FYS4150
Autumn 2016

Project 4: Phase transitions in magnetic system

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November 18, 2016

Abstract

In this project our aim is to study a widely popular so-called Ising model to simulate phase transitions, our goal is to numerically find the critical temperature or transition temperature for the two dimensional Ising model by using the metropolis algorithm with periodic boundary conditions. We will begin with testing the implementation of the algorithm, first by comparing with the theoretical values calculated for a small system. And then we will see if the algorithm behaves as expected according to our physical intuition for a larger system. We will look at the thermodynamic properties of a system under Ising model and see how these behave around the critical temperature. Finally, we estimate the critical temperature of the thermodynamic limit. When we have found a estimate for the critical temperature, we will compare it to Lars Onsagers analytical result. We should end up with an acceptable estimate, but to see that we would like to have time to make more accurate time-consuming calculations. All source codes used are hosted on Github, at: `https://github.com/sarahbra/Project4/tree/master/Project4/Project4A`

Contents

1 Introduction

Ising model deals with the physics of phase transition, which occur when a small change in a parameter such as pressure or temperature cause a large-scale qualitative change in the state of a system. Phase transitions are common in physics and can be seen in everyday life: we see one, for instance whenever we put a kettle of water on stove, or when temperature drops very low in winters. Other example includes the formation of binary alloys and the well known phenomenon of ferromagnetic. " Ferromagnetism arises when a collection of atomic spins align such that their associated magnetic moments all point in the same direction, yielding a net magnetic moment which is macroscopic in size. The simplest theoretical description of ferromagnetic is called the Ising model". http://farside.ph.utexas.edu/teaching/329/lectures/node110.html

A second order phase transition at the critical temperature T_c is described by a macroscopic change to a system. At this temperature (T_c) some thermodynamic values approaches zero with an infinite slope and disappears. Other variables are discontinuous or diverge at the critical temperature in the thermodynamic limit. In this report we will look at a second order phase transition by using the Ising model and the metropolis algorithm to simulate results. In other words we will primarily look at Ising model's overall thermodynamic characteristics. The approach used in this project is also applicable for other physical models and therefore very useful and handy.

2 Theory

2.1 Statistical physics in a nutshell

It would be beyond the scope of this report to discuss in detail statistical mechanics of magnetic systems. In this context only the relevant aspects of statistical physics are discussed.

2.2 Observable

In statistical physics, expectation values of quantities such as the energy, magnetization, specific heat etc. -generally called observable- are computed by performing a trace over the partition function Z. Within the canonical ensemble where the temperature T is fixed, the expectation value of an observable $\mathcal{O}$ is given by:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_s \mathcal{O}(s) e^{-\frac{H(s)}{kT}} \tag{1}$$

The sum over all states s in the system, Z is the partition function which normalized the equilibrium Boltzmann distribution. $P_{eq}(s) = \frac{1}{Z} e^{-\beta E_s}$. One can show that internal energy of the system is given by: $E = \langle H(s) \rangle$, whereas the free energy $F = -kTlnZ$. All thermodynamic quantities can be computed directly from the partition function and expressed as derivatives of the free energy. Because the partition function is closely related to Boltzmann distribution. In general we have;

$$\langle \mathcal{O} \rangle = \frac{\sum_s \mathcal{O}(s) e^{-\frac{H(s)}{kT}}}{\sum_s e^{-\frac{H(s)}{kT}}} \tag{2}$$

Equation above can be extended with a distribution for the states, i.e.

$$\langle \mathcal{O} \rangle = \frac{\sum_s [\mathcal{O}(s) e^{-\frac{H(s)}{kT}} / P(s)] P(s)}{\sum_s [e^{-\frac{H(s)}{kT}} / P(s)] P(s)} \tag{3}$$

If $P(s)$ is the Boltzmann distribution then the factors cancel out and we get:

$$\langle \mathcal{O} \rangle = \frac{1}{M} \sum_k \mathcal{O}(s_k) \tag{4}$$

Now states s_k are selected according to the Boltzmann distribution. Problem now is to find an algorithm that allows for a sampling of the Boltzmann distribution, this method is known as the metropolis algorithm. The explanation of this method will be given later.

2.3 The Ising model

Magnetism in matter is caused by charged particles moving in closed orbits or spinning around their axes. Recall that a current loop creates a magnetic field according to Ampere's law. A spinning charge particle has a magnetic moment associated with it. A simple classical approximation to an atomic or electronic magnetic moment is provided by an Ising spin. The simplicity and rich behavior of the Ising model makes it the prefect platform to study magnetic systems, as well as for testing of algorithms. For simplicity, it is assumed that the magnetic moments can only point in one space direction. The classical spins $s_k = \pm 1$ are placed on a hyper cubic lattice with nearest-neighbor interactions. Therefor the Hamiltonian or the interaction energy can be approximated by:

$$H = \sum_{<kl>} J_{kl} s_k s_l - H \sum_k s_k \tag{5}$$

The first term describes the pairwise interaction between two neighboring spins s_k and s_l. The force between two magnets falls off rather rapidly, like r^{-3}, so a reasonable approximation is to assume that any spin interacts only with its 4 nearest neighbors- north, south, east and est. When $J_{kl} < 0$ the energy is minimized by aligning all spins, i.e. ferromagnetic order, whereas when $J_{kl} > 0$ the energy is minimized by ensuring that the product over all neighboring spins is negative. In this case anti-ferromagnetic order is obtained. The " $\langle kl \rangle$ " represents a sum over nearest neighbor pairs of spins on the lattice. The second term represents an external magnetic field which couples to the magnetization $M = \sum_k s_k$. This model is exactly solvable in 1D and in 2D for $H = 0$. In space dimensions larger than one it undergoes a finite-temperature transition into on ordered state. The temperature-dependent transition in the ferromagnetic case is to measure the magnetization of the system. At low temperature when all spins are aligned, the magnetization is close to unity. For larger temperature; much larger than the transition temperature T_c, spins fluctuate widely and so on average, the magnetization is zero. For this reason, the magnetization plays the role of an order parameter that is large in the ordered phase and zero otherwise. Amazingly the Ising model captures all interesting phenomena found in statistical physics and phase transitions.

