The Ising model and phase transitions in magnetic systems

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Abstract

In this report, Metropolis' algorithm is used for solving the two dimensional Ising model. By storing the energy and magnetization of the accepted states, thermodynamic quantities like the mean energy $\langle E \rangle$, mean absolute magnetisation $\langle |M| \rangle$, specific heat C_V and susceptibility χ is calculated for different temperatures T and lattice sizes $L \times L$. By looking at the lattice size $L = 20$ for temperatures $T = 1$ and $T = 2.4$ with an unordered and ordered initial configuration of the lattice, I find that an ordered initial configuration gives a much shorter thermalisation time for the lower temperature. For the higher temperature, there seems to be no big difference in thermalisation time for the two starting configuration, with an thermalisation time of about 10^4 Monte Carlo sweeps (mcs). I also find that for higher temperatures, new states are accepted more often, and there are more possible energy states. Examining the peak in C_V as a function of T, and comparing different lattice sizes, I get an estimate of the critical temperature T_C of 2.259 ± 0.015 for a low temperature resolution run, and 2.363 ± 0.007 for a high temperature resolution run, both within one standard deviation of the analytical value.

1 Introduction

One of the pillars of modern physics is statistical mechanics. It is crucial when studying a system with a large number of degrees of freedom, and can be used to understand the thermodynamic behaviour of a large system. By studying fluctuations around a value, one can connect microscopic states to macroscopic observations. Since an analytical solution involves all possible states of a system, in general, only small systems allow an analytical solution. However, numerical methods makes it possible to solve larger and more complex systems. Such a method is the Monte Carlo method, where random samples are used to determine the results. One of the most popular algorithms in the Monte Carlo family is the Metropolis' algorithm.

Starting with the methods section, I will shortly introduce how some thermodynamic properties are calculated, before describing the Ising model and phase transitions in this model. I will then introduce the Metropolis' algorithm for solving the Ising model. Before the result section, a method for finding the probability distribution $p(E)$ and the implementation of the algorithm is described. In the results section, properties of the model are precented, before a time evolution of different thermodynamic properties are shown for a variety of lattice sizes, together with an estimate of the critical temperature in the thermodynamic limit of a infinite sized lattice. Finally, the results are discussed.

2 Methods

2.1 Thermodynamic properties

In this report I will study different thermodynamic properties of a Canonical Ensemble in

the form of a spin lattice. The probability distribution in such a system is given by the Boltzmann distribution,

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}, \tag{1}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, and E_i is the energy in a given microstate. Z is the partition function given by

$$Z = \sum_i e^{-\beta E_i}. \tag{2}$$

The expectation value of a given variable A is given by

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{N} D_i A_i e^{-\beta E_i} \tag{3}$$

where A_i is the value of the variable in question for the state i. Equation (3) gives a method for finding the expectation value of the energy E and mean magnetization $|M|$. Further, the specific heat at a constant volume C_V can be expressed as

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}, \tag{4}$$

while the susceptibility χ is given by

$$\chi = \frac{\langle |M|^2 \rangle - \langle |M| \rangle^2}{k_B T}. \tag{5}$$

For a derivation of these expressions, see for example [3].

2.2 The Ising model

The Ising model consists of variables s that can exist in two states, typically +1 or -1. These variables represent magnetic dipole moments of atomic spin, and are ordered in a two dimensional lattice consisting of $L \times L$ spins. Given that there is no external magnetic field, the energy of the system is modelled as

$$E = -J \sum_{\langle ij \rangle} s_i s_j, \tag{6}$$

where J is a coupling constant expressing the strength of the interaction between neighbouring spins. The symbol $\langle ij \rangle$ means that the sum is over neighbouring spins. The magnetisation of the system is simply the sum of all the spins

$$M = \sum_i s_i. \tag{7}$$

For smaller systems, it is possibly to calculate the expectation values analytically by finding and counting all the possible states. The different states for a 2×2 lattice are listed in Table 1, and will be used together with equation (3) and (1) to test if the algorithm produces the expectation values.

