FYS3150 - Project 4

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Disclaimer In this project I worked together with Gunnar Lange. Due to the fact that he has had thermodynamics, while I haven't, makes the theory part concerning this topic very much like his. While we wrote the rest of the project together, this part especially was written under direct guidance from Gunnar (but is written and understood by me).

Abstract

In this article we are going to investigate the Ising model, and its application to phase transitions. We are going use the Metropolis algorithm to simulate grids of spin up to 140 for temperatures around $2 - 3$ Kelvin, and use the results to find the critical temperature for phase transition. We are also going to look at the time it take such systems to reach the equilibrium state of lowest energy. All scripts and data can be found in our GIT-page[1].

Contents

[1] https://github.com/dulte/Comp-Phys/tree/master/Project4Final

1 Introduction

The Ising model is a simple but very popular model for modeling every thing from materials [6] to bird song [1]. In our case we are going to look at a lattice of atomic spins, where the only possible values are *up* or *down*. This is a very popular method is statistical physics, in particular to study ferromagnetic phenomena.

We will use the Metropolis algorithm to look at how some interesting thermodynamic quantities, including heat capacity, magnetic susceptibility, mean magnetization and mean energy, behave over time in the Ising model. And how they behave near the phase transition. For smaller systems we are able to compare this with analytical expressions. For larger systems we are interested in looking at the critical temperature where the phase transition happen. We will also use analytical expressions for this.

We will also see how the equilibrium state is reached using ordered and disordered start configurations, and much time this takes. We will do this at different temperatures to see how this affect the time.

2 Theoretical model

2.1 The Ising model

We want to look at a lattice of spins. The spins can either be up or down(± 1). This is the Ising model, a microcanonical system. What we are interested in studying is how energy, magnetization, heat capacity and magnetic susceptibility develop in this system with temperature.

We are going to look at quite an easy system. For this kind of system, the Ising model is given as

$$E = -J \sum_{\langle kl \rangle} s_k s_l \tag{1}$$

E is the energy of the system. The sum is over the nearest neighbors. This is a simplification of "reality", quantum mechanics makes this expression more complicated, but in this classical version all the quantum mechanical details are backed into the constant J. We will use $J = 1$ for all our investigations.

The other quantity we are interested is the magnetization, which is given as:

$$\mathcal{M} = \sum_i s_i \tag{2}$$

and is simply a sum over all the spins.

These quantities can be used to compute the quantities that we are really interested in [5]. The first is the heat capacity, C_v:

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2} \tag{3}$$

The second is magnetic susceptibility:

$$\chi = \frac{\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2}{kT} \tag{4}$$

k will be set to 1 in this article.

2.2 Thermodynamic quantities

For building more understanding of the Ising model, we can use Boltzmann statistics. The distribution for such a system is given by:

$$P(E) = \frac{1}{Z} e^{-\frac{E}{kT}} \tag{5}$$

Where E is the energy of a microstate. T is the temperature in kelvin, and k is Boltzmann's constant. To make the notation easies, we're going to define $\beta = 1/(T)$. Since we are dealing with a probability distribution, we have to make sure the function is normalized, by summing over all the possible microstates. This is what the partition function Z is:

$$Z = \sum_i e^{-\beta E_i} \tag{6}$$

When calculating the heat capacity and magnetic susceptibility we need to calculate the moments – the mean is the first moment – of E and $\mathcal{M}$. The moment of some quantity X^n is given by:

$$\langle X^n \rangle = \frac{1}{Z} \sum_i X_i^n e^{-\beta E_i} \tag{7}$$

Where X_i the quantity at microstate i.

2.3 Phase transitions in the Ising model

There exists a so called critical temperature T_c at which phase transitions occur in the Ising model [2]. The T_c heat capacity and magnetic susceptibility will converge. Near the critical temperature, the quantities can be modelled as [4]

$$\begin{aligned} \langle \mathcal{M}(T) \rangle &\sim (T - T_C)^\beta \\ C_V(T) &\sim |T_c - T|^{-\gamma} \\ \mathcal{X}(T) &\sim |T_C - T|^{-\alpha} \end{aligned} \tag{8}$$

Where α, β and γ are critical exponents, given by: $\alpha = 0,\ \beta = 1/8,\ \gamma = 7/4$

Find the value we want the T_c we need to simulate a lattice size close to infinity. This is numerically impossible. But we can estimate , we have to use a using that [3]

$$T_C(N) - T_C(N = \infty) = aN^{-1/\nu} \tag{9}$$

$\nu = 1$. This means that we can use critical temperature of two finite lattices, an calculate the constant a. This constant is given by:

$$a = \frac{T_C(N_1) - T_C(N_2)}{N_1^{-1/\nu} - N_2^{-1/\nu}} \tag{10}$$

.

2.4 Starting State, State between Temperatures and the Equilibrium of the system

There are two main ways of configuring the the start lattice. The easiest is just to have all the spins start in the same direction. The other way is to start the spins with some random distribution. We want the system to reach the an equilibriums state, this is where the energy of the system is at its minimum. The sign that this state is reached is that all the thermodynamical quantities has an equilibrium, where, due to the now low acceptance of flips, they varies little. If we look at how these quantities evolve, we are capable of determining when the system is in equilibrium.

We want to wait until this state is reached before we begin to sample data. But which starting configuration is the fastest to give us this state. This is a difficult question. Low temperature has an equilibrium were all(or most) spins point in one direction. In this case the homogeneous start should be the best. For higher temperature, the question is more complicated, but the random start may often be faster.

If we are looking at a series of temperatures, we can consider how to make the start state for the next temperature in the series. One way is to use the same methods as above, but one smart way of doing it is to use the last state of the previous temperature. The equilibrium states of two adjacent temperatures should have similar equilibrium states, and since the last state of the previous temperature was in equilibrium, we should expect it to be close to equilibrium state of this temperature. It may therefor be smart of choosing this state as a start state.

2.5 Analytic solution for the 2x2 case with periodic boundary conditions

We will now derive an analytic solution for a simple system, which only contains 4 spins, organized in a square, and labelled as shown in figure 1 below: We begin with investigating the magnetiza-

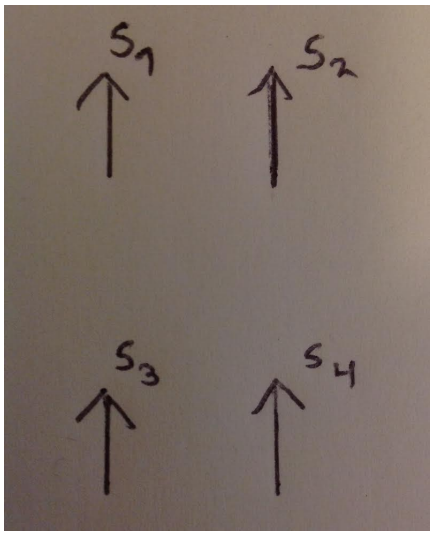


Figure 1: Labelling of our 2×2 lattice(Drawn by Gunnar Lange.

tion for the system. This is rather straightforward - we simply sum over all spins.

