University of Oslo

FYS3150

Computational Physics

Project 4 - Studies of phase transitions in magnetic systems

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December 8, 2016

Contents

Abstract

When the phase space of physical systems become very large, Monte Carlo[1] methods play an extremely important role when it comes to numerical simulations of these systems. The Metropolis algorithm and Markov chains are used in this paper and is analyzed in terms of sweeps per lattice which will be our indication of runtime. The two dimensional Ising model illustrates the efficiency of the Monte Carlo method where we study the phase transition from a ferromagnetic material to a paramagnetic material at a critical temperature called the Curie temperature. This stochastic method proves to be highly applicable for these kinds of problems. The accuracy of the method is illustrated by calculating the critical temperature at which the phase transition takes place and is compared to the analytical result of Lars Onsager[1] in the thermodynamical limit where the lattice size $L \to \infty$. The values are in good agreement, and is further underlined by the use of finite size scaling.

Github repository: `https://github.com/VebjornG/FYS3150/tree/master/Project4`

1 Introduction

Ferromagnetic materials lose their magnetic behavior when they reach a critical temperature. This was discovered by Pierre Curie and is called the Curie temperature. The electrons in the material has spin up or down with a magnitude of $\pm 1/2$, and it is this trait we exploit in the Ising model which is based on analyzing critical points of phase transitions in these kinds of materials. The vital thing about this model is that it can predict the behavior of the neighboring electrons for a given set of spins. We will study the phase transition between the ferromagnetic and the paramagnetic materials using Metropolis as the algorithm of our choice. We apply this algorithm in order to compute the heat capacity, magnetization, susceptibility and the energy of the system at equilibrium. These values will be studied in order to get an idea of the efficiency and accuracy of the Metropolis algorithm. Because computers and infinity do not get along, we will utilize finite size scaling in order to make an estimate for the critical temperature in the thermodynamical limit using the data we find and compare it to Onsager's analytical value.

[1]The Monte Carlo method got it's name from Ulam, Fermi, Von Neumann and Metropolis during the second world war at Los Alamos.

2 Theory

2.1 The 2D Ising model with periodic boundary conditions

In statistical physics we don't have the capability to solve all of the systems analytically and thus we need alternative schemes to determine these kinds of thermodynamical quantities. Although we can solve the two dimensional Ising model analytically for $H = 0$, a solution for the general case where $H \neq 0$ has yet to be found. The task at hand introduces another obstacle, namely the fact that one cannot, in most cases, take into account every possible configuration of the system when it becomes large. This means that we need a set of configurations that are representative for the entire ensemble. To do so we consider a two dimensional lattice with degrees of freedom that are spins $S_i = \pm 1$ at every vertex i, and in the $2D$ case there can be $N = 2^{L \times L}$ of them where L is the dimension of the lattice. The Hamiltonian representing the Ising model can be described as

$$H = -J \sum_{\langle kl \rangle} S_k S_l.$$

The parameter J represents the strength of the interaction between the spins and the sum runs over all pairs of the nearest neighbours as shown in figure 1. We assume that $J > 0$ which means that the material is ferromagnetic[2].

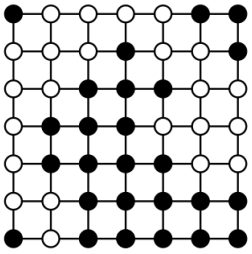

Figure 1: 2D Ising model with nearest-neighbor interactions in terms of lines that connect the dots. The black circles represent $S_i = +1$ and thus the white ones represents $S_i = -1$. This figure can also represent a binary system, without the need for physics.

There are numerous choices when it comes to boundary conditions, and one of the more efficient ones takes into account the geometrical aspect of the lattice. We can maximize the interaction of the spins at the edges by letting them interact with their geometrical counterparts. This means that the first spin at the left edge of each row

can see the the last spin on the same row as its neighbor and vice versa. This also applies to the rows at the top and the bottom. To get a better view of this one can visualize the lattice as a torus as shown in figure 2.

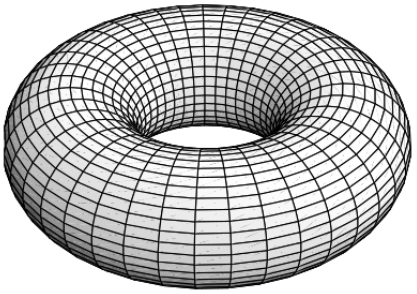

Figure 2: The periodic boundary conditions in the two dimensional lattice represented as a torus.

It's evident that we need some thermodynamical quantities in order to study this system, and the statistical properties of this physical system can be obtained from the partition function which is defined as

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

where $\beta \equiv 1/k_B T$ at a fixed temperature T in the canonical ensemble. The partition function is extremely useful due to the fact that the probability of the system existing as a configuration in a set of microstates is given by

$$P(i) = \frac{1}{Z} e^{-\beta E_i}$$

Using the partition function we can find a multitude of expressions, that is, the mean energy of the system, the heat capacity, the magnetization and the susceptibility. Hence,

$$\langle E \rangle = -\frac{\partial}{\partial \beta} lnZ = \frac{1}{Z} \sum_{i=1}^{N} E_i e^{\beta E_i} \tag{1}$$

$$\langle C_v \rangle = \frac{1}{k_b T^2} \frac{\partial^2}{\partial \beta^2} lnZ = \frac{1}{k_b T} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{2}$$

$$\langle M \rangle = \frac{1}{Z} \sum_i M_i e^{-\beta E_i} \tag{3}$$

$$\langle \chi \rangle = \frac{1}{k_b T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{4}$$

where $M_i = \frac{1}{N}\sum_i S_i$.

