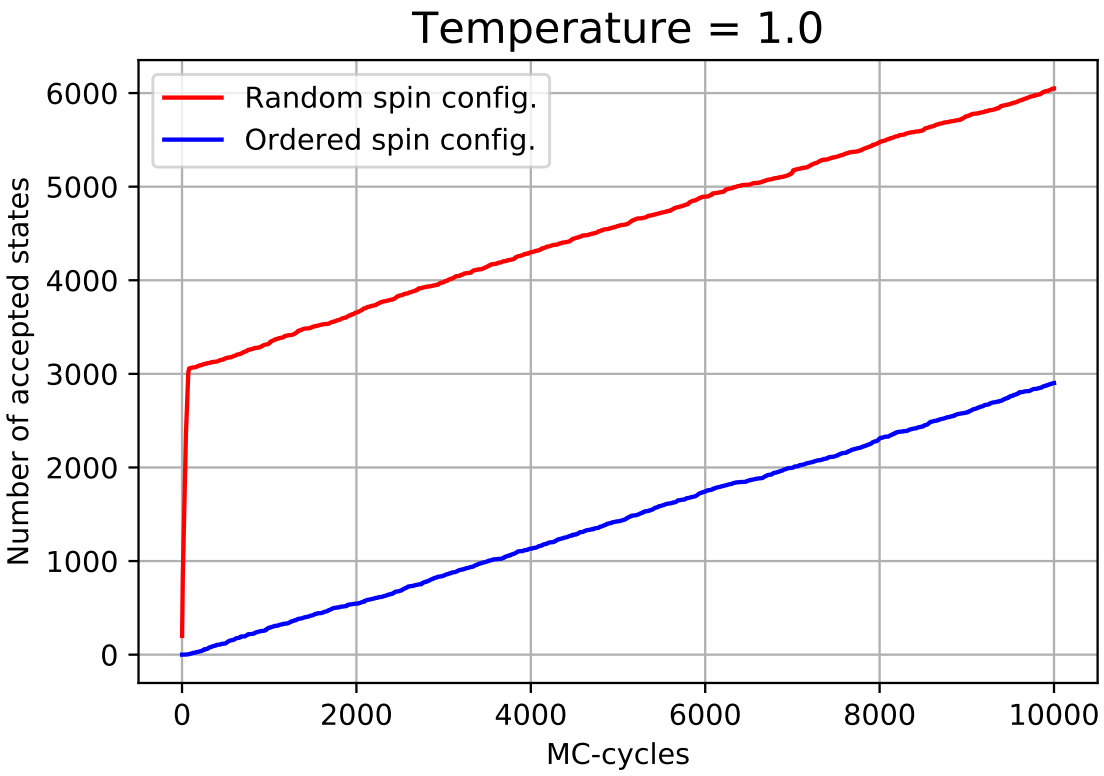

Figure 9: Number of accepted states as a function of temperature, T = 1.0, MC-cyles = $1e4$