We now investigate the energy of each of the 16 microstates. We write the the energy as:

$$E = -J\left[s_1 s_2 + s_2 s_1 + s_1 s_3 + s_3 s_1 + s_2 s_4 + s_4 s_2 + s_3 s_4 + s_4 s_3\right]$$

Let us now look at what happens for different spin arrangement. Let us first assume that all spins point upwards (+1). Then, the energy will be $E = -8J$. Similarly, if all spins point downwards (-1), the energy will be $E = 8J$. If one spin points up, whilst all other point down, the energy will be zero, because half the terms change sign. Finally, if two spins point up, the energy depends on whether or not these spins neighbor each other. If they are next to each other, all terms involving the interaction of these two spins will have a positive sign. This will be two terms (notice that, because of the periodic boundary conditions, all interactions are reciprocal). The interaction between the two remaining spins will also be positive (as they have the same sign). However, all cross terms will give a negative contribution to the energy. Because of symmetry, these cross-terms must be the same as the not cross terms. Therefore the energy must be zero in this case. If, on the other hand, the two flipped spins are not neighbors, then there will be no interaction whatsoever between the flipped spins. Thus, all interacting spins have opposite signs, which gives the energy as $E = 8J$. This is summarized in the following table:

Table 1: The possible energies and magnetizations

Spins up	Number of microstates	Energy [J]	Magnetization[J/T]
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	+	6-2
0	1	-8J	-4

Then we can define the microcanonical partition function as::

$$Z = \sum_{i=1}^{16} e^{-\beta E_i}$$

Calculations give:

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

Or, recalling some hyperbolic trigonometric functions:

$$Z = 4\cosh(8J\beta) + 12$$

The energy is now given by:

$$\langle E \rangle = \sum_i \Delta E_i e^{-\beta \Delta E_i} \tag{11}$$

Which gives, after some substantial but elementary algebra:

$$\frac{-16Je^{8\beta J} + 16Je^{-8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 12}$$

Now C_V is easy:

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2}$$

Where $\langle E^2 \rangle$ is:

$$\langle E^2 \rangle = \frac{1}{Z} \sum_{i=1}^{16} E_i^2 e^{-\beta E_i}$$

The sum is easy:

$$\sum_{i=1}^{16} E_i^2 e^{-\beta E_i} = 128J^2 \left(e^{8J\beta} + e^{-8J\beta}\right)$$

So that:

$$\langle E^2 \rangle = \frac{256J^2 \cosh(8J\beta)}{4\cosh(8J\beta) + 12}$$

And thus:

$$C_V = \frac{1}{kT}\left(\frac{256J^2\cosh(8J\beta)}{4\cosh(8J\beta)+12} - \left(\frac{-8J\sinh(8J\beta)}{\cosh(8J\beta)+3}\right)^2\right) \tag{12}$$

Magnetization is easier, as it can be computed as:

$$\langle M \rangle = \frac{1}{Z}\sum_{i=1}^{16} M_i e^{-\beta E_i}$$

Which, however, gives:

$$\sum_{i=1}^{16} M_i e^{-\beta E_i} = 4e^{8J\beta} + 8 - 8 - 4e^{8J\beta} = 0$$

$\langle \mathcal{M}^2 \rangle$ can similarly be computed as:

$$\langle M^2 \rangle = \frac{8e^{8\beta J} + 8}{\cosh(8J\beta) + 3}$$

Now it is easy to compute the susceptibility:

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT} = \frac{1}{kT}\left(\frac{8e^{8\beta J}+8}{\cosh(8\beta J)+3}\right) \tag{13}$$

Note, however, that we in application frequenty substitute $\langle \mathcal{M} \rangle$ with $\langle |\mathcal{M}|$ in place of $\angle \mathcal{M} \rangle$, for reasons explained **HERE**. Therefore, we also compute the expected value of the absolute value of the magnetization, which gives:

$$\langle |M| \rangle = \frac{1}{Z}\sum_{i=1}^{16} |M_i| e^{-\beta E_i} = \frac{1}{Z}\left(4e^{8J\beta} + 4\cdot 2 + 4\cdot 2 + 4e^{8J\beta}\right) = \frac{2e^{8J\beta}+4}{\cosh(8J\beta)+3} \tag{14}$$

2.6 A brief introducton to the Metropolis Algorithm

The Metropolis algorithm is very common in Monte Carlo simulations. It is an extremely elegant algorithm, based on the ratio of probabilities, as explained here [3]. The idea is that the Boltzmann factor, $e^{-\beta \Delta E}$, tells us something about how probably it is to change state. If the energy difference bewteen the states is negative, the transition should be likely to occur, whereas if the energy difference is positive, it should be unlikely to occur. This is exactly what the Boltzmann factor expresses. The question is what to compare this factor to. This is at the heart of the simplest form of the Metropolis algorithm - simply choose a number, a from a uniform distribtuion of values betweenn 0 and 1. Compare this number to $s^{-\beta J}$. If a is less than $e^{-\beta J}$ (where ΔE is the energy different between two states. If a is less than $e^{-\beta \Delta E}$, flip the spin. This simple recipe, surprisingly, gives the correct thermodynamic behavior.

2.7 Periodic boundary condition

One problem of this model is how to treat the boundaries. The easiest way is to say that the spins on the boundaries have no neighbors. Real materials have close to infinite atom spins, so the boundaries are negligible. But we can't simulate infinite lattices, so we have to find another. With periodic boundary conditions, the spins at the boundary treats the spins at the opposite boundary as its neighbor. This will make a good approximation to an infinite lattice, since every spin has a neighbor. Because of this does the boundary condition corresponds better with reality.

3 Methods

3.1 Finding the Energy

The fastest and easiest way of implement the Ising method is to flip one spin at the time. This is because the energy difference ΔE in the system only will depend on the energy difference of a single spin. ΔE of a spin only depends on its closest neighbors, and can only have one of five values [3]

$$\Delta E = \{-8J, -4J, 0, 4J, 8J\}$$

This means that all the values for $e^{\beta \Delta E}$ can be precomputed. This saves us a lot of this in large simulations.

For each spin flip, we calculate the ΔE by checking the spin of the neighbor spins, and using 3.3.

Before starting the Metropolis algorithm the energy of the system has to be calculated this is done by looping though all the spins and calculating:

```
for i in range(Nspins):
    for j in range(Nspins):
        energy -= spinMatrix(i,j)*(spinMatrix(i-1,j)+ spinMatrix(i,j-1));
```

3.2 The Periodic Boundary Conditions

The easiest way of implementing the boundary conditions is with modular division. Every time we want to calculate ΔE, we have to use four nearest neighbors, but this neighbor may not exist. If the spin we are calculating ΔE is x_{N-1}, then its neighbor x_N does not exit. Instead we will check $periodic(N)$, where

$$periodic(i) = (i + N) \text{mod} N \tag{15}$$

We can check this we can test with $periodic(N)$ which should be 0

$$periodic(N) = (N + N) \text{mod} N = 0 \tag{16}$$

So as we can see this loops to the other side of the lattice.

3.3 Implementing the Metropolis algorithm

We implemented the Metropolis algorithm by looping over two nested for-loops. The outer for-loop loops over the number of Monte Carlo cycles, while the inner loops over the number if spin. Inside the loops a spin in the lattice is chosen to be flipped. The then energy difference is calculated from

$$\Delta E = 2J \sum_k s_i s_k$$

we use this to to find the precalculated Boltzmann factor, and compare this with a random variable $\zeta \in [0, 1]$, as described in 2.6, and check if this flip is acceptable.

Here is psudo-code describing the implementation of the Metropolis algorithm. Periodic boundary conditions are not implemented:

```
for i in range (MCSteps):
    for k in range(N*N):
        x=int(random.uniform(0,1)*N)
```

```
y=int(random.uniform(0,1)*N)
dEnergy=2*grid(x,y)*(grid(x+1,y)+grid(x-1,y)+grid(x,y+1)+grid(x,y-1))
boltzmann=boltzmann_factor(dEnergy) //Precomputed factors
if random.uniform(0,1)=<boltzmann: //Metropolis test
    lattice(x,y)*=-1
    energy +=dEnergy
    magnetic_moment=2*lattice(x,y)
```

3.4 Investigating the time to reach at the most likely state, and probability distribution

We are interested in seeing how long it takes the system to reach the most likely state, and if this depends on the temperature. We also wish to see if the start configuration change this time. We want to check when the mean energy and the mean absolute value of the magnetization smooth out and converges to a value. Since is difficult to do in a qualitative way, so we are just going to plot these values against the Monte Carlo cycles, and look for the cycle where this happens. We will also look at the number of accepted flips, since, as discussed in section 2.4, we also want the accepted flips to converge as we reach equilibrium.