2.1.1 Phase transitions and finite size scaling

The spins in the material will fluctuate depending on the temperature, that means that for low temperatures, the spins are aligned and the magnetization is close to 1. However, as the temperature rises, the spins fluctuate wildly. When the temperature reaches a critical point T_C, the magnetization tends to 0 with an infinite slope and the material loses it's magnetic properties. This phase transition is characterized as a discontinuity in the first and second order derivatives of the quantities that are related to the potential of the system. Because we cannot model this phase transition in the actual thermodynamical limit where $L \to \infty$, a problem arises when it comes to recognizing the point at which this transition occurs. It is therefore necessary to construct a way for which we can extrapolate the theoretical value for T_C using our limited resources, i.e. computers. We use a critical exponent lambda which is given by $\lambda = \lim_{t\to 0} \frac{|F(t)|}{|t|}$ and this can be written as $F(t) \sim |t|^\lambda$ for $t = T - T_C$. The critical exponents that are involved in the Ising model are represented as

$$\begin{aligned} \xi(T) &\sim |T - T_C|^{-\nu} \\ \langle M(T)\rangle &\sim (T_C - T)^\beta \\ C_v &\sim |T_C - T|^\alpha \\ \chi &\sim |T_C - T|^\gamma \end{aligned}$$

where $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$ represents the critical exponents. The correlation length $\xi(T)$ is expected to be of the order lattice spacing for $T >> T_C$. Also, the correlation length increases when T approaches T_C because the spins become more and more correlated. To illustrate this we can consider how the correlation length changes with temperature. Once it reaches some point L, we can get closer to T_C but ξ will no longer grow. This is like a tree growing inside but cannot grow any further because of the ceiling where the ceiling represents L. That is, if the system is very small the saturation of ξ will occur when the temperature is quite far from T_C and thereby much closer to T_C when the system is large. This means that in the thermodynamical limit $L \to \infty$ the critical temperature scales as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{5}$$

where a is a constant. The rest of the quantities scales as

$$\begin{aligned} \langle M(T)\rangle &\sim (T_C - T)^\beta \to L^{-\beta/\nu} \\ C_v &\sim |T_C - T|^\alpha \to L^{\alpha/\nu} \\ \chi &\sim |T_C - T|^\gamma \to L^{\gamma/\nu}. \end{aligned}$$

2.1.2 The 2×2 lattice

Using the energy and the partition function given in the introduction to the Ising model, we can find the exact expressions for the different quantities that we want to calculate for a 2×2 lattice. That is,

$$E_i = -J(s_1 s_2 + s_1 s_3 + s_2 s_1 + s_2 s_4 + s_3 s_1 + s_3 s_4 + s_4 s_3 + s_4 s_2)$$

where $s_i = \pm 1$. If we calculate the energies for the $N = 2^{2\times 2} = 16$ spin configurations we get three possible values for the energy, namely $-8J, 0, 8J$ where $-8J$ occurs for the two configurations where all of the pins point either up or down. There are 12 configurations which share the energy 0, and two states that share $8J$ where both of the rows in the configuration contains a spin up and down and the diagonal contains equal spins. Thus, the partition function becomes

$$\begin{aligned} Z = \sum_i e^{-\beta E_i} &= 2e^{8J\beta} + 12 + 2e^{-8J\beta} \\ &= 4\cosh(8J\beta) + 12. \end{aligned}$$

Equation (1) yields

$$\langle E \rangle = -\frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3}$$

The heat capacity can be found using eq. (2), which essentially consists of finding the derivative of $\langle E \rangle$.

$$\begin{aligned} \langle C_v \rangle &= \frac{1}{kT^2} \frac{\partial^2}{\partial \beta^2} \ln Z \\ &= \frac{1}{kT^2} \frac{\partial}{\partial \beta} \left[\frac{\partial}{\partial \beta} \ln Z \right] \\ &= \frac{1}{kT^2} \left[\frac{64J^2 \cosh(8J\beta)\left(\cosh(8J\beta) + 3\right) - 8J \sinh(8J\beta) 8J \sinh(8J\beta)}{\left(\cosh(8J\beta) + 3\right)^2} \right] \\ &= \frac{1}{kT^2} \left[\frac{64J^2 \cosh(8J\beta)}{\cosh(8J\beta) + 3} - \frac{64J^2 \sinh^2(8J\beta)}{\left(\cosh(8J\beta) + 3\right)^2} \right] \\ &= \frac{64J^2\beta}{T} \left[\frac{1 + 3\cosh(8J\beta)}{(\cosh(8J\beta + 3)^2)} \right] \end{aligned}$$

When we calculate the mean magnetization we get 0, and so we need to find $\langle|M|\rangle$, hence

$$\begin{aligned}\langle M\rangle &= \frac{1}{Z}\left[-4e^{8J\beta} - 8 + 8e + 4e^{8J\beta}\right] = 0\\ \langle|M|\rangle &= \frac{1}{Z}\left[4e^{8J\beta} + 8e^{0} + 8e^{0} + 4e^{8J\beta}\right]\\ &= \frac{16 + 8e^{8J\beta}}{4\cosh(8J\beta) + 12} = \frac{4 + 2e^{8J\beta}}{\cosh(8J\beta) + 3}\end{aligned}$$

With this, we can find the susceptibility of the system given by equation (4), but in order to do so we need $\langle M^2\rangle$.

$$\begin{aligned}\langle M^2\rangle &= \frac{1}{Z}\left[16e^{8J\beta} + 16e^{0} + 16e^{0} + 16e^{8J\beta}\right]\\ &= \frac{32\left(e^{8J\beta} + 1\right)}{4\cosh(8J\beta) + 12} = \frac{8\left(e^{8J\beta} + 1\right)}{\cosh(8J\beta) + 3},\end{aligned}$$

and so the susceptibility for $\langle M\rangle = 0$ and $\langle|M|\rangle$ becomes

$$\begin{aligned}\langle\chi\rangle &= \frac{1}{kT}\left(\frac{8\left(e^{8J\beta} + 1\right)}{\cosh(8J\beta) + 3} - 0^2\right) = \frac{8\left(e^{8J\beta} + 1\right)}{kT\left(\cosh(8J\beta) + 3\right)}\\ \langle|\chi|\rangle &= \frac{1}{kT}\left(\frac{8\left(e^{8J\beta} + 1\right)}{\cosh(8J\beta) + 3} - \left(\frac{4 + 2e^{8J\beta}}{\cosh(8J\beta) + 3}\right)^2\right),\end{aligned}$$

respectively. The possible values for the energy and magnetization are listed in table 1.