# spins up	D	E	M
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: The different states for a 2×2 lattice. For each possibility of number of spins up, the degeneracy (D), energy (E) and magnetisation (M) is listed.

In the Ising model you can have both open and periodic boundary conditions. In this report, periodic boundaries are used. This can be visualized as the lattice being wrapped around itself so that all ends meet, i.e. if you move to the end of a row/column, you go back to the beginning of that row/column.

Two different initial configurations will be presented in this report. One is an ordered configuration, which means that all spins point

in the same direction. In an unordered configuration, each spin has a random direction.

2.2.1 Phase transitions and critical temperature in the Ising model

A phase transition is an often discontinuous change in properties of a system as a result of changing external conditions, for example a change in temperature. The two dimensional Ising model exhibits a phase transition at a critical themperature T_C. For temperatures below T_C, the mean magnetisation is different from zero, while above T_C we have $\langle M \rangle = 0$. This phenomena occurs because of the two competing principles of maximizing entropy and minimizing energy. In the thermodynamic limit of an infinite large lattice, the specific heat C_V and susceptibility χ is discontinuous at T_c. In the case of a finite lattice we will not observe that these quantities diverge. We will however observe a maxima in C_V. The critical temperature of an infinite and finite lattice is connected by the following relation

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{8}$$

where a is a constant, and ν is connected to the correlation length. See [1] for a more detailed description. By setting $\nu = 1$, you can obtain the following expression for T_C in the thermodynamic limit of $L \to \infty$:

$$T_C(L = \infty) = \frac{T_C(L_i)L_i - T_C(L_j)L_j}{L_i - L_j}. \tag{9}$$

$T_C(L_i)$ and $T_C(L_j)$ can be found by finding the temperature when C_V reaches its maximum value in the solution for the Ising model with lattice size L_i and L_j. For $\nu = 1$, the exact solution is given by $kTC/J = 2/\ln\left(1 + \sqrt{2}\right) \approx 2.269$ [2].

2.2.2 Metropolis' algorithm

One possibly way of solving the Ising model is by using the so called Metropolis' algorithm. The key concept in this algorithm is to generates steps in a Marcov chain, with a method for rejecting new steps. The Markov chain will eventually reach the most likely state. Algorithm 1 shows Metropolis' algorithm adapted for Ising's model, and is based on the algorithm found in [1]. For each spin in the lattice, a random spin is flipped. The energy difference is then computed, and the transition probability w is computed as

$$w = e^{-\beta \Delta E}. \tag{10}$$

In order to determine if the new state is accepted, the transition probability is compared with a number r given by a random number generator (RNG) with an uniform probability distribution. If $w \geq r$, the new state is accepted. The new state is also accepted if the new state has a lower energy. Each sweep over the lattice is called a Monte Carlo cycle or Monte Carlo sweep (mcs). After a given number of mcs, the expectation values of the system will have reached equilibrium and the most likely configuration is reached. There can still be variations in E an $|M|$, but they will fluctuate around a given value. This is called the thermalisation time, where mcs is used as an unit of time. In order to get good estimates for the expectation values, the sampling should start after the thermalization time is reached.

2.2.3 Probability distribution of the energies

One of the properties of the Ising model addressed in this report is the probability distribution of the energy states $p(E)$. In order to determine the distribution, the number of times each energy appears after the termalization time is counted, and then divided by the total number of samples. This is done for temperatures 1.0 and 2.4. The resulting probability distribution is then compared with the

```
Initzialise a state with energy E;
for i = 1, ..., mcs do
    foreach s do
        Flipp random spin;
        Calculate ΔE;
        if ΔE ≤ 0 then
            Accept new state;
        else
            Calculate transition probability
             w;
            Generate random number
             r ∈ [0, 1];
            if r ≤ w then
                Accept new state;
            else
                Keep old state;
    Update expectation values;
Calculate mean expectation values;
```

Algorithm 1: Metropolis' algorithm for solving the Ising model.

variance of the energy, given as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 . \tag{11}$$

2.3 Implementation

Algorithm 1 can be calculation-heavy when using a large number of Monte Carlo cycles. In order to get a more efficient code, the calculations are parallelised. This is done using MPI. Each CPU is assigned only a fraction of the total number of mcs, and then all the expectation values are collected and the mean is calculated.