We also want to look at the probability distribution of the equilibrium state. This is done by counting the number of times a certain E appears. We then have to use what we found above, and start when the equilibrium state is started.

3.5 The Phase transitions

We already have an analytical temperature for $T_C(N = \infty)$ from section 2.3, $\sim 2.269K$ [4]. We are there for only going to look at temperatures in an interval around this temperature while investigating the phase transitions. At the critical temperature the heat capacity and the magnetic susceptibility are going to diverge, but since we are using finite lattices, they aren't going to go to diverge, but they are going to show a value much higher then for the surrounding. This spike will give the critical temperature, which we can compare with the equations from section 2.3.

3.6 Parallelizing with MPI

Monte Carlo methods have an error(variance)

$$\sigma \sim \frac{1}{\sqrt{N}}$$

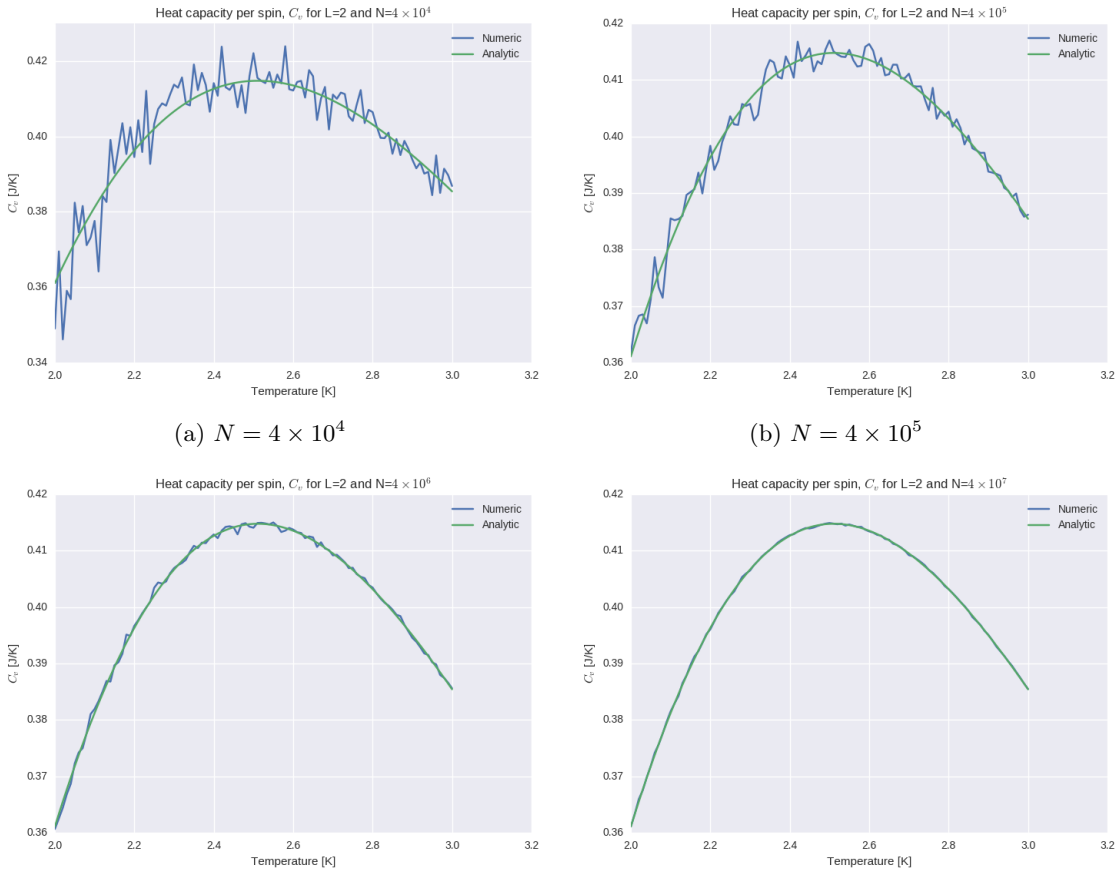
This means that the higher the number of cycles we use, the more accurate the simulation will be. One way of getting more cycles without increasing the run time is with parallelization. MPI lets us use all the core of the CPU. The Monte Carlo calculation is sent to the cores, and when the they are done, they(the slaves) send to data to a master core/node. This node will calculate the mean of all the data. We are mainly using 4 cores, so with MPI, we will get 4 times the Monte Carlo cycles, and more accurate data. [2]

[2]Note that we initially intended to run on a larger cluster but, due to time constraints, this was not possible.

4 Results

4.1 Numerical vs Analytical results for a 2 × 2 lattice

Before going on to larger lattices, we want to check if our program works. The one system we have an analytical results for is the 2x2 lattice 2.5. We want to look at how many Monte Carlo cycles it take to get a numerical result which corresponds well to the analytical. The most characteristic quantity is the heat capacity, so we choose to use this for the comparison. To make the plots as general as possible, all quantities are per spin.



(a) $N = 4 \times 10^4$

(b) $N = 4 \times 10^5$

(c) $N = 4 \times 10^6$

(d) $N = 4 \times 10^7$

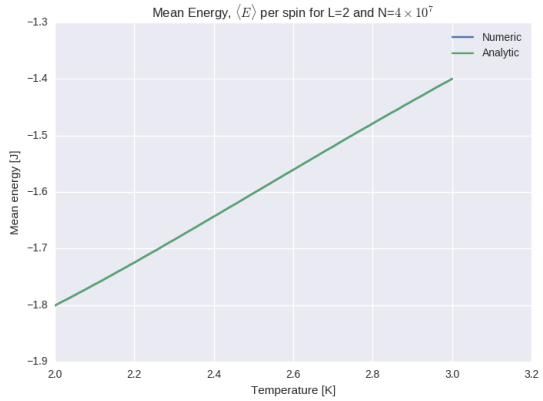
Figure 2: Comparison of the numeric and analytic solution of heat capacity and mean energy per spin for the 2×2 lattice. We plot multiple Monte Carlo steps, N, to find where the correspondence becomes good. This was done with temperatures in the interval $kT/J = 2$ to $kT/J = 3$, with 10 steps inbetween.

We also compare explicitly the value from the Ising model and the analytic solution at $kT/J = 1$ in table 2 below.

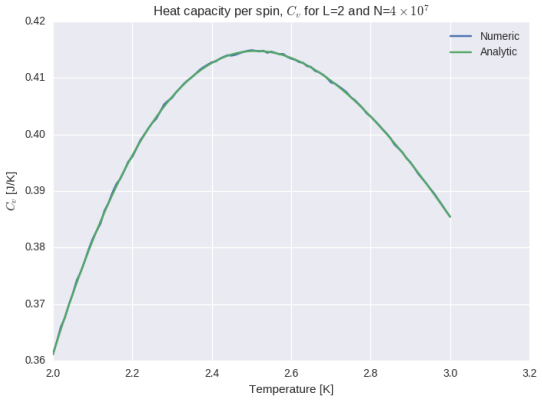
Table 2: Explicit comparison for the 2×2 lattice at the point $kT/J = 1$ for different Monte Carlo cycles, N.