Number of spins up	E	M	Multiplicity
0	$-8J$	-4	1
1	0	-2	4
2	$8J$	0	2
2	0	0	4
3	0	2	4
4	$-8J$	4	1

Table 1: Table of the different energies and the magnetization for the 2×2 system with the multiplicity of the configurations.

2.2 The Monte Carlo process

2.2.1 The Metropolis algorithm and Markov chains

Although Markov chains can be challenging to fully understand, the underlying principle is quite simple. That is, the future of the present state is independent of it's past. In order to make this more precise we need to elaborate a bit. Markov chains makes use of random walks to generate random states which depends on a probability distribution function $w(x,t) \to w_i(t)$ which is normalizable. In a small timestep ϵ this process can be described as

$$w_i(t+\epsilon) = \sum_j W(j \to i) w_j(t)$$

where $W(j \to i) = W_{ij}$ is the transition probability matrix where $0 \leq W_{ij} \leq 1$. This means that the matrix representation of this can be described as

$$\hat{\boldsymbol{w}}(t+\epsilon) = \hat{\boldsymbol{W}}\hat{\boldsymbol{w}}(t).$$

We reach the most probable state when $t \to \infty$, that is

$$\hat{\boldsymbol{w}}(\infty) = \hat{\boldsymbol{W}}\hat{\boldsymbol{w}}(\infty),$$

but at this point a problem arises, namely that we don't know what the transition matrix is due to the complicated behavior of the system, and in order to get to know the transition matrix we need the Metropolis algorithm. The Metropolis algorithm works like a supporter at a Trump rally, some states get rejected and some are accepted. The way it determines whether the random states are accepted or rejected is by first defining the transition matrix as

$$W(j \to i) = T(j \to i) A(j \to i)$$

where $T(j \to i)$ represents the probability of making a move from $j \to i$ and $A(j \to i)$ represents the acceptance of the move $j \to i$ that the random walk offered. The detailed balance, i.e. the equilibrium situation, can be described as

$$\begin{aligned} w_j T(j \to i) A(j \to i) &= w_i T(i \to j) A(i \to j) \\ \Rightarrow \frac{w_i}{w_j} &= \frac{T(j \to i) A(j \to i)}{T(i \to j) A(i \to j)} \end{aligned}$$

where $w_i = P_i(\beta) = \frac{e^{-\beta E_i}}{Z(\beta)}$. This yields

$$\begin{aligned} \frac{w_i}{w_j} &= \frac{T(j \to i) A(j \to i)}{T(i \to j) A(i \to j)} \\ &= \frac{e^{-\beta E_i}}{e^{-\beta E_j}} = e^{-\beta(E_i - E_j)} = e^{-\beta \Delta E} \end{aligned}$$

which is known through the statistical properties of the ferromagnet at hand. With $T(j \to i) = T(i \to j)$ we can write the acceptance as $A(j \to i) = e^{-\beta \Delta E}$ which becomes a probability defined as

$$A(j \to i) = \begin{cases} e^{-\beta \Delta E} & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0. \end{cases}$$

This ensures that the accepted transitions result in a lower energy configuration. If, however the energy of the new state is higher than the one preceeding it, we go on to generating a random number a such that if $a > e^{-\beta \Delta E}$, the transition is accepted. The good thing about the Metropolis algorithm is that we don't have to calculate the partition function due to the fact that it can be nearly impossible to calculate in some cases.

3 Methods and algorithms

3.1 The Metropolis algorithm

As discussed in section 2.2.1, there are numerous advantages to the Metropolis algorithm. The first thing to do is to randomize the lattice to form an initial state, and then randomly choose a site i. Then, when we flip s_i, ΔE is calculated and we go on to choosing whether to accept the flip or not. This is repeated from the step where we choose a site i until the iterations have reached the size of the lattice. Figure 3 shows more explicitly how this would work.