2.4 The Ising model in 2D

Without an external magnetic field ($H = 0$) the energy of the Ising model can be written as;

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{6}$$

where spin can take values; $S_k = \pm 1$. N is the total number of spin and variable J represents a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $\langle kl \rangle$ indicates that we sum over nearest neighbors only, as explained earlier. Assuming a ferromagnetic ordering, viz $j > 0$ we will use periodic boundary conditions and metropolis algorithm. This means that the particles along the edge 'looks for ' particles along the opposite edge. For example if we 'have' a particle at position (L, L) in the grid, both the particle at position (1, L) and (L, 1) and interacts with this particle as if they were neighbors. This represents that we have lattice structure, the system we are looking at is repeated further in all directions. We choose to use a square lattice of L spins in x and y direction. The total number of spins is then $N = L^2$ and the total number of micro-states, the different configurations the spins can have is given by $M = 2^N$. The partition function for such system is expressed as:

$$Z = \sum_{i=1}^{M} e^{\beta E_i} \tag{7}$$

where the sum extend over all micro state M, and β being inverse of temperature $[\beta = \frac{1}{k_B T}]$, k_B is Boltzmann constant.

2.5 A simple 2×2 lattice, analytical expression

Let us first assume that there is only two spins in each dimension [in x and y direction], that is $L = 2$. Which means $N = 2 * 2 = 4 \Rightarrow M = 2^4 = 16$. whence 16 micro states or possible configurations. For finding the expression for partition function we have to find the energies: $Z = e^{-\beta E_1} + e^{-\beta E_2} + ... + e^{-\beta E_{16}}$. We can visualize the spin system in a two dimensional matrices on the following form:

$$\begin{bmatrix} (0,0) & (0,1) \\ (1,0) & (1,1) \end{bmatrix}$$

$E_1 = 0$ $\begin{pmatrix} \uparrow & \uparrow \\ \downarrow & \downarrow \end{pmatrix}$	$E_2 = 0$ $\begin{pmatrix} \uparrow & \downarrow \\ \uparrow & \downarrow \end{pmatrix}$	$E_3 = 0$ $\begin{pmatrix} \downarrow & \uparrow \\ \downarrow & \uparrow \end{pmatrix}$	$E_4 = 0$ $\begin{pmatrix} \downarrow & \downarrow \\ \uparrow & \uparrow \end{pmatrix}$
$E_5 = 0$ $\begin{pmatrix} \uparrow & \uparrow \\ \uparrow & \downarrow \end{pmatrix}$	$E_6 = 0$ $\begin{pmatrix} \uparrow & \uparrow \\ \downarrow & \uparrow \end{pmatrix}$	$E_7 = 0$ $\begin{pmatrix} \uparrow & \downarrow \\ \uparrow & \uparrow \end{pmatrix}$	$E_8 = 0$ $\begin{pmatrix} \downarrow & \uparrow \\ \uparrow & \uparrow \end{pmatrix}$
$E_9 = 0$ $\begin{pmatrix} \downarrow & \downarrow \\ \downarrow & \uparrow \end{pmatrix}$	$E_{10} = 0$ $\begin{pmatrix} \downarrow & \downarrow \\ \uparrow & \downarrow \end{pmatrix}$	$E_{11} = 0$ $\begin{pmatrix} \uparrow & \downarrow \\ \downarrow & \downarrow \end{pmatrix}$	$E_{12} = 0$ $\begin{pmatrix} \downarrow & \uparrow \\ \downarrow & \downarrow \end{pmatrix}$
$E_{13} = 8J$ $\begin{pmatrix} \uparrow & \downarrow \\ \downarrow & \uparrow \end{pmatrix}$	$E_{14} = 8J$ $\begin{pmatrix} \downarrow & \uparrow \\ \uparrow & \downarrow \end{pmatrix}$	$E_{15} = -8J$ $\begin{pmatrix} \downarrow & \downarrow \\ \downarrow & \downarrow \end{pmatrix}$	$E_{16} = -8J$ $\begin{pmatrix} \uparrow & \uparrow \\ \uparrow & \uparrow \end{pmatrix}$

Table 1: Spin configurations with their corresponding energies for two spin system

$E_1 = 0$ $\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}$	$E_2 = 0$ $\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$	$E_3 = 0$ $\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix}$	$E_4 = 0$ $\begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}$
$E_5 = 0$ $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	$E_6 = 0$ $\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$	$E_7 = 0$ $\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$	$E_8 = 0$ $\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$
$E_9 = 0$ $\begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}$	$E_{10} = 0$ $\begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}$	$E_{11} = 0$ $\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}$	$E_{12} = 0$ $\begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$
$E_{13} = 8J$ $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$	$E_{14} = 8J$ $\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$	$E_{15} = -8J$ $\begin{pmatrix} -1 & -1 \\ -1 & -1 \end{pmatrix}$	$E_{16} = -8J$ $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Table 2: Spin configurations with their corresponding energies for two spin system

From table 2.1 and table 2.2 we see that there are only three possible value of energy for the different configurations, $E \in [-8J, 0, 8J]$ with corresponding multiplicity $[2, 12, 2]$. We observe from table 2.2 that there are two configurations with $E = 8J$ corresponding to the configuration with spin aligned in the two diagonals. There are two configurations with $E = -8J$ which corresponds to configuration with all the spin aligned in both directions. Leaving all the other twelve configurations with $E = 0J$. As mentioned in theory section the particle on position (L, L) in the grid with spin (1, 1) has a neighbor at position (0, L) with corresponding spin (0,1) twice. The product of $s_k s_l$ must be calculated once. For finding the energy we sum over the nearest neighbors for all the spin in the system as follow;
$E = -J\left(s(0,0)[s(1,0) + s(0,1)] + s(0,1)[s(1,1) + s(0,0)] + s(1,0)[s(0,0) + s(1,1)] + s(1,1)[s(0,1) + s(1,0)]\right)$.
Thus the partition function can be found as:

$$Z = 2e^{-\beta(-8J)} + 2e^{-\beta 8J} + 12e^{-\beta 0J} = 2e^{-\beta(-8J)} + 2e^{-\beta 8J} + 12 = 2(e^{+\beta 8J} + e^{-\beta 8J}) + 12.$$

which can be written further by using the trigonometric function $cosh(x) = \frac{1}{2}(e^{-x} + e^{(}x))$ in following final form:

$$2(e^{\beta 8J} + e^{-\beta 8J}) + 12 \Rightarrow 4cosh(\beta 8J) + 12$$

The partition function will help us calculating a range of values, such as expectation value of the energy, magnetic moment, heat capacity and susceptibility. We begin with finding the expectation value for the energy by using equation 1 :

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

$$\Rightarrow \frac{1}{Z}\left[2(-8J)e^{\beta 8J} + 2(8J)e^{-\beta 8J}\right] = -\frac{16J}{Z}\left[e^{\beta 8J} - e^{-\beta 8J}\right]$$

by using trigonometric function this expression can be rewritten as;

$$-\frac{32J}{Z} sinh(\beta 8J)$$

.