N	4×10^4	4×10^5	4×10^6	4×10^7	Analytic
$\langle E \rangle [J]$	-1.9961	-1.9962	-1.9961	-1.9960	-1.9960
$\langle \lvert M \rvert \rangle$ [J/T]	3.9946	3.9946	3.9948	3.9946	3.9946
C_v [J/K]	0.0315	0.0305	0.0311	0.0321	0.0320
χ [J s^2]	3.950	3.991	3.984	3.993	3.993

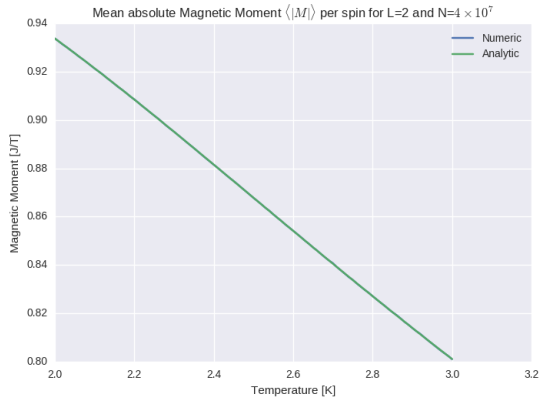
We gave each core a $N = 10^n$; with 4 cores, this means that our simulation runs with $N = 4 \times 10^n$ cycles. We see from the plots that if use $N = 4 \times 10^7$, we get a very good correspondence between the analytic and the numeric solution. We will therefor plot the other thermodynamic quantities in the 2×2 lattice for this value of N.



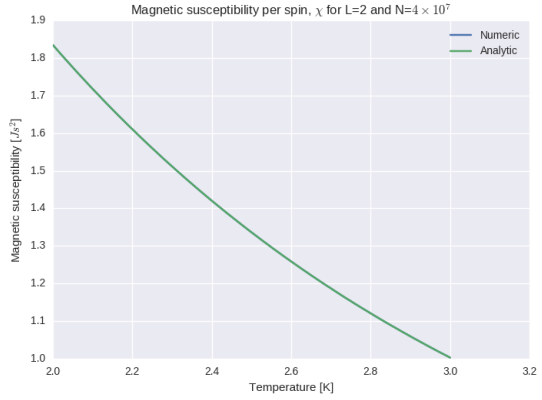
(a) Mean energy per spin



(b) Heat capacity per spin



(c) Mean absolute magnetic moment per spin



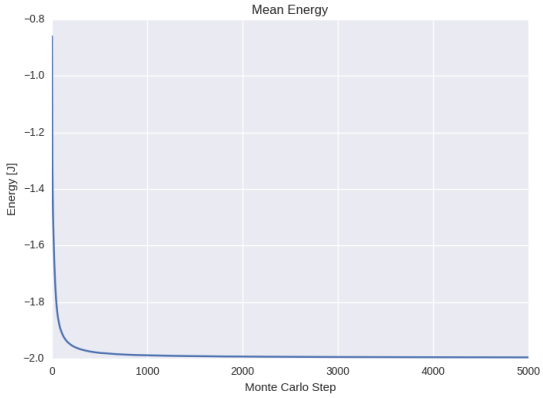
(d) Magnetic susceptibility per spin

Figure 3: Comparison of the numeric and analytic solution for the mean energy per spin, heat capacity per spin, mean absolute magnetic moment per spin and magnetic susceptibility of the 2×2 lattice, running 10^7 Monte Carlo cycles for each temperature.

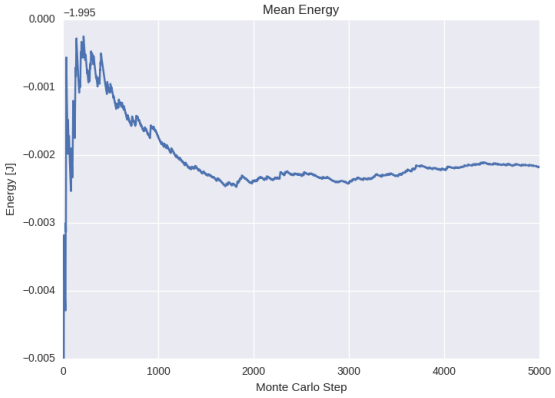
4.2 Results for the equilibration time

We were now interested in find the N were the equilibrium state is reach. For this we used a larger lattice, 20×20 spins. We are going to start with a temperature of $kT/J = 1.0$. We are interested in seeing where the quantities converges to there equilibrium value. We want to look at both the

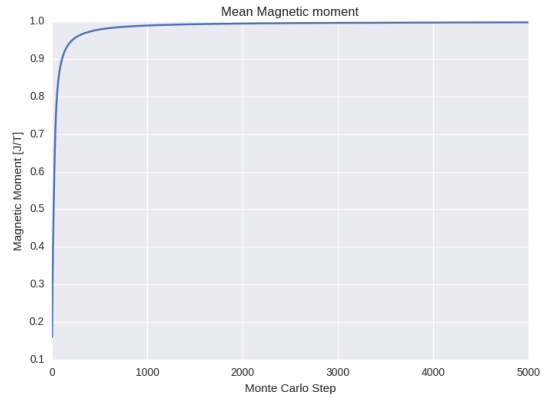
random and homogeneous start. Here are the plots of mean energy and mean absolute value of the magnetization:



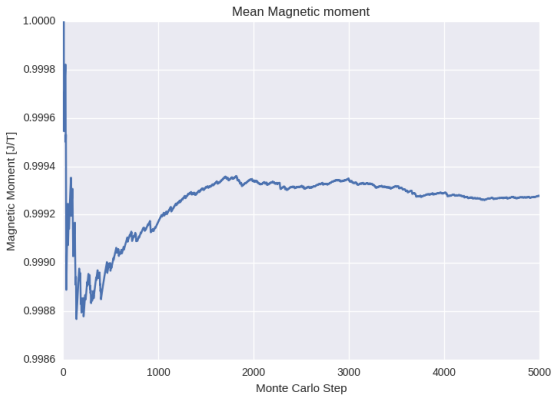
(a) Mean energy per spin from disordered state



(b) Mean energy per spin from ordered state



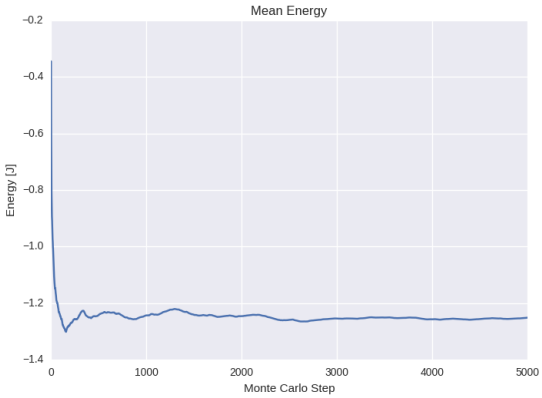
(c) Mean absolute magnetic moment per spin from disordered state



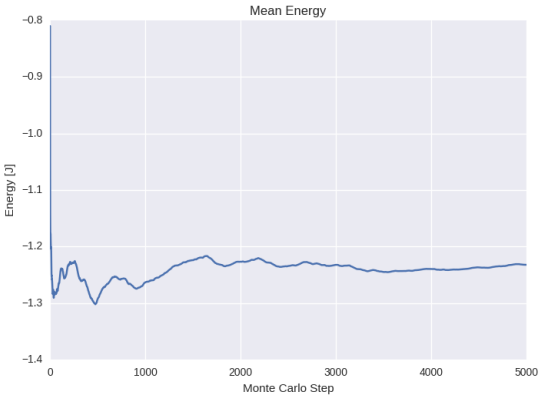
(d) Mean absolute magnetic moment per spin from ordered state

Figure 4: Time development of mean energy and mean magic moment per spin for two different initial configurations.Here $L = 20$ and $kT/J = 1.0$.