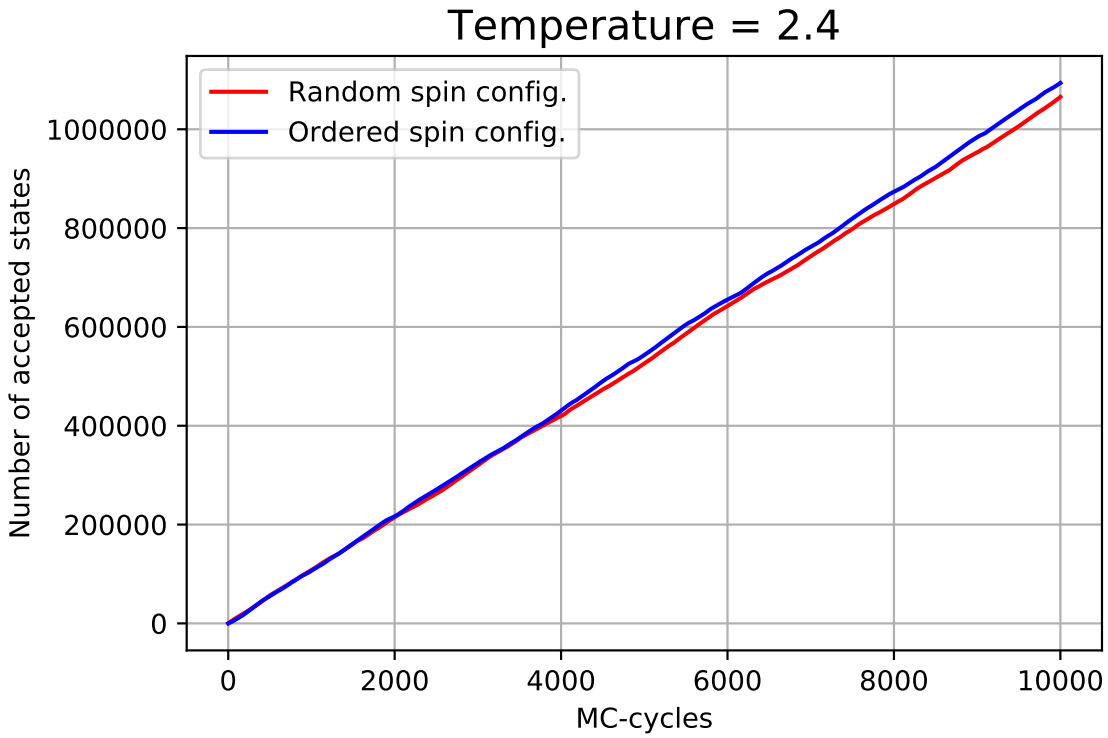

Figure 10: Number of accepted states as a function of temperature, T = 2.4, MC-cycles = $1e4$