S ↑	E	M	Micro-states
4	-8J	4	1
3	0	2	4
2	0	0	4
2	8J	0	2
1	0	-2	4
0	-8J	-4	1

Table 3: M with the corresponding E and multiplicity for the spin two system.

From table 2.3 we can see that for the expectation value of $|M|$ we have one configuration with $M = 4$ and another with $M = -4$ corresponding to the lattice with all the spins aligned in the same direction, either all up or down. We also know that both of these configuration have energy $E_i = -8J$. Then we have four configuration with $M = 2$ and four with $M = -2$ corresponding to the lattices with 3 spin aligned in one direction and one in the opposite direction [see table 2.1]. In our case all these configurations have $E_i = 0J$, and all other six configurations have $M = 0$. Since we define the magnetization M as the sum of all spins s. We can easily see that for 2×2 system there are 5 possible values for M, $M \in [4, 2, 0, -2, -4]$. The expectation value of the magnetization and the magnetization squared reads as:

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{M} M e^{-\beta E_i} \tag{8}$$

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{i=1}^{M} M^2 e^{-\beta E_i} \tag{9}$$

Since we are considering the absolute value of magnetization, the configuration with opposite M have to be put together. The micro-states with opposite magnetization have the same multiplicity so they cancel each other out. By looking at the table 2.2 and equation of $< M >$ we see that the expectation value of the magnetization is zero for all temperatures. For simulation of a very large system with large L, the numerical value of $< M >$ will not reach zero unless the simulation is run for extremely long time. It happens due to a long time for the simulation to run through all the possible micro-states after the simulation have reached a steady state. Since we want to minimize the execution time for the simulation and want to measure a reasonable large amount of measurements for the magnetization and susceptibility, we must choose the absolute value of the magnetization in defining the susceptibility. For the absolute value of magnetization we thus have only three possible values. $M \in 4, 2, 0$. By using multiplicity and magnetization we can calculate the absolute value of magnetization as:

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |M| \, e^{-\beta E_i} = \frac{1}{Z}\left(8 \cdot e^{-\beta(-8J)} + 16\right)$$

$$\Rightarrow \frac{8(e^{\beta 8J} + 2)}{4cosh(\beta 8J) + 12} = \frac{2(e^{\beta 8J} + 2)}{cosh(\beta 8J) + 3}$$

similarly we get the value of the $\langle |M^2| \rangle$:

$$\langle |M^2| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |M^2| \, e^{-\beta E_i} = \frac{1}{Z} \left(32 \cdot e^{-\beta(-8J)} + 32 \right)$$

$$\frac{32}{Z} \left(e^{\beta 8J} + 1 \right) = \frac{8(e^{\beta 8J} + 1)}{cosh(\beta 8J) + 3}.$$

Heat capacity C_v is defined as; $C_v = \frac{1}{k_B T} \sigma_E^2 = \frac{1}{k_B T} \left(\langle E^2 \rangle - \langle E \rangle^2 \right)$. Where k_B is Boltzmann constant, T is temperature, from this expression we see that we need to calculate the term $\langle E^2 \rangle$. We have already found an expression for $\langle E \rangle$ which means we only need to find the expectation value of energy squared using same approach.

$$\langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^{M} E_i^2 e^{-\beta E_i} = \frac{1}{Z} \left[2 \cdot (-BJ)^2 e^{\beta 8J} + 2 \cdot (8J)^2 e^{-\beta 8J} \right] = \frac{64 J^2 cosh(\beta 8J)}{cosh(\beta 8J) + 3}$$

Inserting into C_v-term gives:

$$C_v = \frac{1}{k_B T} \left[\frac{64 J^2 cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(- \frac{8J sinh(\beta 8J)}{cosh(\beta 8J) + 3} \right)^2 \right]$$

after some algebra and rearrangement we get:

$$\frac{64 J^2 \beta}{T} \left[\frac{1 + 3cosh(\beta 8J)}{(cosh(\beta 8J) + 3)^2} \right]$$

Finally we can calculate the susceptibility by same approach and by the term $\chi = \frac{1}{k_B T} (\langle |M^2| \rangle - \langle |M| \rangle^2)$:

$$\chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle |M| \rangle^2) = \frac{1}{k_B T} \left[\left(\frac{2(e^{(}\beta 8J) + 2)}{cosh(\beta 8J) + 3} \right) - \left(\frac{8(e^{\beta 8J} + 1)}{cosh(\beta 8J) + 3} \right)^2 \right]$$

$$= 4\beta \left[\frac{2(e^{\beta 8J} + 1)(cosh(\beta 8J) + 3) - (e^{\beta 8J} + 2)^2}{(cosh(\beta 8J) + 3)^2} \right].$$

In order to test the implementation of the numerical method for the "$L = 2$" system, the theoretical values which will be used, should be expressed in terms of scaled temperature. This include the equation for the expectation values, the heat capacity and the susceptibility.

$$T^* = T \frac{k_b}{J} \Rightarrow T = T^* \frac{J}{k_b} \Rightarrow \beta = \frac{1}{k_b T} = \frac{1}{k_b T^* (\frac{J}{k_b})} = \frac{1}{T^* J}$$

Set $J = 1$, such that;

$$\beta = \frac{1}{T^*} \Rightarrow T^* = \frac{1}{\beta}$$

We will use T^* in the numerical calculations. Scaling the heat capacity as:

$$C_v^* = \frac{C_v}{k_b} = \frac{64}{T^* 2} \frac{1 + 3cosh(8/T^*)}{(cosh(8/T^*) + 3)^2}$$

For the 2×2 system the expectation values and the susceptibility can be written in term of T^* as:

$$\langle E \rangle = - \frac{8 sinh(8/T^*)}{cosh(8/T^*) + 3}$$

$$\langle E^2 \rangle = \frac{64 J^2 cosh(8/T^*)}{cosh(8/T^*) + 3}$$

$$\langle |M| \rangle = - \frac{2(e^{8/T^*} + 2)}{cosh(8/T^*) + 3}$$

$$\langle M^2 \rangle = \frac{8(e^{8/T^*} + 1)}{cosh(8/T^*) + 3}$$

$$\xi = \frac{4}{T^*} \frac{2(e^{8/T^*} + 1)(cosh(8/T^*) + 3) - (e^{8/T^*} + 2)^2}{(cosh(8/T^*) + 3)^2}$$

2.6 Phase transitions

Physically a phase transition is a point in parameter space, where the physical properties of a many-body system undergoes a sudden change. An example is the para-magnet to ferromagnetic transition in Iron(Fe) or Nickel(Ni). Mathematically a phase transition is a point in parameter space, where the Helmholtz free energy $F = -k_B T ln Z$ becomes a non-analytic function of one of its parameters *i.e. free energy or some of its derivatives obtains singularity or becomes discontinuous* in the thermodynamic limit. For a finite system this can never happen, because, the partition function $Z = \sum_k e^{-\frac{E(k)}{k_b T}}$ is a finite sum over finite, positive terms. Therefor all derivatives are finite and well defined as well. Phase transitions are usually characterizes in two categories:

First Order Phase Transitions. In this case the free energy is continuous, but a first derivative is discontinuous. At the transition there is phase coexistence, meaning that two or more different phases can exists simultaneously(e.g. water and ice at some specific temperature and pressure) . The magnetization per site is a first order derivative of the free energy with respect to the magnetic field H. Therefore the phase transition at $H = 0$ is first order see figure 1.