We also plot the same quantities for a temperature of $kT/J = 2.4$ in the figure below:



(a) Mean energy per spin from disordered state



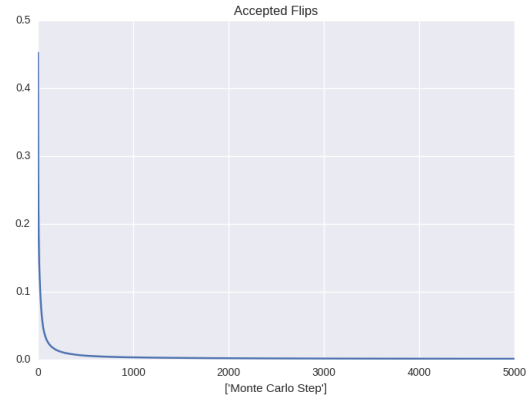
(b) Mean energy per spin from ordered state

(c) Mean absolute magnetic moment per spin from disordered state

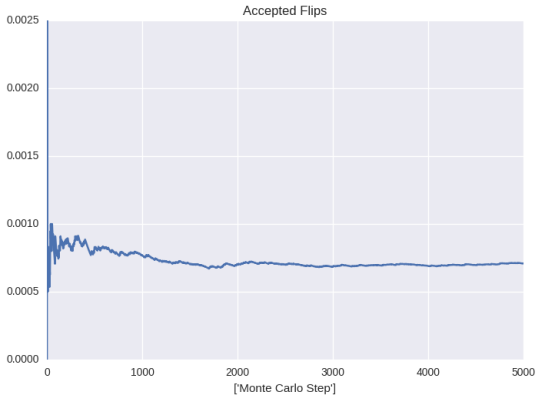
(d) Mean absolute magnetic moment per spin from ordered start

Figure 5: Time development of mean energy and mean magic moment per spin for two different initial configurations. Here $L = 20$ and $kT/J = 2.4$.

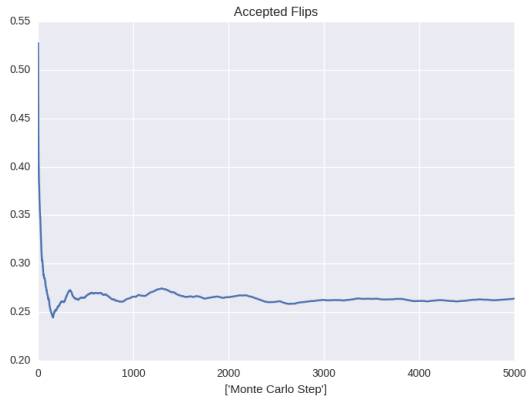
We also plot the number of accepted flips per spin per time:



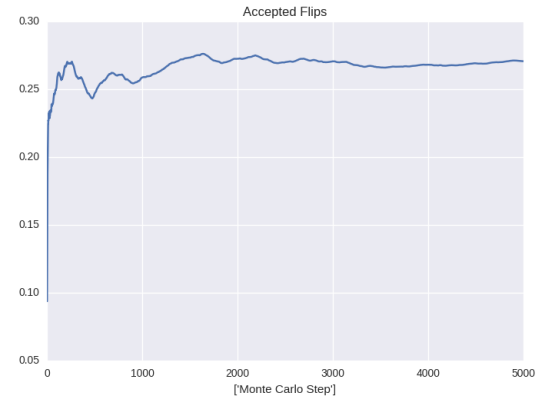
(a) With disordered initial state, at $kT/J = 1$



(b) With ordered initial state, at $kT/J = 1$



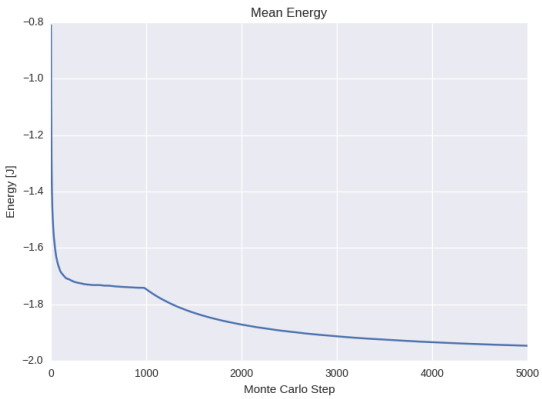
(c) With disordered initial state, at $kT/J = 2.4$



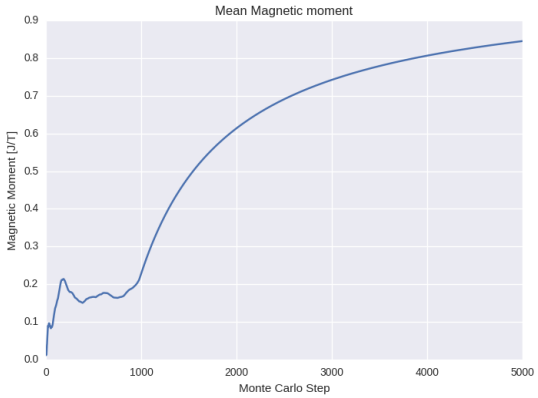
(d) With ordered initial state, at $kT/J = 2.4$

Figure 6: Mean number of accepted flips per spin per Monte Carlo cycle for different initial states and different temperatures.

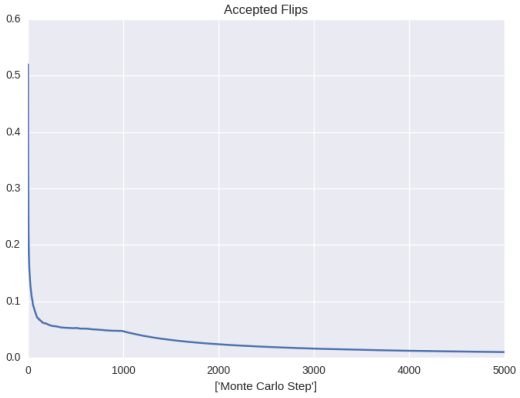
It seems that most of the qualities reach the equilibrium after $1-2000$ with the low temperature, while it longer for the higher temperature. For the rest of the results, where the data it retrieved after equilibrium, 5000 cycles are waited before the data collection – to be on the safe side–. We did also encounter an interesting case, where we hit a local minimum. They can be described here:



(a) Mean energy per spin from ordered state



(b) Mean magnetic moment per spin from ordered state



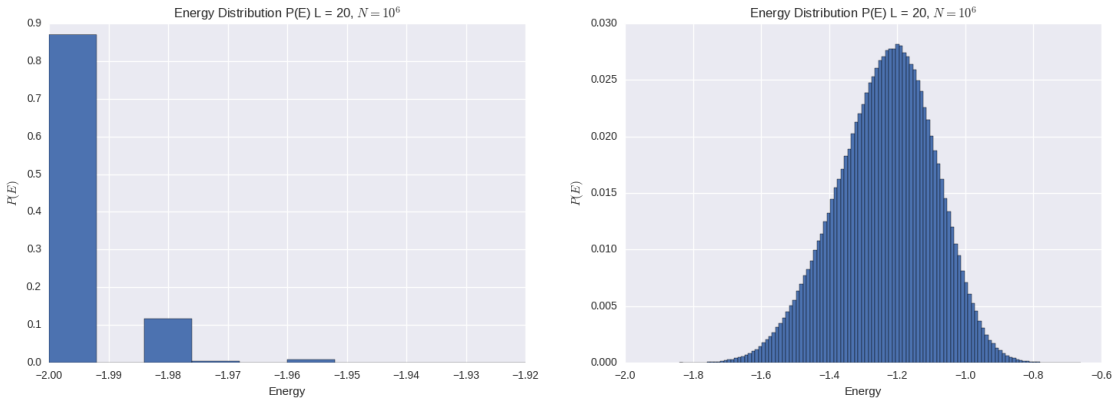
(c) Mean number of accepted flips per spin per Monte Carlo cycle from ordered state

Figure 7: Time development of mean energy, mean magnetic moment and mean number of accepted flips per spin per Monte Carlo cycle for a system with $L = 20$, $kT/J = 1$, with all spins initially pointing up.