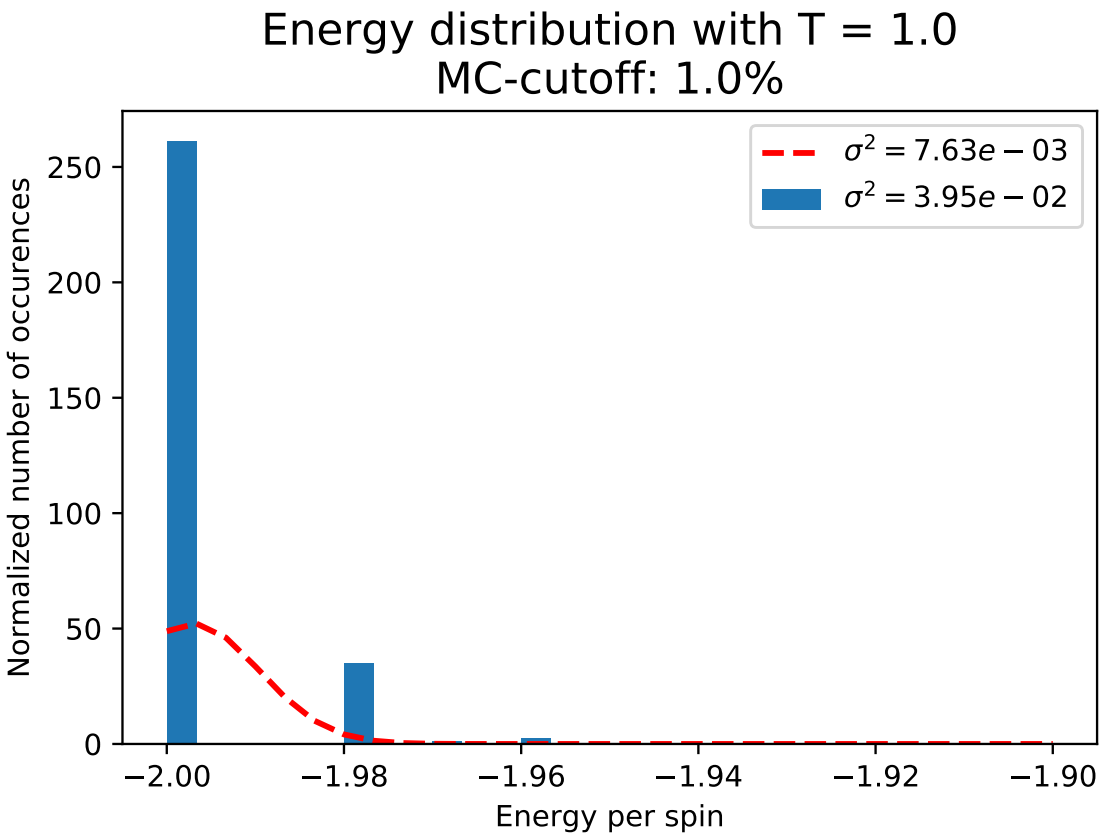

Figure 11: Energy distribution at T = 1.0

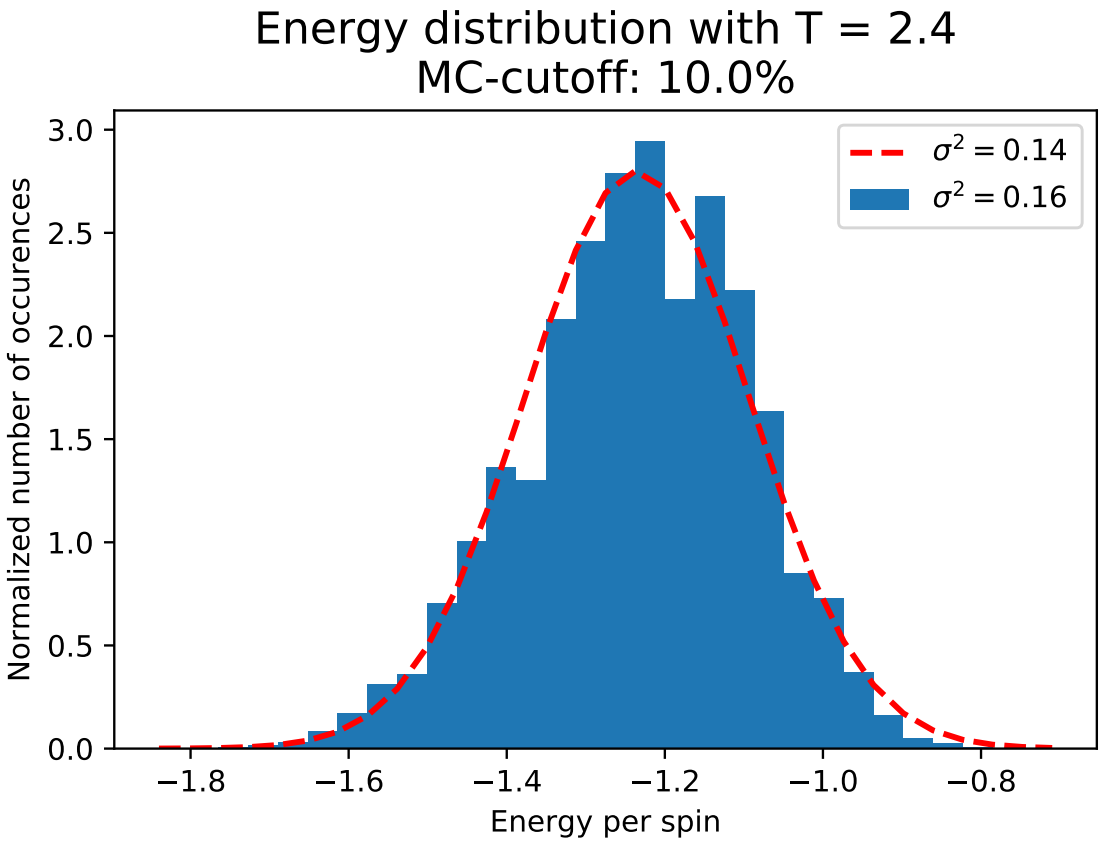

Figure 12: Energy distribution at T = 2.4