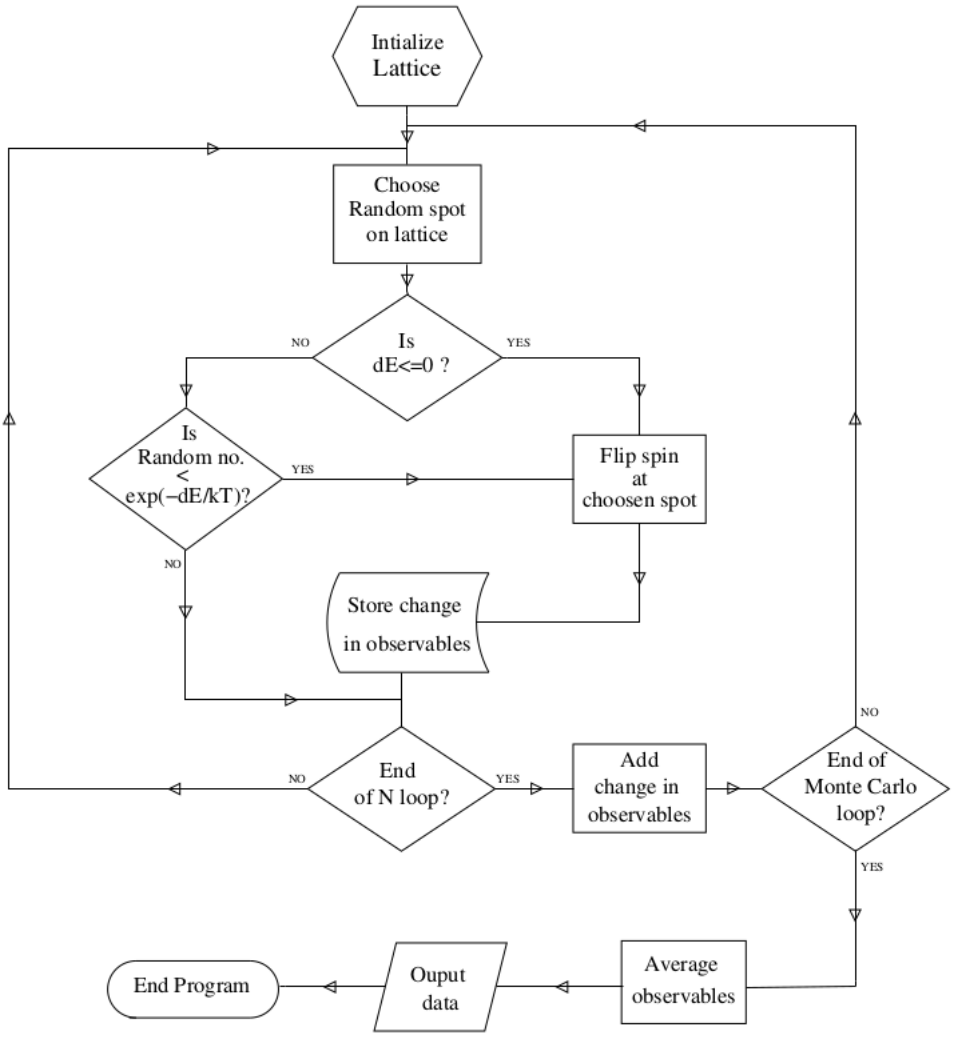

Figure 3: Flowchart of the Metropolis algorithm[3].

3.2 Efficient implementation of ΔE and ΔM

The simulation of the phase transition takes a lot of computational power and time which is the motivation behind not only optimizing the code, but also finding expressions that can be calculated with less effort and reduce the number of floating point operations. In the case of ΔE we get

$$\Delta E = E_2 - E_1 = -J \sum_{\langle kl \rangle}^{N} s_k^2 s_l^2 + -J \sum_{\langle kl \rangle}^{N} s_k^1 s_l^1$$

where 1 and 2 are the indices, k is the neighbors of l and l is the index of the flipped spin. Because we flip one spin at a time, the neighbors of s_l doesn't change. This implies that $s_k^2 = s_k^1 = s_k$. Hence,

$$\Delta E = J \sum_{\langle kl \rangle}^{N} s_k (s_l^1 - s_l^2).$$

This is a binary system, and for that reason the spin s_l^1 can only take the values ± 1. In the case of $s_l^1 = 1$, the value of $s_l^2 = -1$ and $\Delta s_l^{1,2} = 2$. However, if $s_l^1 = -1$ we would get $s_l^2 = 1$ and we end up with a difference of -2. This allows us to write $\Delta s_l^{1,2} = s_l^1 - s_l^2 = 2s_l^1$ which further simplifies the calculation. That is,

$$\Delta E = J \sum_{\langle kl \rangle}^{N} s_k 2 s_l^1 = 2J s_l^1 \sum_{\langle kl \rangle}^{N} s_k.$$

As for the magnetization we get

$$\Delta M = M_2 - M_1 = \sum_{i}^{N} s_i^2 - \sum_{i}^{N} s_i^1 = \sum_{i}^{N} (s_i^2 - s_i^1) = s_l^2 - s_l^1 = -2s_l^1$$
$$\implies M_2 = M_1 - 2s_l^1.$$

It is unnecessary to calculate $e^{-\beta \Delta E}$ every time the current energy is lower than the trail energy. When we flip one spin, ΔE can only take five values, namely $\Delta E \in \{-8, -4, 0, 4, 8\}$ and so we only have calculate the minimum energy four times and the maximum energy eight times. In fact, this can be extended if we recognize that we're only interested in the values for which $\Delta E > 0$ which means that $\Delta E \in \{4, 8\}$. Ultimately we end up with a faster runtime which is a highly desired trait in a program of a system like this.

4 Results and discussion

4.1 Numerical results of 2×2 lattice

It is interesting to see how well the numerical calculations of the 2×2 lattice fare when we compare them to the analytical cases. In section 2.1.2 we found the analytical expressions for the expectationvalues $\langle E \rangle$, $\langle C_v \rangle$, $\langle |M| \rangle$ and $\langle |\chi| \rangle$. With $\beta = J = 1$

the analytical values for the expectationvalues are given by

$$\begin{aligned}\langle E\rangle &= -1.99598\\ \langle C_v\rangle &= 0.0320823\\ \langle |M|\rangle &= 0.998661\\ \langle |\chi|\rangle &= 0.00401074.\end{aligned}$$

The numerical values agree quite well at about 10^7 Monte Carlo cycles as shown in table 2 below. However, the expectationvalue of the energy and the absolute value of the magnetization agrees with the analytic number to some extent already at 10^4 Monte Carlo cycles.

MC cycles	$\langle E\rangle_{Rel.Err.}$	$\langle C_v\rangle_{Rel.Err.}$	$\langle \|\chi\|\rangle_{Rel.Err.}$	$\langle \|M\|\rangle_{Rel.Err.}$
10^4	$1.10 \cdot 10^{-3}$	0.54	0.59	$7.61 \cdot 10^{-4}$
10^5	$2.42 \cdot 10^{-4}$	0.12	0.12	$1.61 \cdot 10^{-4}$
10^6	$2.41 \cdot 10^{-5}$	0.01	0.04	$3.48 \cdot 10^{-5}$
10^7	$1.25 \cdot 10^{-5}$	$6.27 \cdot 10^{-3}$	$8.22 \cdot 10^{-3}$	$9.65 \cdot 10^{-6}$

Table 2: Table of the relative error between the analytical values for the expectationvalues of the dimensionless thermodynamical quantities and the numerical values for $kT/J = 1.0$ which is considered to be a low temperature. The calculations are done with the different Monte Carlo cycles given in the table.

4.2 Equilibrium state for the observables

When the equilibrium situation is reached we want to calculate the thermodynamical quantities at hand due to the fact that we're interested in the system at a constant temperature. To better the realism of our experiment due to the fact that there are normally more than 4 spins in a large scale ferromagnet, we now choose a lattice size of 20×20. The simulation of the system in the ground state compared to a random configuration of spins at low and high temperatures, that is $T = 1.0$ and $T = 2.4$ respectively, will give us a good idea of the behavior of the system before the equilibrium state and of course when it actually reaches that state. We calculate the average energy and magnetization for 5000 M.C. cycles and we can see from figure 4 that they each an equilibrium state quite early. The average energy for the ground state reaches equilibrium as early as after 1000 Monte Carlo cycles for $T = 2.4$, and about the same for the random configuration. As for the lower temperature $T = 1.0$ the equilibrium situation is reached after quite a bit less cycles. Although there are some fluctuations in the average magnetization in the ground state it also stabilizes between 1000 and 2000 cycles which also applies to the random configuration. It is

therefore safe to say that we can start calculating the averages of the observables after about 5000 cycles.