As we can see using 5000 cycles also ensure that local equilibrium states aren't interfering with our data.

4.3 Results for the probability distribution

We found the probability distribution for the same 20x20 lattices as above, but only were taken after equilibrium. The distributions are plotted her as a histogram:



(a) $KT/J = 1$ (b) $KT/J = 2.4$

Figure 8: Histogram showing the probability of different energies occurring for two different temperature. This is for a lattice with $L = 20$, simulated with $N = 10^6$ Monte Carlo cycles, excluding an equilibration time of 5000 cycles. The histograms are normalized.

We can see that for the lower temperature that the energy is -2.0 is dominating, while the energy are more gaussian distributed with the mean -1.2.

We also computed the variance of the energy per spin, simply by computing:

$$\text{Var}(E) = \langle E^2 \rangle - \langle E \rangle^2$$

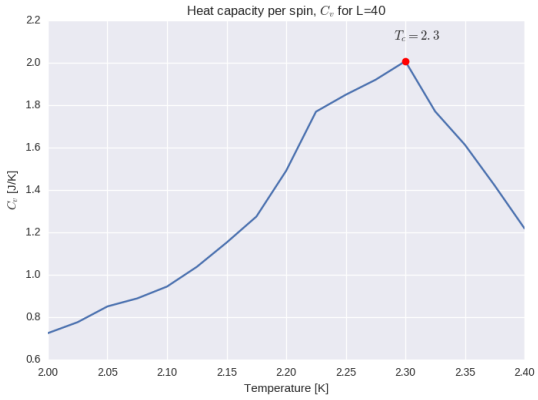
Where the energy is per spin. Writing this out for the last points (where we have simulated the longest) gives:

Table 3: The variance of the energy for the temperatures above

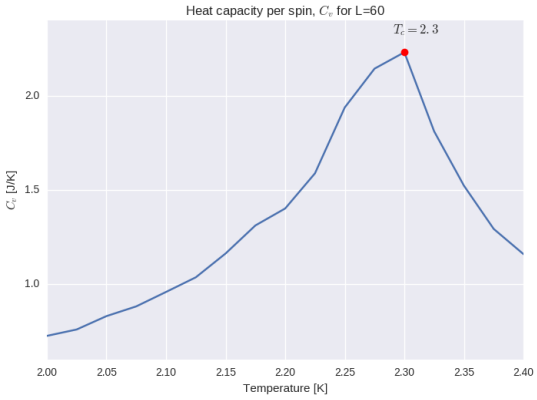
Temperature [kT/J]	Variance of energy [J^2], σ^2
1.0	9.949×10^{-5}
2.4	0.02035

4.4 Results for phase transitions

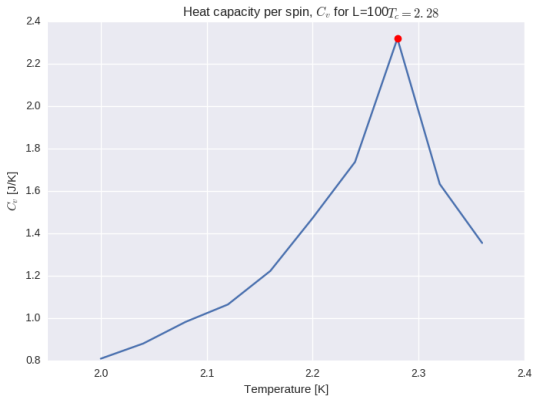
To find the critical temperature, we can look at the critical temperature and the magnetic susceptibility for 4 different lattice sizes, and see where the spike is:



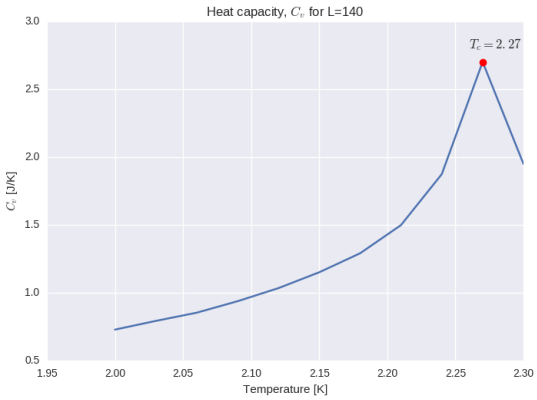
(a) Heat capacity for $L = 40$



(b) Heat capacity for $L = 60$

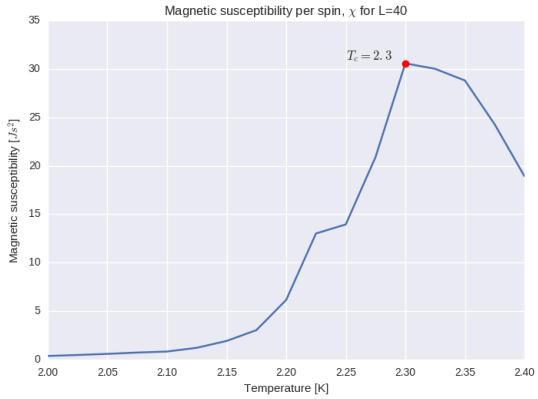


(c) Heat capacity for $L = 100$

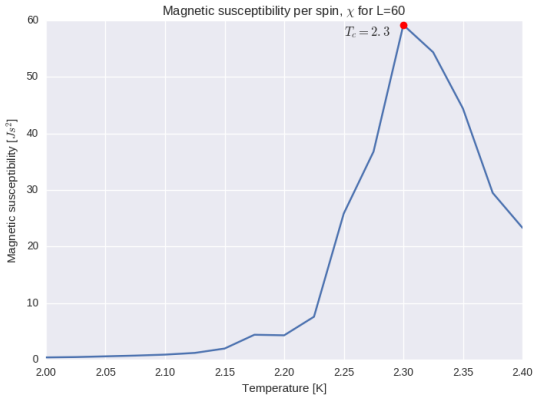


(d) Heat capacity for $L = 140$

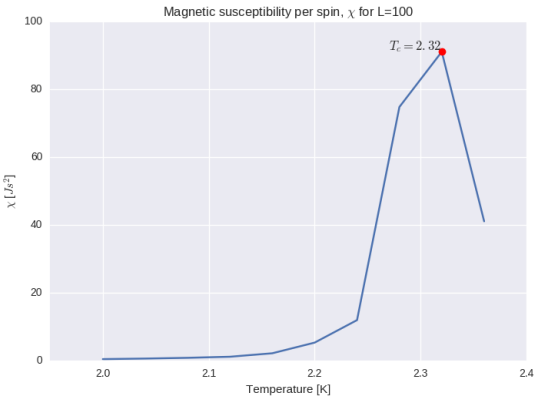
Figure 9: Development of the heat capacity for systems of different sizes, as a function of temperature. We simulated 10^5 Monte Carlo cycles, excluding an equilibration time of 5000 cycles.