Second Order Phase Transitions. These are characterized by a divergence in one of the higher order derivatives ("susceptibilities") of the free energy. In this project our task is to study the second order phase transitions. Figure 1 and figure 1 shows a schematic of phase transitions.

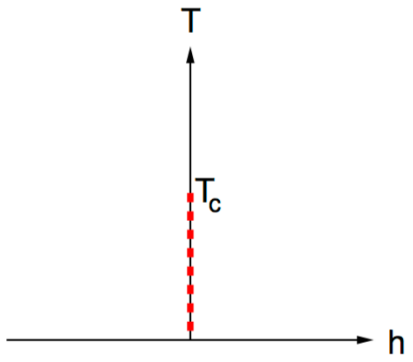

Figure 1: The first order phase transition as a function of T for $h = 0$.

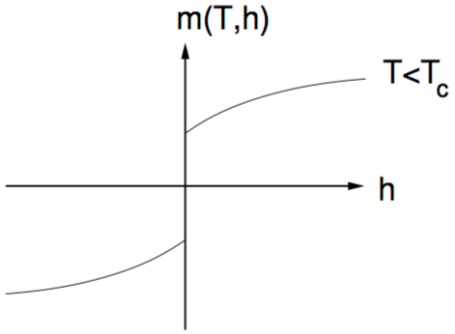

Figure 2: Phase diagram for the para-magnetic to ferromagnetic transition. The magnetization per site $m(T, h)$ jumps when crossing zero for $T < T_c$.

Continuous phase transitions have no latent heat at the transition and are easier to describe. At a continuous phase transition the free energy has a singularity that usually manifests itself via a power-law behavior of the derived observable at criticality. In other words near T_c critical temperature where the phase transition occurs, we can characterize the behavior of many physical quantities by power-law. As an example the mean magnetization of the Ising model is given by

$$\langle M(T) \rangle \approx (T - T_c)^{\beta}$$

where $\beta = \frac{1}{8}$ is a so-called critical exponent. The magnetization does not diverge, but has a singular link at T_c with $\beta > 0$. The specific heat c_V has a singularity at T_c with a similar relation:

$$c_V(T) \approx |T_c - T|^{-\alpha}$$

where α can be both negative and positive, but is zero in this case. Similar relation applies to susceptibility as well: $\chi(T) \approx |T_c - T|^{\gamma}$, and $\gamma = \frac{7}{4}$. The correlation length ξ which gives us the measure of correlations and order in a system ("is expected to be of the order of the lattice spacing for $T >> T_c$, because the spins are more and more correlated as T approaches T_c") diverges at the transition.

$$\xi(T) \approx |T - T_c|^{-v}$$

A second order phase transition is characterized by a correlation length which spans the whole system. How can we determine the critical exponents of a system by simulating finite lattice? When the systems are not infinitely large, the critical behavior is smeared out. One can show that the non-analytic part of a given observable can be described by a finite size scaling. In other words; Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice, i.g. it can be shown that the critical exponents are related via scaling relations. Through scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. Models in statistical physics generally obey universal behavior, if the lattice geometry is kept the same, the critical exponents only depends on the order parameters symmetry. Therefor is is enough to determine the location of the transition temperature T_c, as well as two independent critical exponents to fully characterize the universality class of the system. The transition/critical temperature is scale as:

$$T_c(L) - T_c(L = \infty) = aL^{-\frac{1}{v}}$$

with a a constant and v defined (see at the end of this section). We set $T = T_c$ and obtain a mean magnetization

$$\langle M(T) \rangle \approx (T - T_C)^{-\beta} \rightarrow L^{\frac{-\beta}{v}}$$

a heat capacity

$$c_V(T) \approx |T_c - T|^{-\gamma} \rightarrow L^{\frac{-\alpha}{v}}$$

and susceptibility

$$\xi(T) \approx |T_c - T|^{-\alpha} \rightarrow L^{\frac{\gamma}{v}}$$

with defined $v = 1$ in the expression of ξ, we can estimate the critical temperature with the numerical results and compare with the theoretical values of the critical temperature $T_c = 2/ln(1+\sqrt{2} \approx 2.269$. Rewrite the equation of critical temperature given above and using $T_c(L = \infty)x$ for the variable we want to estimate and using two values of L and combining them we obtain.

$$x = \frac{T_c(L*)L* - T_c(L)L}{L* - L}$$

2.7 Equilibrium time

In order to obtain a correct estimate of an observable $\mathcal{O}$, it is necessary to ensure that one actually sample an equilibrium state. Because in general the initial configuration of the simulation can be chosen at random, the system have to evolve for several MC-steps before an equilibrium state at a given temperature is obtained. The time until the system is in thermal equilibrium is called equilibrium time (τ_{eq}) and depends on the size of the system (e.g the number of spins $N = L^d$) and increases with decreasing temperature. In general it is measured in units of Monte Carlo sweeps i.e. $1MCS = N$ spin updates. In practice all measured observably should be monitored as a function of MCS to ensure that the system is in thermal equilibrium. Some observable such as energy reaches equilibrium faster than others such magnetization and thus the equilibrium times of all observable measured need to be considered.