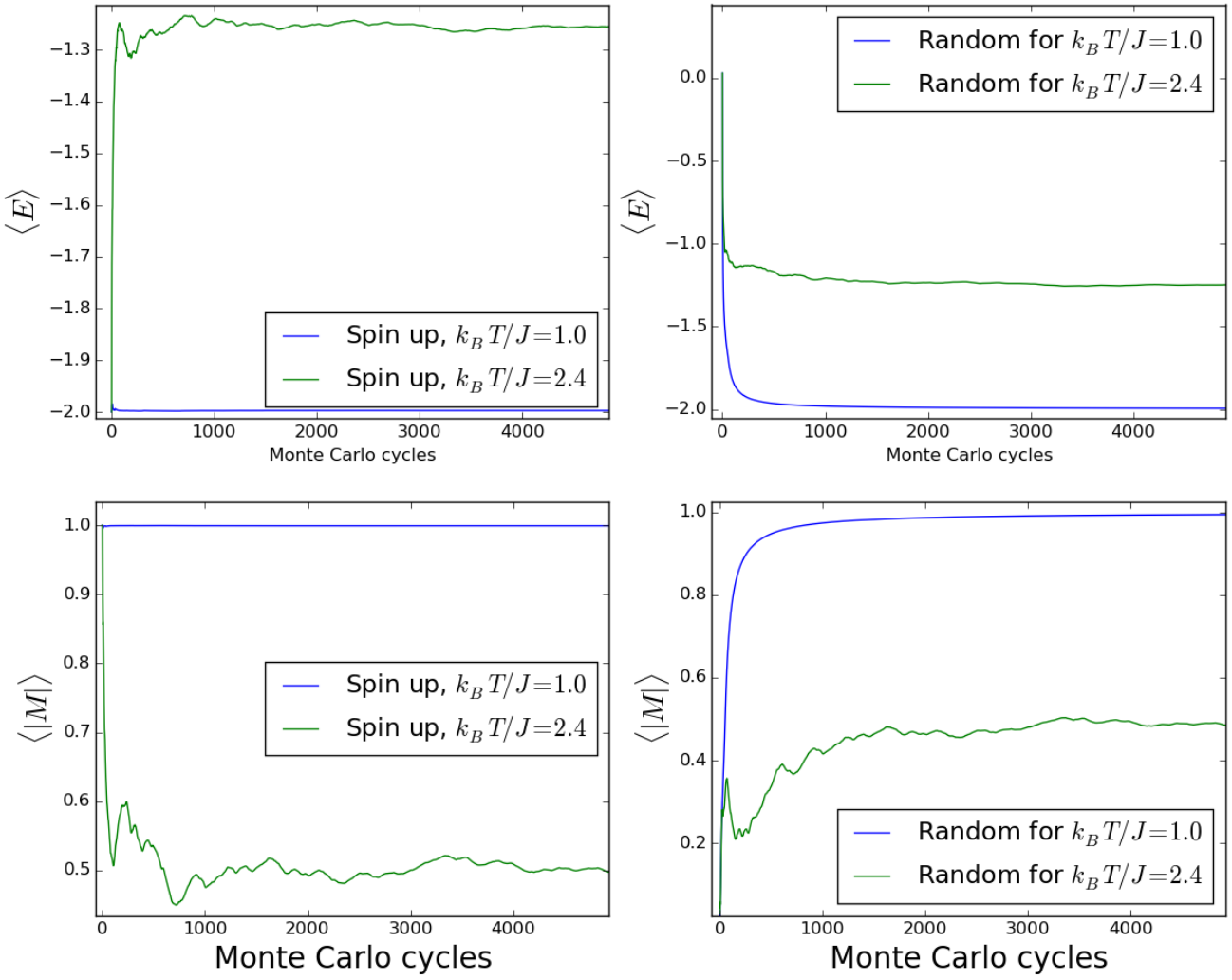

Figure 4: Plots of the averages of the magnetization and energy per spin at different temperatures for 5000 cycles. The averages are calculated with the systems starting out with all spins up which corresponds to the ground state, and in a random configuration.

The number of accepted spins are displayed in figure 5 as a function of Monte Carlo cycle. The striking difference between the two plots lies in the sheer number of accepted states for the temperature $T = 2.4$. This is due to the fact that the spins can move more freely in the system at that temperature. For $T = 1.0$ there are way more accepted states initially for the random configuration than for the ordered configuration, also known as the ground state. This is due to the fact that there are more spins to flip in an unordered state, than in an ordered state. In other words, this happens as a consequence of the comparison between the factor $e^{-\Delta E/T}$ and a random number.