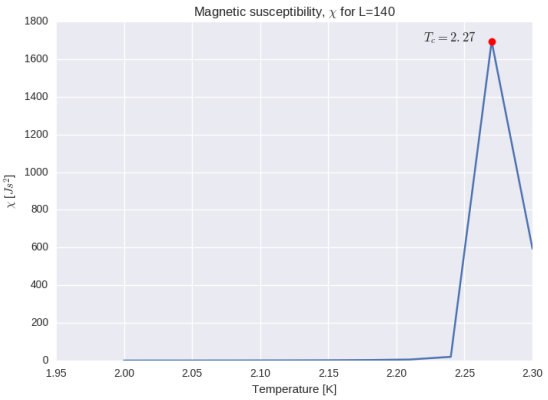
(a) Magnetic susceptibility for $L = 40$



(b) Magnetic susceptibility for $L = 60$



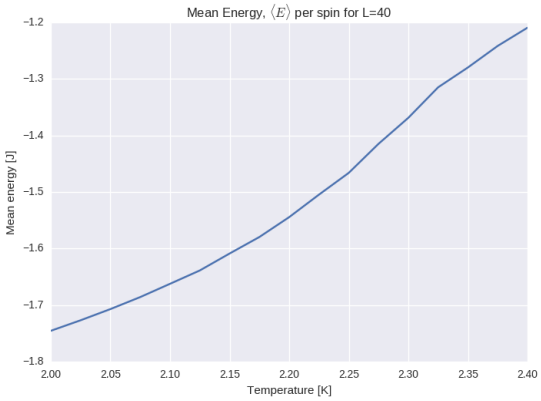
(c) Magnetic susceptibility for $L = 100$



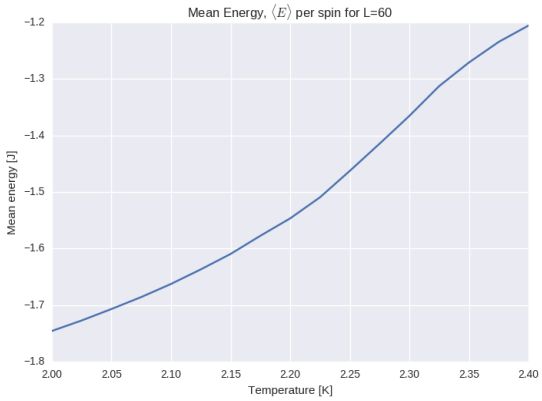
(d) Magnetic susceptibility for $L = 140$

Figure 10: Development of the magnetic susceptibility for systems of different sizes, as a function of temperature. We simulated 10^5 Monte Carlo cycles, excluding an equilibration time of 5000 cycles.

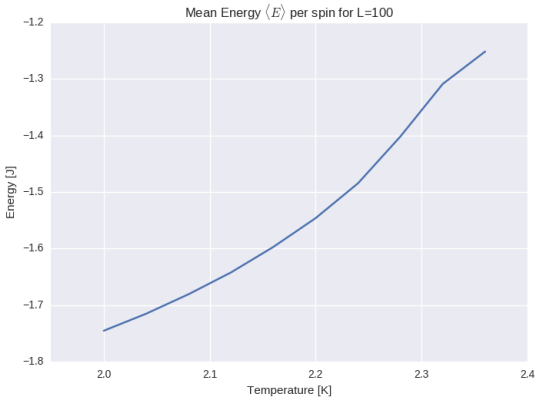
The mean energy and mean absolute magnetic moment are also included:



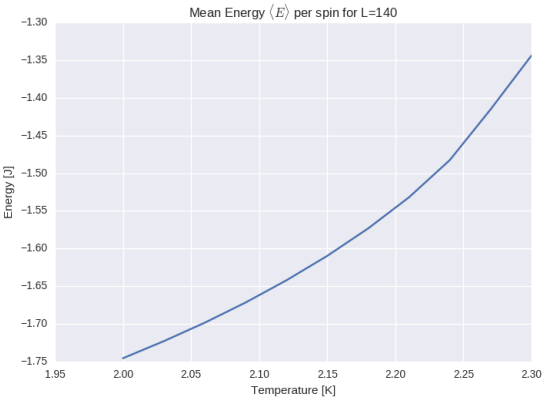
(a) Mean energy per spin for $L = 40$



(b) Mean energy per spin for $L = 60$

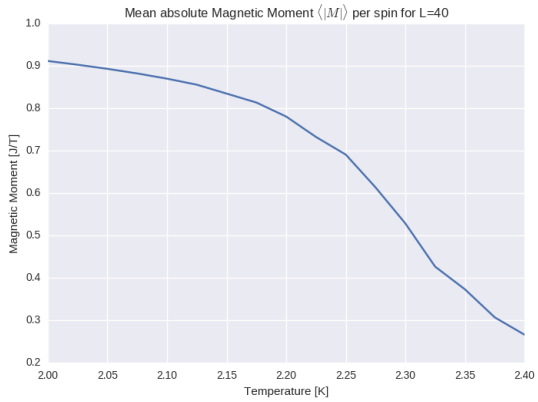


(c) Mean energy per spin for $L = 100$

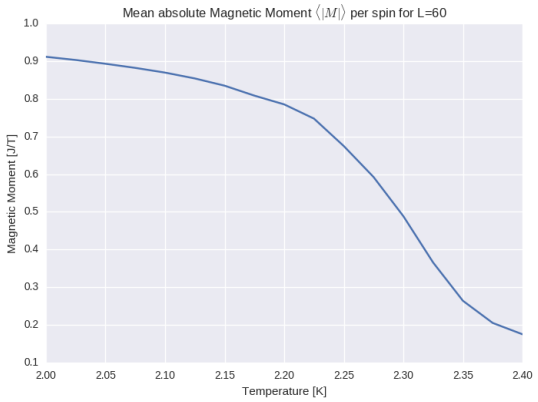


(d) Mean energy per spin for $L = 140$

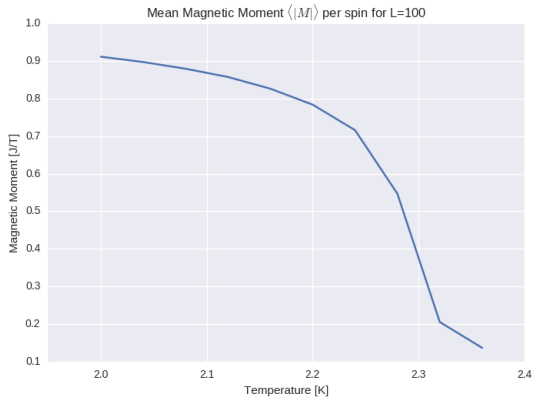
Figure 11: Development of the mean energy per spin for systems of different sizes, as a function of temperature. We simulated 10^5 Monte Carlo cycles, excluding an equilibration time of 5000 cycles.



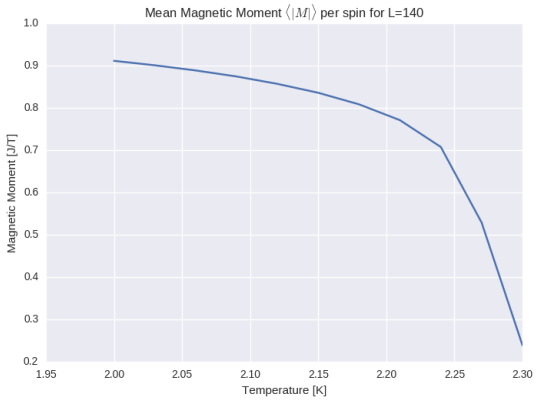
(a) Mean absolute value of the magnetic moment per spin for $L = 40$



(b) Mean absolute value of the magnetic moment per spin for $L = 60$



(c) Mean absolute value of the magnetic moment per spin for $L = 100$



(d) Mean absolute value of the magnetic moment per spin for $L = 140$

Figure 12: Development of the mean absolute value of the magnetic moment per spin for systems of different sizes, as a function of temperature. We simulated 10^5 Monte Carlo cycles, excluding an equilibration time of 5000 cycles.