All programs are written in C++, using python3.6 together with Numpy, Matplotlib and Seaborn to produce figures and tables. The code can be found in the GitHub repository of alpsjur[1].

[1] https://github.com/alpsjur/FYS3150prosjekt4

3 Results

Figure 1 shows the expectation values for the energy and absolute magnetisation as a function of mcs with both an ordered and unordered initial configuration. Results for a low temperature 1.0 (in units of k_BT/J) and a higher temperature 2.4, which is above the critical temperature, are shown. One can see that the expectation values stabilises almost immediately when an ordered starting configuration is chosen for the lower temperature. But when an unordered configuration is chosen, the values does not stabilise until about 25000 mcs. As for the higher temperature, both an ordered and unordered initial configuration gives a result that stabilises quite fast around a value, with some fluctuations. This happens after about 5000 mcs for the energy, and after about 10000 mcs for the magnetisation.

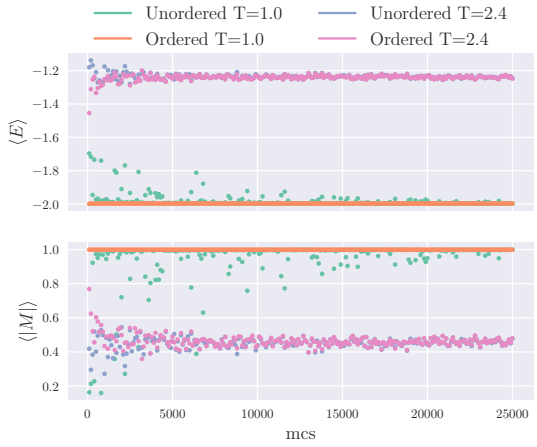

Figure 1: Plot over expectation values for energy E per spin and absolute magnetisation $|M|$ per spin as a functions of Monte Carlo sweeps mcs. The expectation values are plotted for $T = 1.0$ and $T = 2.4$ with both an ordered and unordered initial state. Lattice size $L = 20$, and a step size of 100 was used.

In Figure 2, the number of accepted configurations as a function of Monte Carlo cycles

is shown. Again this is plotted for temperatures 1.0 and 2.4, with both an unordered and ordered initial configuration.

In the case of an ordered initial configuration for the lower temperature, the graph is linear in the logarithmic space, with a slope of about 1. Looking at the graphs for the higher temperature, the same trend can be seen, with the graphs shifted upward a distance of about 3 in log space compared to the lower temperature. For few mcs, one can see that the higher temperature graph with an unordered initial configuration lays slightly over the graph for the ordered initial configuration.

The graph for the lower temperature with an unordered starting configuration starts of with about 10^3 accepted new configurations for 10 mcs, well above the ordered case. From about 10^4 mcs and out, the two graphs follow each other.

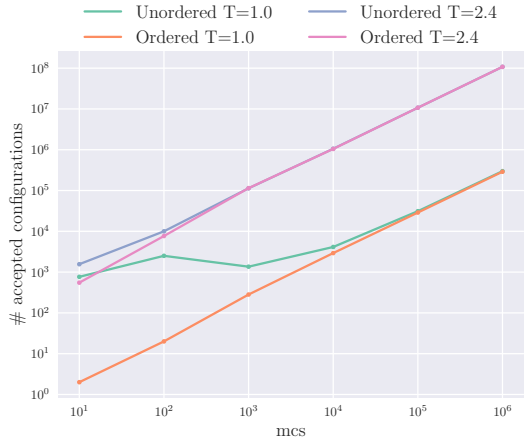

Figure 2: Plot over the accumulated number of accepted configurations as a function of Monte Carlo sweeps mcs. The number of accepted configurations are plotted for $T = 1.0$ and $T = 2.4$ with both an ordered and unordered initial state. Lattice size $L = 20$ was used. The scale is logarithmic, with an step size of 10 in log space.