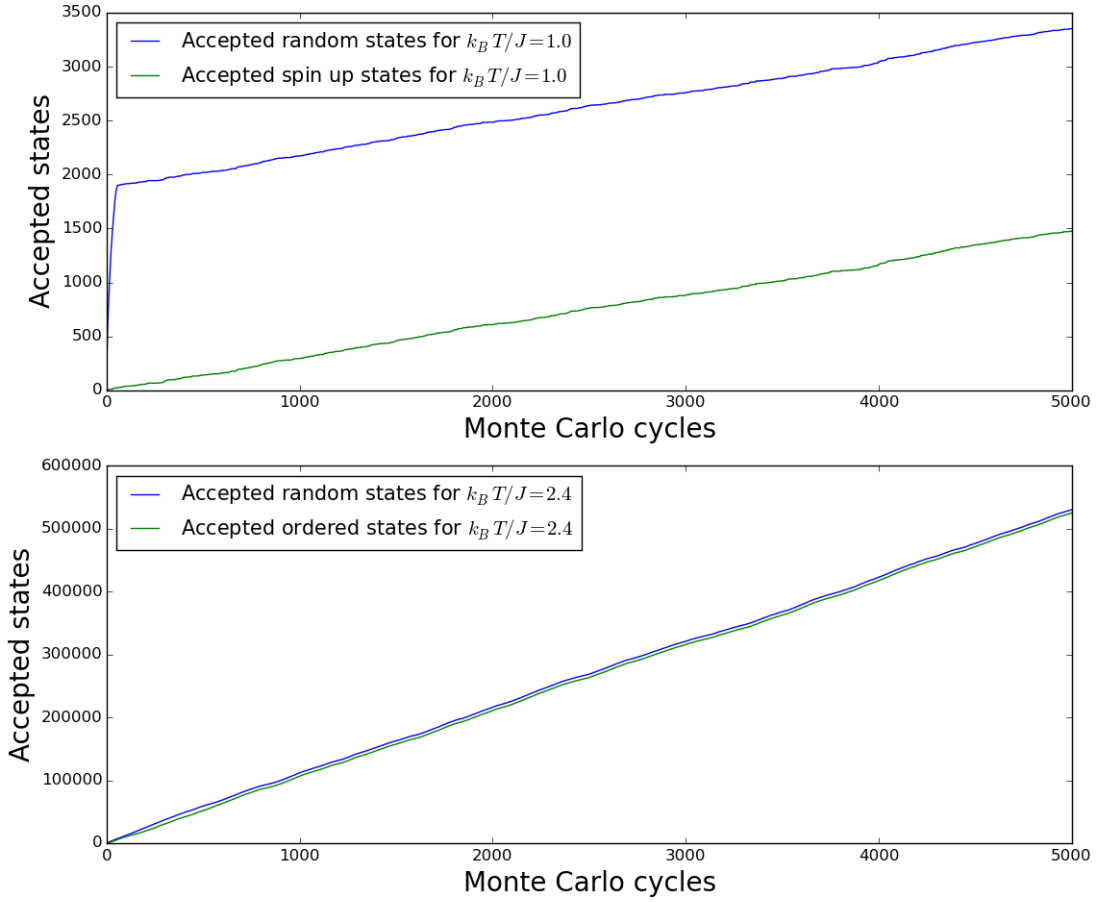

Figure 5: The accepted states in the two different configuration for the temperatures 1.0 and 2.4, respectively.

We can explain the phenomena more precisely if we also conduct a study of the probability of a spin flip as a function of temperature. This can be done by using the same algorithm and simply count the number a given energy E_i occurs, and so the probability is given as the number of times that particular energy was measured divided by the total number of measurements which makes the quantity normalized. That is,

$$P(E_i) = \frac{N_i}{\sum_i N_i}.$$

This will ultimately give us the variance and the expectationvalue of E, and is equivalent to the one we use in the Metropolis algorithm. The variance in the probability of a given energy for $T = 1.0$ is low as one would expect, it's largely oriented around $E = -2.0$ and $E = -1.98$ which matches the analytical expectationvalue well. The reason we expect such a distribution is that the spin system is extremely ordered in the equilibrium state due to the low temperature. As for the higher temperatures, which in our case is at $T = 2.4$, the variance is somewhat larger. The number of possible microstates increases with temperature, which means that this behavior is also what one would expect in such a system.

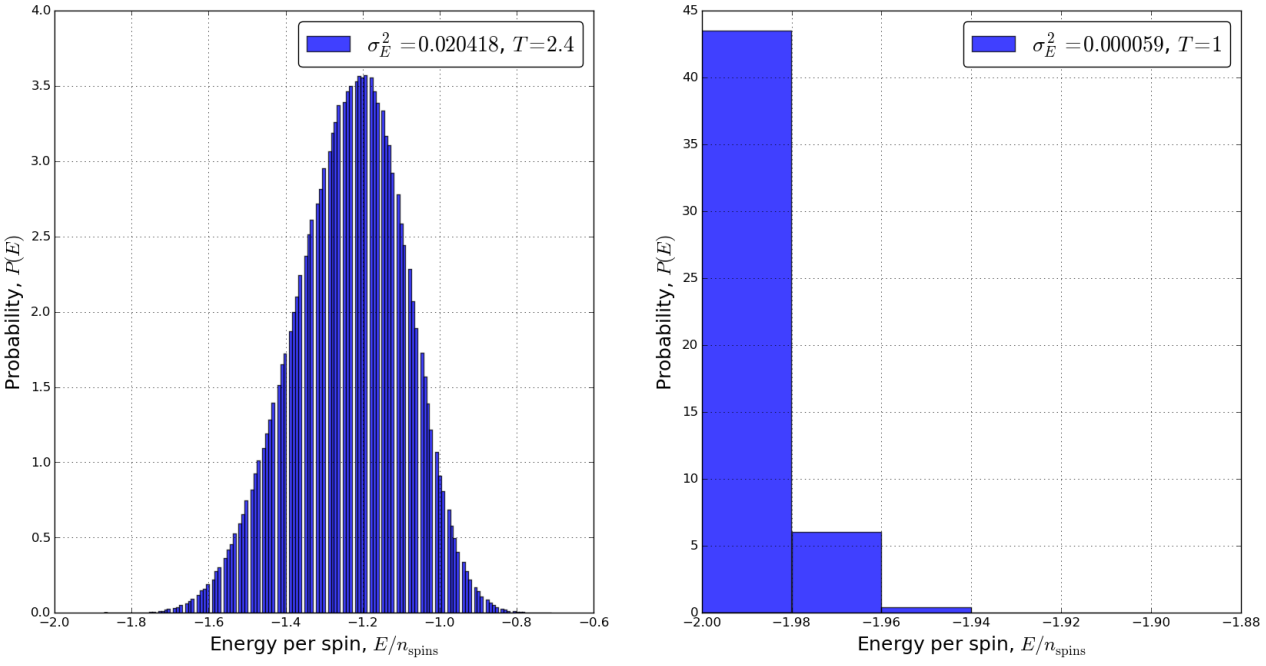

Figure 6: Probability distributions of the energy at temperatures $kT/J = 1.0$ and $kT/J = 2.4$.