3 Methods or Algorithms

3.1 Metropolis algorithm

The idea of Metropolis is the following: In order to evaluate equation. 2 we generate a Markov chain of successive states, $s_1 \rightarrow s_2 \rightarrow ...$, the new state is generated from the old state with transition probability $\mathcal{P}(s \rightarrow s^{'})$ such that it occurs with a probability given by the equilibrium Boltzmann distribution. In the Markov process the state s occurs with probability $\mathcal{P}_k(s)$ at the kth time step, expressed by equation:

$$\mathcal{P}_{k+1}(s) = \mathcal{P}_k(s) + \sum_{s^{'}}[\mathcal{T}(s^{'} \rightarrow s)\mathcal{P}_k(s^{'}) - \mathcal{T}(s \rightarrow s^{'})\mathcal{P}_k(s)] \tag{10}$$

The sum is over all states $s^{'}$ and the first term in the sum describes all processes reaching state s, while the second term describes all processes leaving state s. The aim is that for $k \rightarrow \infty$ the probability $P_k(s)$ reach a stationary distribution described by the Boltzmann distribution. The transition probability $\mathcal{T}$ can be modified such that for $\mathcal{P}_k(s) = \mathcal{P}_{eq}(s)$ all term in sum vanish, i.e. for all s and $s^{'}$ the condition balance $\mathcal{T}(s^{'} \rightarrow s)\mathcal{P}_{eq}(s^{'}) = \mathcal{T}(s \rightarrow s^{'})\mathcal{P}_{eq}(s)$ must hold. The ratio of transition probabilities depends only on the change in energy ΔE when the system has assumed the equilibrium probabilities. The pseudo code for Metropolis algorithm (for a Monte Carlo simulation) as follows:

1. The system is in one spin state with energy E.
2. Establish an initial configuration.
3. Make a trail change the initial configuration, for example, choose a spin and flip it.
4. Compute the change in energy of the system $\Delta E = E_t - E_b$ due to the trail change
   - If $\Delta E <= 0$, accept the trial state(new configuration) as the new state and repeat step $2-5$.
   - If ΔE is positive, calculate the "transition probability" $\omega = e^{-b\Delta E}$
5. Generate a random number r in the interval $[0, 1]$
   - If $r <= \omega$, then accept the new configuration as new state, otherwise retain the previous configuration.

   Step 2-5 are repeated $L \times L$ times to obtain sufficient number of configurations or "trails" (one Monte Carlo cycle) Update various expectation values. One MC cycle correspond to one loop with the possibility of flipping one spin throughout the lattice. Meaning that when we have summed over all spins.

3.2 $\Delta E, \Delta M$ and ω

Since we want to simulate a large numbers of MC cycles, therefor it is necessary to code the calculation of ΔE efficiently. The energy difference is written as follow:

$$\Delta E = E_2 - E_1 = -J \sum_{<kl>}^{N} s_{k,2}s_{l,2} + J \sum_{<kl>}^{N} s_{k,1}s_{l,1} \tag{11}$$

where the index k is the neighboring spin of spin l, l was flipped. As mentioned earlier we flip one spin at a time, the spin of s_l are unchanged i.g. $s_{k,2} = s_{k,1} = s_k$. The ΔE can be expressed as:

$$\Delta E = J \sum_{<kl>}^{N} s_k s_{l,1} - J \sum_{<kl>}^{N} s_k s_{l,2} = J \sum_{<kl>}^{N} s_k(s_{l,1} - s_{l,2}) \tag{12}$$

We know that the spin can only take two values, meaning that $s_{l,1}$ can be either 1 or -1. If $s_{l,1} = 1$ then after flipping it will take value $s_{l,2} = -1$ and $s_{l,1} - s_{l,2} = 1 - (-1) = 2$. If $s_{l,1} = -1$ then

$s_{l,2} = 1$ and $s_{l,1} - s_{l,2} = -1 - 1 = -2$. Therefor $s_{l,1} - s_{l,2} = 2s_{l,1}$ and we get new expression for ΔE as:

$$\Delta E = J \sum_{<kl>}^{N} s_k \cdot 2s_{l,1} = 2Js_{l,1} \sum_{<kl>}^{N} s_k \tag{13}$$

similarly we get expression for ΔM:

$$\Delta M = M_2 - M_1 = \sum_{i}^{N} s_{i,2} - \sum_{i}^{N} s_{i,1} = s_{l,2} - s_{l,1} = -2s_{l,1} \Rightarrow M_2 = M_1 - 2s_{l,1} \tag{14}$$

These expression; equation 6 and equation 8 of differences makes the execution time much shorter/faster for the algorithm of flipping the spin. Since we want to avoid calculating the exponential of the energy difference, the value $\omega = e^{-\beta \Delta E}$ for the trail energy is higher than the current energy for every time. This can be avoided because we know that in 2D the ΔE takes only five possible values when we flip only one spin at a time, i.e. $\Delta E \in [-8, -4, 0, 4, 8]$. Thus the energy maximum have to change in 8 steps and the energy minimum in steps of 4 when flipping one spin at a time. There are only 5 possible values for ω for a given temperature, we use ω only when $\Delta E > 0$ which means $\Delta E \in [4, 8]$. Thereby for a given temperature we only calculate two values of ω and pass it to the metropolis test which use the corresponding value to the energy difference ΔE.

4 Implementation and results

4.1 The 2×2 system

We begin with comparing the result for metropolis algorithm with the theoretical values for the $L = 2$ system calculated in theory section. We have collected data we got through Metropolis algorithm with different number of Monte Carlos cycles. The analytic value of energy is $\langle E \rangle = -7.9839J$ and the analytic value of heat capacity is $C_V = 0.03208233$ while the analytic value of susceptibility is $\xi = 0.0004010739$. Table 4 below shows the numerical values of heat capacity and susceptibility.

MC cycles	Energy	$\lvert M \rvert$	Numeric C_v	Numeric ξ	
10^0	-8	4.0	0	0	
10^1	-8	4.0	0	0	
10^2	-8	4.0	0.047856	0.005984	
10^3	-7.976	3.9960000	0.0494462	0.00638236	
10^4	-7.98144	3.9952000	0.0370339	0.00465039	
10^5	$-7.98364 \cdot 10^6$	3.9946200	0.0326531	0.0041823824	
10^6	$-7.9838 \cdot 10^7$	3.9946756	0.032488	0.0040636711	
10^7	$-7.9837 \cdot 10^7$	3.9946486	0.0321948	0.0040242065	

Table 4: Numerical values of heat capacity and susceptibility

We can see from table 4 that as the Monte Carlo cycles increases the numeric value of the heat capacity C_v and the susceptibility ξ approaches the analytic values. For Monte Carlos cycles of order 10^7 we see that the numeric value of heat capacity and susceptibility matches quite well with the analytic value, but at the cost of CPU time.