The probability distribution of E per spin is shown in Figure 3. For the temperature 1.0 the possible states are all close to -2.0, with two states highly more probable than the others. For the temperature 2.4, the distribution is closer to a gamma distribution, with the most probable states around -1.2. The expectation value and variance of E for the same temperatures are shown in Table 2.

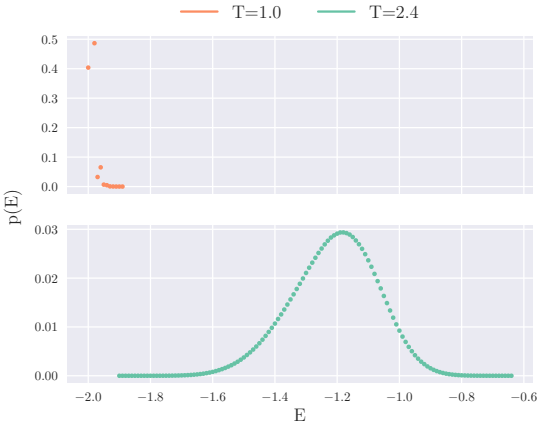

Figure 3: Plot over probabilities for a given energy E per spin. The top plot is for temperature $T = 1.0$ while the bottom plot is for temperature $T = 2.4$. 10^6 mcs were used. Lattice size $L = 20$ was used.

T	$\langle E \rangle$	σ^2
1.0	-1.997	0.025
2.4	-1.237	8.116

Table 2: The expectation values $\langle E \rangle$ and variances σ^2 of the energy per spin after 10^6 mcs for temperatures $T = 1.0$ and $T = 2.4$. Lattice size $L = 20$ was used.

Table 3 shows a timing analysis for some selected runs of the parallelised code. One can see that the running time with two nodes is about half of the running time with only one node.

Figure 4 and 6 shows the expectation values for the energy and the absolute magnetisa-

L	T_1	T_2	T_1/T_2
40	25.957	13.391	1.938
60	58.681	30.853	1.902
80	104.561	58.587	1.951
100	163.892	84.191	1.947

Table 3: The CPU-time used for computing one temperature step with 10^5 mcs with one node (T_1) and two nodes (T_2). The ratio of the two is also listed.

tion from $T = 2.0$ to $T = 2.3$, while Figure 5 and 7 shows the specific heat and susceptibility for the same temperature interval. In all these plots results for lattices with size $L = 40, 60, 80$ and 100 are shown.

In the energy plot, all expectation values are negative, and increases as temperature increase. For temperatures under 2.25, all the lattices gives the same results, but for higher temperatures, the values slightly diverge from each other.

A similar trend is found in the plot of the absolute magnetisation. The values for the different lattices are very similar until a temperature of about 2.20, and then diverge. Comparing the energy and magnetisation plots, the magnetisation values diverge more strongly from each other. All the magnetisation values are positive, and decrease as the temperature increases.

The plots over the specific heat and the susceptibility does also feature a divergent trend in the temperature interval 2.20 to 2.30. In addition, the plots are less smooth in this interval. The specific heat values increase with temperature until they reach a maxima between 2.25 and 2.30. The maximum values are slightly shifted towards lower temperatures, and becomes larger, as L increase. In the susceptibility plot, only the results for the lattice size $L = 100$ has a maxima in this interval. Also here the maximum values increase as the lattice size increases.