4.3 The phase transition at the critical temperature

The number of Monte Carlo cycles plays a crucial role when it comes to the accuracy when we plot the data produced by the program. It is safe to say that 10^6 cycles produces results worth looking at in terms of stability. Lars Onsager calculated the critical temperature of the phase transition in the thermodynamical limit where $L \to \infty$ to be about $T_C = 2.269$. This is impossible for us to achieve at this point, but we can increase the lattice size enough to approximate the exact behavior of the transition. To illustrate the evolution of the transition we have plotted the different observables for $L \in \{40, 60, 100, 140\}$ as a function of temperature in the range $T \in \{2.0, 2.4\}$. As discussed earlier, we can safely say that the system reaches equilibrium after about 5000 cycles and so the measurements are made after this point.

The computation time increases drastically with larger L, so code optimization is key at this point. The Message Passing Interface(MPI) is an excellent tool to drive the runtime down to a minimum together with optimization flags. The runtime for the 140×140 lattice with a temperature step of 0.02 was at about 6 hours which is a lot, but acceptable.

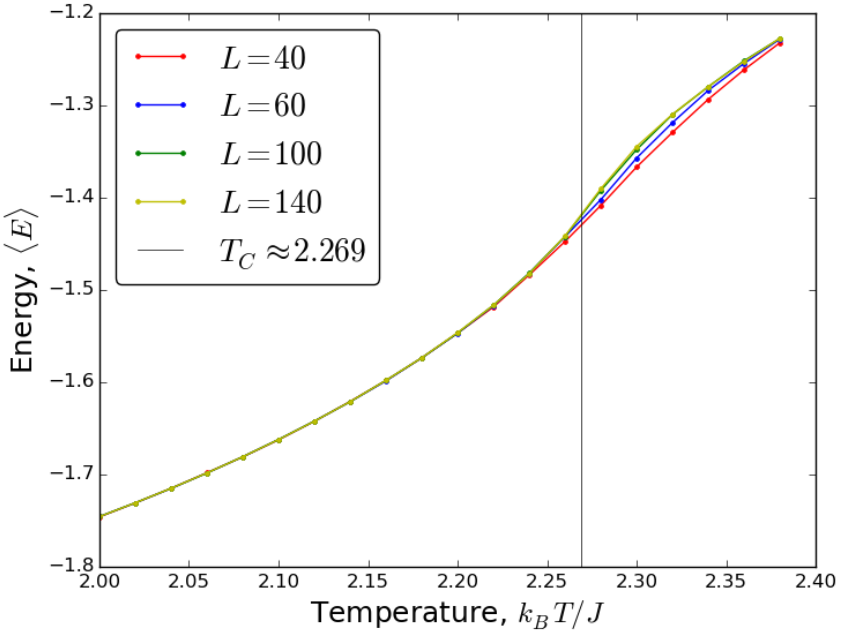

Figure 7: Mean value of the energy in a 40×40, 60×60, 100×100 and 140×140 lattice with the critical temperature calculated by Lars Onsager[1]

Although we cannot replicate the exact result of Onsager's article, there is a distinct change around T_C in the plot of the average energy in figure 7. That is, the energy suddenly increases faster than it does before that point. It is also evident that the statistical data gets better with a larger lattice which is illustrated in figure 8 due to the fact that the real system would be a lot larger than what we're dealing with.

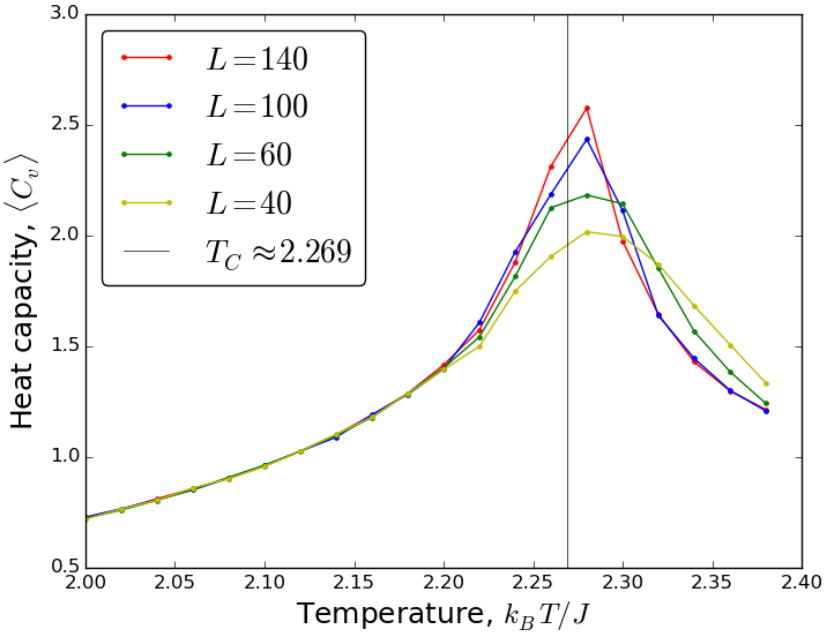

Figure 8: Mean value of the heat capacity in a 40×40, 60×60, 100×100 and 140×140 lattice with the critical temperature calculated by Lars Onsager[1].

The analytical value of the critical temperature is shown in figures of the mean observables that we consider, and the calculated critical temperatures are quite close to the analytical value in the thermodynamical limit. That is, we can see the behavior of the shift towards Onsager's T_C quite clearly in the plots for larger lattice sizes. The computed critical temperatures for the heat capacity is given in table 3 below.

L	$T_C(C_V)$
40	2.295
60	2.285
100	2.280
140	2.275

Table 3: Table of the critical temperatures of the heat capacity measured with a timestep for the temperature of $T_{step} = 0.005$ in the range $[2.25, 2.31]$ to get more accurate results.

Although the value of the critical temperature is the same in the case of the heat capacity for $L = 40$ up to $L = 140$, we can see that the peak gets sharper, so the value would probably vary more with a more accurate step in the temperature.