4.2 Equilibrium state, $L = 20$ system

In this exercise we want to study how much time or how many Monte Carlo cycles one needs in order to reach equilibrium state, and thus compute the expectation values of the system. First we set $T = 1.0$ and all spins of the matrix pointing upwards, and then set $T = 2.4$ keeping the ordered configuration. Then we make the calculation of absolute magnetization and energy as a function of MC cycles. We then repeat the same process setting $T = 1.0$ and $T = 2.4$ and using random spin matrix. Figure 3 shows an ordered initial state, where we have plotted the expectation value of the mean energy and the absolute magnetization as a function of the number of Monte Carlo cycles. From the plot below (Figure 3) it is quite obvious that after 10^2 Monte Carlo cycles the

values start to oscillate around an equilibrium state, while it takes around 10^3 cycles with higher temperature $T = 2.4$, I refer to figure 5. In figure 3 we see the "strange" behaviors of the curves, we notice that in the beginning the magnetization "humps" down and the energy "humps" up and start increasing and decreasing respectively. We observe that the magnetization increase with increasing MC cycles while the energy decrease with increasing MC cycles. From bottom plot of figure 3 and figure 4 we observe that the number of accepted configuration increases with increasing MC cycles. Figure 5 gives us an opposite behavior of the curves we have seen recently, here we see that the magnetization decreases while the energy increases with increasing MC cycles.

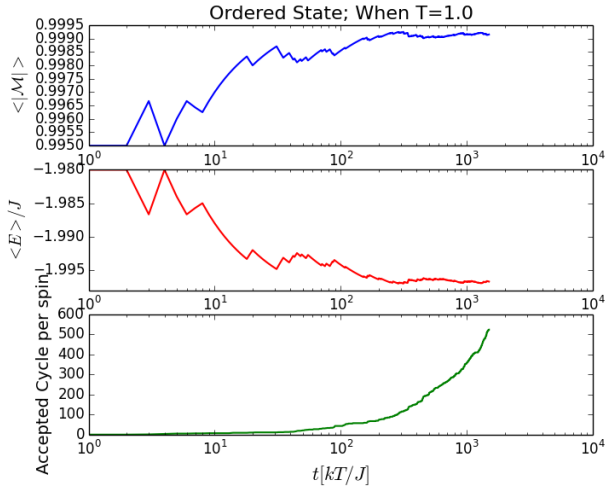

Figure 3: Ordered initial state (all spins up). Top: Expectation value of the absolute magnetization per spin as a function of Monte Carlo cycles. Middle: Expectation value of the energy per spin as a function of Monte Carlo cycles. Bottom: Accepted configurations per spin as a function of MC cycles. The size of the lattice is $L = 20$ and the temperature is $T = 1$ in $[\frac{kT}{J}]$units, here we have used **logarithmic scale**.

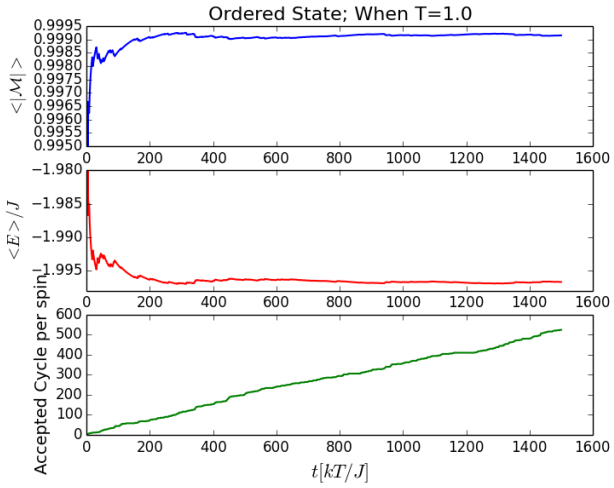

Figure 4: Ordered initial state (all spins up). Top: Expectation value of the absolute magnetization per spin as a function of Monte Carlo cycles. Middle: Expectation value of the energy per spin as a function of Monte Carlo cycles. Bottom: Accepted configurations per spin as a function of MC cycles. The size of the lattice is $L = 20$ and the temperature is $T = 1$ in $[\frac{kT}{J}]$units.

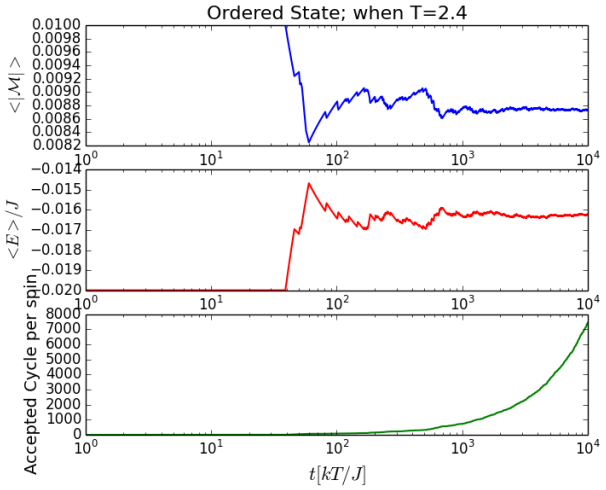

Figure 5: Ordered initial state (all spins up). Top: Expectation value of the absolute magnetization per spin as a function of Monte Carlo cycles. Middle: Expectation value of the energy per spin as a function of Monte Carlo cycles. Bottom: Accepted configurations per spin as a function of MC cycles. The size of the lattice is $L = 20$ and the temperature is $T = 2.4$ in $[\frac{kT}{J}]$units, with **logarithmic scale**.

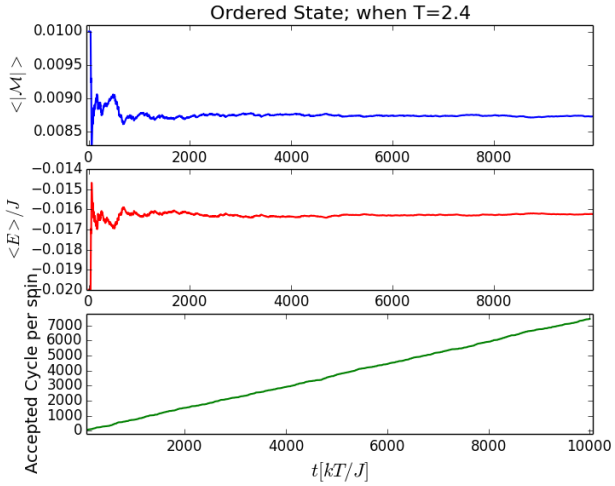

Figure 6: Ordered initial state (all spins up). Top: Expectation value of the absolute magnetization per spin as a function of Monte Carlo cycles. Middle: Expectation value of the energy per spin as a function of Monte Carlo cycles. Bottom: Accepted configurations per spin as a function of MC cycles. The size of the lattice is $L = 20$ and the temperature is $T = 2.4$ in $[\frac{kT}{J}]$units.