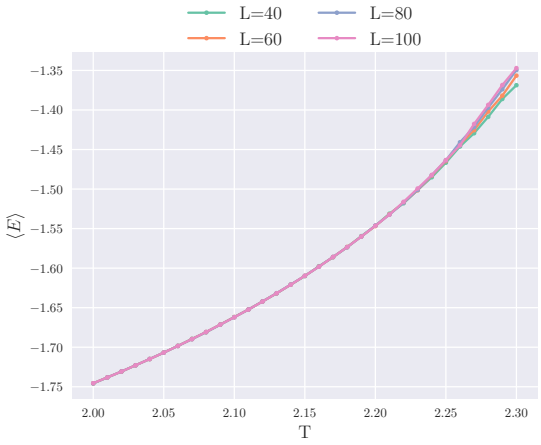

Figure 4: Plot over the expectation values for the energy per spin $\langle E \rangle$ as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 mcs were used for each step.

Figure 8 shows results for the specific heat in the temperature interval 2.26 to 2.30 with a higher resolution than Figure 5. In addition, a running mean is shown.

Table 4 lists the calculated values for the critical temperature T_C in the thermodynamic limit $L \to \infty$ using the data shown in Figure 5 and 8. One can see that all means are within one standard deviation from the analytical value. The higher resolution data set (Figure 8) gives a mean value closer to the analytical value. There mean value of the results using a running mean is the same as when no running mean is applied.

4 Discussion

When a model is used in order to understand behaviour of a system, or for predicting certain quantities, it is important to understand how the model responds to different initial conditions, and how computations and parameters

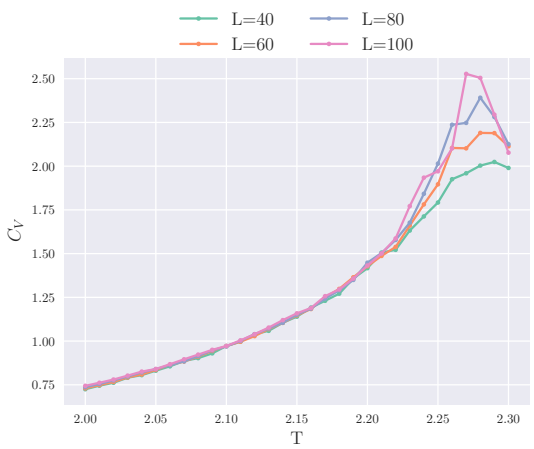

Figure 5: Plot over the expectation valuess for the specific heat per spin C_V as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 mcs were used for each step.

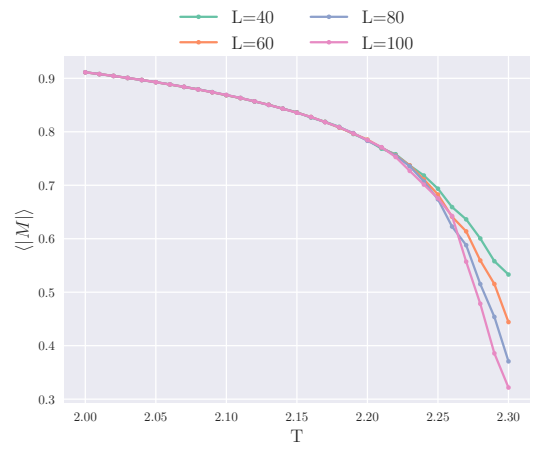

Figure 6: Plot over the expectation value for the absolute magnetisation per spin $\langle |M| \rangle$ as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 mcs were used for each step.

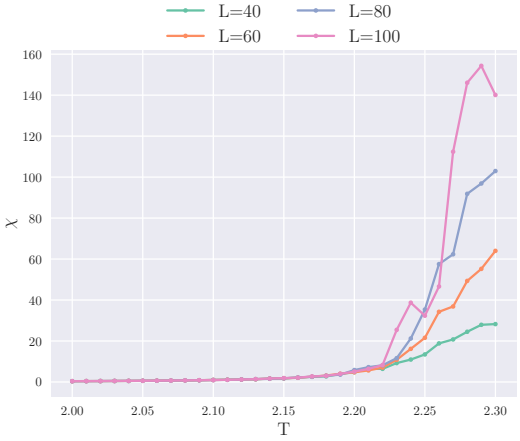

Figure 7: Plot over the expectation values for the susceptibility per spin χ as a function of temperature T with step size 10^{-3}.The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 mcs were used for each step.