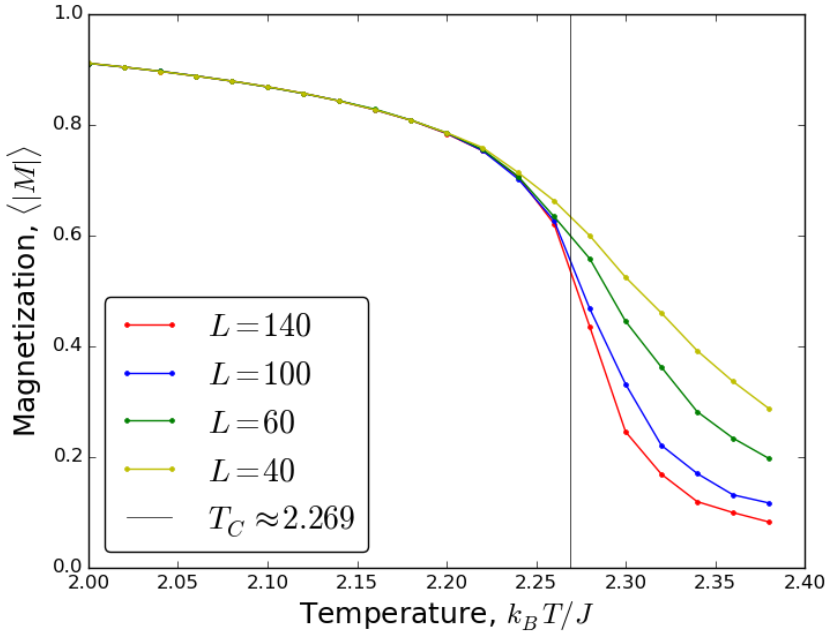

Figure 9: Mean value of the absolute magnetization in a 40×40, 60×60, 100×100 and 140×140 lattice with the critical temperature calculated by Lars Onsager[1]

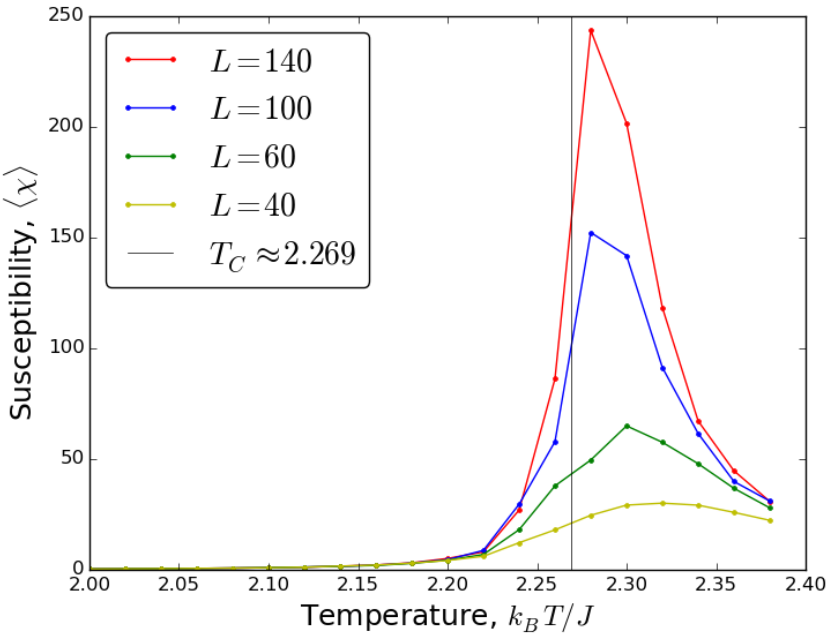

Figure 10: Mean value of the susceptibility in a 40×40, 60×60, 100×100 and 140×140 lattice with the critical temperature calculated by Lars Onsager[1]

In the section 2.1.1 we discussed the phase transitions in the limit $L \to \infty$ and we can make an estimate for T_C using eq.(5) which relates the critical temperature at an infinite lattice size to the finite case that we have to work with. In order to do so one can write a simple python script with the critical temperatures found in the simulation.

$$T_C(L \to \infty) = 2.265 \pm 0.004$$

Which is the mean of both the heat capacity and the susceptibility. The individual values are $T_C(L \to \infty) = 2.266 \pm 0.003$ for the heat capacity and $T_C(L \to \infty) = 2.263 \pm 0.006$ for the susceptibility. The result is quite good compared to Onsager's result, and the error is about 0.004. One way the error could have been made smaller is to add more data points to the calculations, that is, we could for example set $T_{step} = 0.01$ or even $T_{step} = 0.005$, and increase the lattice size, but given the computational power at hand it would be somewhat tedious. A way around this would be to decrease the interval to lie closer to the analytical critical temperature, on the other hand it's interesting to see the behavior some time before and after the phase transition occurs.

5 Conclusion

The simulation of a phase transition in ferromagnetic materials is no laughing matter when it comes to computational speed, and an exact Ising model for this process is not easily accomplished on a computer. This problem, however, can be made considerably more tractable by considering the Metropolis algorithm together with a stochastic process like Monte Carlo. Computers have no concept of infinity, but they do know about large numbers, and for that reason we needed an alternative finite description of the infinite case which was provided by the Monte Carlo simulation and it compared favorably with the theoretical result of Lars Onsager as well as in terms of efficiency. Furthermore, the accuracy of the method is quite good even for small lattices. The use of the absolute magnetization rather than simply the magnetization plays a more vital role than one might initially expect. This is because spontaneous magnetization can arise which would have dire consequences for the susceptibility and the magnetization which would consequently yield inaccurate results for the finite size scaling of the thermodynamical quantities. This approximation of the analytical Ising model is effective and produces good results compared to the theoretical values, but obviously with some small deviations. The finite size scaling was in good agreement with the theoretical exponents as well. The calculated observables around the critical temperature matches the analytical ones well which indicates that the stochastic method used works as it should and is a good method to use for the two dimensional Ising model.

References

[1] Lars Onsager. Crystal statistics i. a. two-dimensional model with an order-disorder transition. Sterling Chemistry Laboratory, Yale University. Physical Review, October 4, 1943.

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[3] Jacques Kotze. Introduction to monte carlo methods for an ising model of a ferromagnet. arXiv:0803.0217v1 [cond-mat.stat-mech] 3 Mar 2008. `http://arXiv.org/abs/0803.0217v1`.