4.5 Results from parallelizing our code

Table 4: Comparison of speed with and without parallelization for a 20×20 lattice. We compare for numbers of Monte-Carlo cycles, N.

N	With MPI [s]	Without MPI [s]
$4 \cdot 10^5$	4.08	11.296
$4 \cdot 10^6$	45.347	109.675

5 Discussion

5.1 The 2×2 lattice

Figure 2 shows how for bigger N the numerical results converges towards the analytical result for heat capacity. After $N = 10^7$ the results become near indistinguishable. This is also true for the other quantities. So for the optimal results in our other investigation this is the N we ought to

use. But while the 2x2 was fast to run with this N, the bigger systems run much slower. The run time goes like $O(L^2)$, so even for 20x20 this takes a very long time. So we had to use 10^5 for the larger systems. We hope that this, with the fact that we start collecting data after the equilibrium state is reached, still gives us reliable data.[3]

5.2 Time required to reach equilibrium

Figure 4 and 5 illustrates how the ordered and disordered systems evolve with Monte Carlo cycles.

There are some interesting points to see here:

The first is that the ordered start reaches the equilibrium before the disordered. This is because for low temperatures, the equilibrium state is close to an ordered state. This means that this start is much closer to the equilibrium than the disordered start.

The second point is that the equilibrium states are different for higher temperature. This is due to the system having more energy from the temperature. In real life a higher temperature would cause the atom to have a higher thermal motion, and thereby making the spins looser bound. Because of this the number of spins pointing in one direction is lower, causing a lower magnetic moment. This is exactly what we see from our data.

The third point is a little more mysterious, and may be because of our implementation of the code. We expect the mean absolute magnetic moment to start at 1.0 for the ordered start, since all the spins start as $+1$. This is not the case in our data. We are not sure why this happens, but one possibility is that, since we are dumping the data to file after the first cycle, then the magnetic moment may have changed from the original state.

Figure 6 show how the mean number of flips per spin per Monte Carlo cycle. We can see that the results are more or less the same as seen above. As the system reaches equilibrium, the Boltzmann factor becomes so large, that few new flips are excepted. We see that both for the low and the high temperature the disordered systems take somewhat longer time to reach equilibrium – this is more pronounced at the low temperature –. It is difficult to see exactly when all the systems are in equilibrium, since the plots have different scales on the axis. But after $2 - 3000$ cycles the number of excepted flips looks to reach equilibrium.

As mentioned in the results section we got local minimums 7 – using the low temperature and ordered start–. This happens when large regions of the lattice by chance acquire the same spin. When we now try to flip one spin, the neighbor all have the same spin, the chance of accepting this spin is very low. The only chance of accepting a flip is to flip a spin on the boundary, where the neighbors have different spins. But this has a low chance of happening, since the stable regions are much more common. But since the lattice is only stable locally, this state will not last for very long, an the system will go on to reach its equilibrium state. With this local minimum, the time for equilibrium will be higher than 2000 cycles. This is why we have decided to wait 5000 cycles before beginning to sample data. This may not always hold, but for the large majority of stats this will due.

5.3 The probability distribution

8 shows the probability distribution. We can see that for low temperatures, the most likely energy is the lowest. This may be because the equilibrium state of this system is where most spins point up, and therefor having the lowest energy -2.0. This is in other words what we expect to see.

[3] We tried using the Smaug cluster. But when we tried to run our program, we got an error stating that MPI couldn't be found. This being the day before the deadline, we decided to go for 10^5 cycles.

For higher temperatures the mean of the energy is higher, and the distribution is gaussian. This make sense since the spins as looser bound, and there for flips will be accepted more often. This makes the energies vary more. Since the acceptance of the flips are governed by a random distribution, we can expect to see the gaussian distribution due to the central limit theorem.

The variances in table 3 corresponds well with our intuitions of the physical systems. But the distributions are not Gaussian, so the variance does not quite characterize the distribution. But the distribution for the for $kT/J = 2.4$ looks very like a Gaussian, so we can give this a standard deviation:

$$\sigma = \sqrt{0.0203} = 0.142$$

The standard deviation for the distribution to $kT/J = 1$ does not make sense, and was not computed.

5.4 The phase transitions

Figures 11, 12, 9 and 10 show the behavior of our system as a function of temperature.

Due to computational times we used different temperatures on the different lattice sizes. With $L = 40$ and $L = 60$ we used temperatures in the interval $[2kT/J, 2.4kT/J]$ with $0.025kT/J$ steps. Now knowing where to find the critical temperature, we could, for the bigger systems $L = 100$, use a smaller interval of $[2kT/J, 2.35kT/J]$ with a step of 0.04, simply to save some time. For $L = 140$ we used a smaller step of 0.03.

We can now look at the critical temperature. As mentioned in section 2.3, the some of the thermodynamical quantities should spike near this temperate (at phase transition). We can especially look at heat capacity9 and magnetic susceptibility 10. We have marked the phase transitions with a red dot and the temperature at which this occurs, the critical temperature. We get a good correspondence between C_v and χ

Table 5: The critical temperatures

L	T_c from C_v	T_c from χ
40 and 60	2.3	2.3
100	2.28	2.32
140	2.27	2.27

We can see that $2.3kT/J$ is a good approximation for the critical temperature.

We will therefore employ equation 10 with $L_1 = 60$ and $L_2 = 140$, as the only viable options. This gives (using the analytic result that $\nu = 1$):

$$a = \frac{2.3 - 2.27}{60^{-1} - 140^{-1}} = 3.15$$

Which gives the critical temperature in the thermodynamic limit as (using equation 9):

$$T_C(L = \infty) = T_C(L) - aL^{-1/\nu} = 2.27 - 3.15 \cdot 140^{-1} = 2.2475$$

The exact analytic expression can be found here [4], and is given by:

$$T_C(L = \infty) = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.269$$

This gives us a relative error of $\epsilon_{\text{rel}} \approx 0.95\%$, a quite good result. If we use $L = 140$ and $L = 40$ instead, we get

$$a = 1.68, \quad T_C(L = \infty) = 2.258, \quad \epsilon_{\text{rel}} \approx 0.48\%$$

.

5.5 Our use of MPI

We can see from 4 that there are quite a speed up from using MPI. This is only with our 4 cores, but when using larger computer clusters with many more cores, the speed up can be huge.

6 Conclusion

6.1 Conclusion

We have looked at various systems using the Ising Model. The first system was the 2x2 lattice. We saw that the Ising model gave a very good correspondence between the numerical and analytical results. We then looked at the time it took for a 20x20 system to reach equilibrium. We found that it took around $2 - 3000$ cycles to reach equilibrium, depending on the temperature and the starting configuration. But due to the occurrence of local minima, we decided to wait 5000 cycles to sample data. We then look at the phase transitions for larger systems, finding the critical temperature to match the analytical values quite well.

6.2 Outlook

While we managed to get a lot out of this investigation, the data should be reproduced with more Monte Carlo cycles to get more accurate data.

Investigating the local minima we found, to see the topography of the regions, and how stable they are, could be very interesting, and could make up a research project by it self.

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[2] David Cimasoni, Hugo Duminil-Copin, et al. The critical temperature for the ising model on planar doubly periodic graphs. *Electron. J. Probab*, 18(44):1–18, 2013.

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