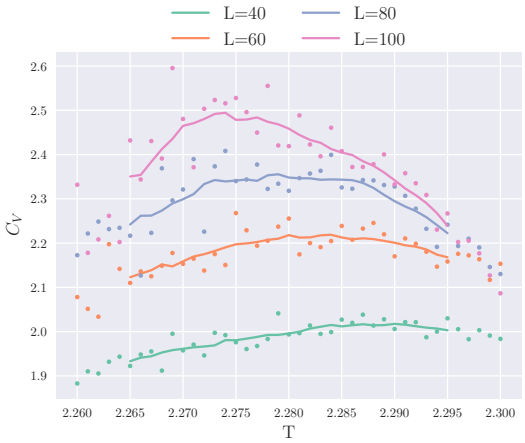

Figure 8: Plot over the expectation values for the specific heat per spin C_V as a function of temperature T with step size 10^{-4}.The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 mcs were used for each step. The dots are the collected data, while the solid line is a running mean with a window size of 11.

L_i	L_j	LR	HR	HRRM
60	40	2.260	2.267	2.272
80	40	2.270	2.269	2.268
80	60	2.280	2.271	2.264
100	40	2.257	2.262	2.263
100	60	2.255	2.260	2.259
100	80	2.230	2.249	2.254
Mean		2.259	2.263	2.263
STD		0.015	0.007	0.006

Table 4: Critical temperature in the thermodynamic limit $L \to \infty$ calculated using eq. 9 for different lattice sizes L. Results using low resolution values (LR) plotted in Figure 5, high resolution values (HR) and the running mean of the high resolution values (HRRM) plotted in Figure 8 are shown. In addition, the mean value and standard deviation (STD) for each set of values are shown.

are connected. Considering Figure 1, one can see a clear difference in the thermalisation time for $T = 1.0$, depending on whether an ordered or unordered initial configuration is used. An ordered configuration, with all spins pointing in the same direction, has a lower energy than an unordered configuration. The expectation value for a system with a low temperature, and then also low energy, will therefore be closer to a system with an ordered configuration.

As for the higher temperature $T = 2.4$, the difference in thermalisation time for an ordered and unordered initial configuration is not that apparent when looking at Figure 1. It is however clear that the expectation values fluctuates more for higher temperatures, than for the lower temperature with an ordered initial configuration. This can be connected with the probability distribution in Figure 3 and the variance in Table 2. Also, the thermalisation time for the absolute magnetisation appears to be longer than for the energy, both for the higher temperature, and for the lower temperature with an unordered initial configuration.

Based on these observations, an ordered initial state appears to be best suited for lower temperatures, while for higher temperatures both unordered and ordered initial configurations appears to give an equally good convergence rate.

Looking at Figure 2, one can see that there are in general more accepted new configuration for higher temperatures. Additionally, the number of accepted new states increases as $\sim$ mcs. An exception to this behaviour is the graph for $T = 1.0$ with an unordered initial configuration, as the number of accepted configurations for few mcs is about the same as for the higher temperatures. This can be seen in relation to the long thermalisation time for this case.

As mentioned, there is a connection between the fluctuations in Figure 1, the probability distribution in Figure 3 and the variance in Table 2. For higher temperatures, there is more and larger fluctuations in expectation values, and therefore more possible energy states, as seen in Figure 3. More possible energy states and a bigger spread in energy leads to a larger variance in the expectation values for higher temperatures. Comparing Figure 3 and Table 2, one can also see that the expectation value for the energy is close to the maxima for the probability distribution.

Finally, let's look at how well the model preforms in predicting the critical temperature in the thermodynamic limit $L \to \infty$. From Table 4, one can see that both the low resolution and high resolution run gives a critical temperature within one standard deviation from the analytical value, and that the higher resolution gives a better approximation than the lower resolution. Further, taking the running mean does not improve the result of the higher resolution run.

References

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