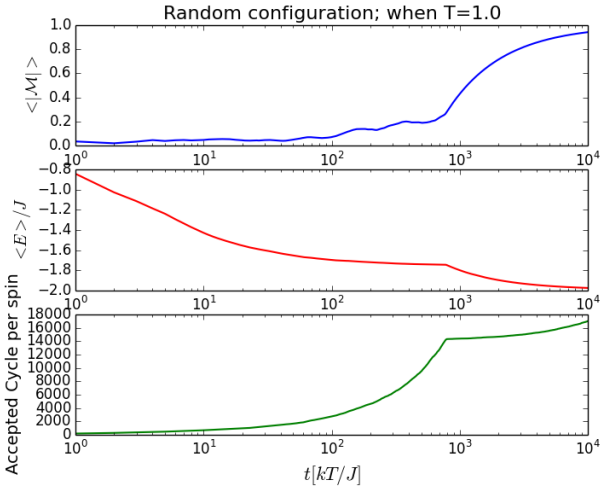

Figure 7: Random configuration. Top: Expectation value of the absolute magnetization per spin as a function of Monte Carlo cycles. Middle: Expectation value of the energy per spin as a function of Monte Carlo cycles. Bottom: Accepted configurations per spin as a function of MC cycles. The size of the lattice is $L = 20$ and the temperature is $T = 1.0$ in $[\frac{kT}{J}]$units, **logarithmic scale**.

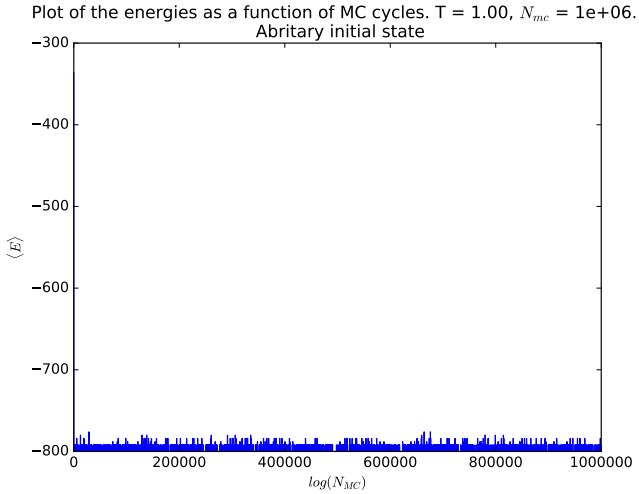

Figure 8: Random configuration: Expectation value of the energy per spin as a function of Monte Carlo cycles. The size of the lattice is $L = 20$ and the temperature is $T = 1.0$ in $[\frac{kT}{J}]$units.

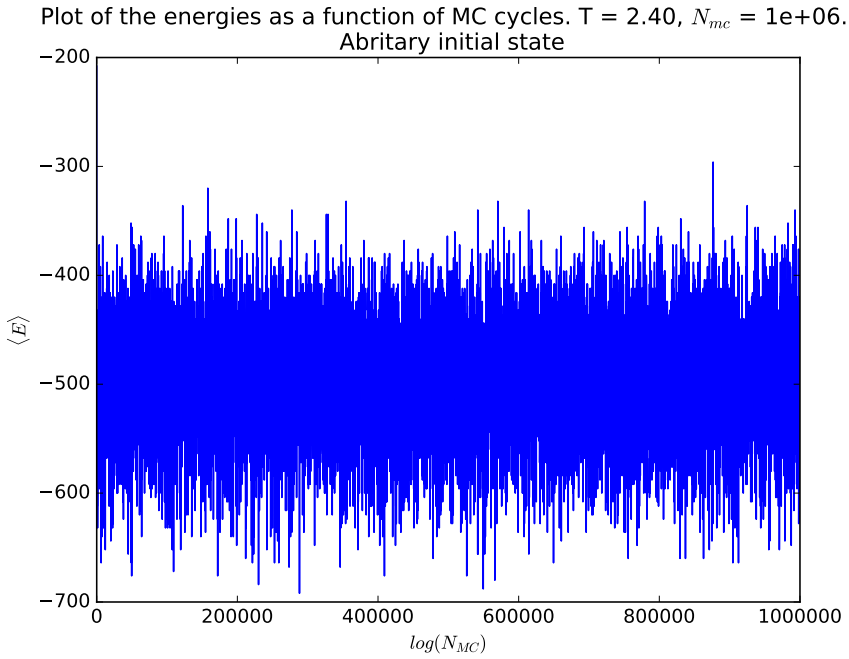

Figure 9: Random configuration: Expectation value of the energy as a function of Monte Carlo cycles. The size of the lattice is $L = 20$ and the temperature is $T = 2.4$ in $[\frac{kT}{J}]$units.

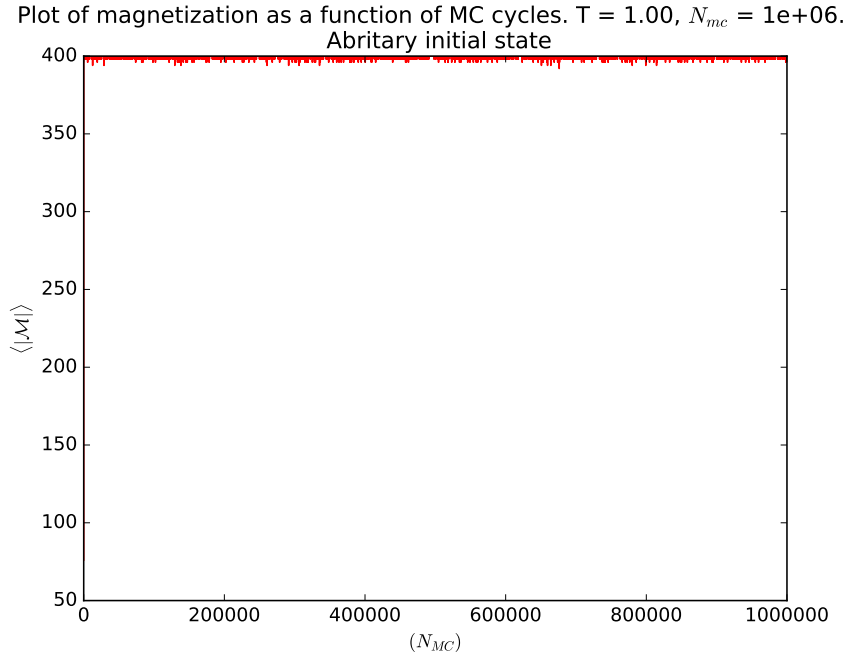

Figure 10: Expectation value of the absolute magnetization as a function of Monte Carlo cycles. The size of the lattice is $L = 20$ and the temperature is $T = 1.0$ in $[\frac{kT}{J}]$units.

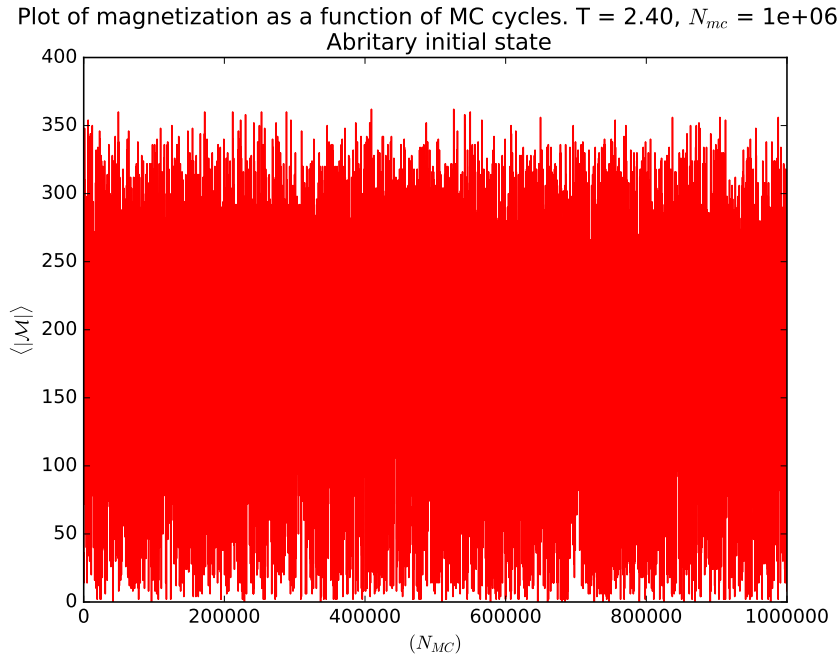

Figure 11: Expectation value of the absolute magnetization as a function of Monte Carlo cycles. The size of the lattice is $L = 20$ and the temperature is $T = 2.4$ in $[\frac{kT}{J}]$units.

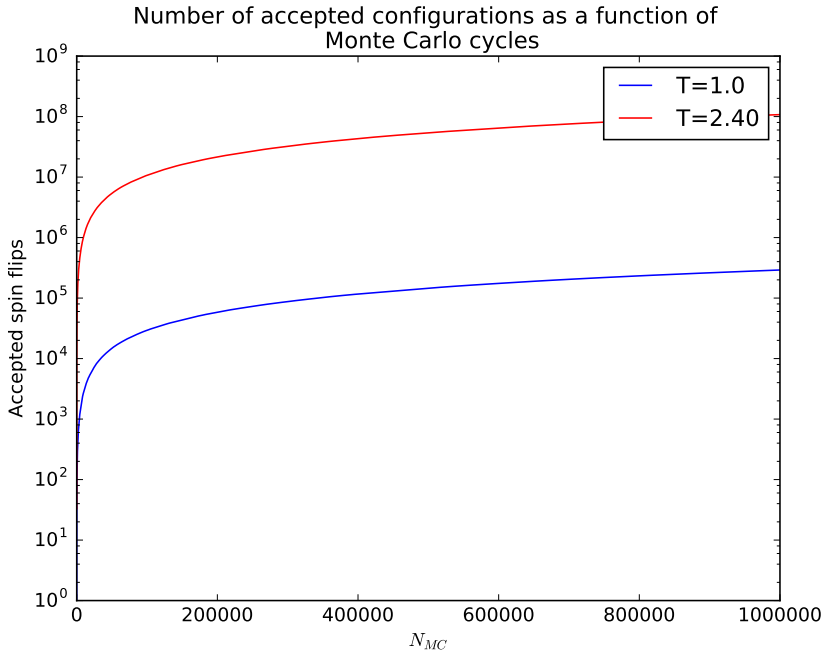

Figure 12: Accepted configurations per spin as a function of MC cycles, for the lattice size $L = 20$ and the temperature $T = 1.0$ and $T = 2.4$ given in $[\frac{kT}{J}]$units.

For Random configuration; given the fact that we start with a random spin value, it takes around "$10^4 - 10^5$" cycles before an equilibrium state is reached. We also notice that the number of accepted configuration increases in the beginning and then stabilizes with increasing MC cycles see figure 12. In conclusion the analysis tell us that after around 10^5 cycles we are in the equilibrium regime and that's where we can start to compute average values of the quantities we are interested to. This approach can be generalized by dividing this value for the size of the matrix. And thus we can state that for a general $L \times L$ case, one can start averaging after N_{start} cycles with:

$$N_{start} = 10^5 \times L^2$$

To explain this phenomena we need to have a closer look at the dependency of the probability of a spin flip as a function of temperature. Since the metropolis algorithm is based on the comparison between the factor $e^{\frac{\Delta E}{T}}$ and a random number, the number of accepted configuration grow with the temperature and is generally higher for ordered spin configuration than the random spin configuration.

4.3 Analysis of the probability distribution

We will now look at the probability for a given energy and see if this matches our physical intuition about the system. We will look at the previous system $L = 20$ and the same temperature $T \in [1.0, 2.4]$. We used the values for the energy after the system have reached a steady state. This is done by letting the simulation run for the equilibrium time first and then start to store the energies as the time goes. We will compare our results with the computed variance in energy σ_E^2. As we stated in theory section, we know that the variance is related to heat capacity as:

$$\sigma_E^2 = C_v k_b T^2 = \left(\langle E^2 \rangle - \langle E \rangle^2\right) k_b T^2$$

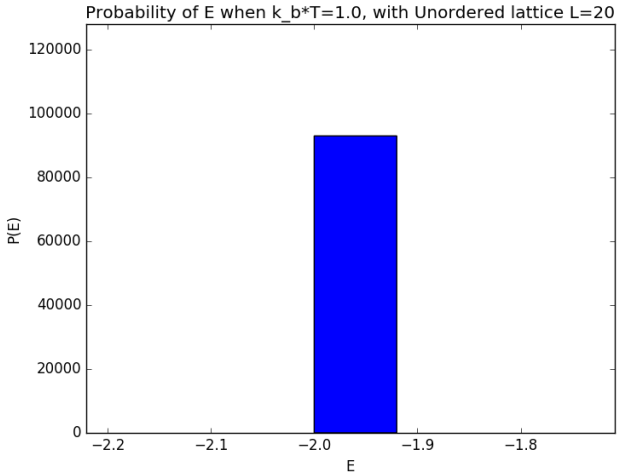

Figure 13: The probability distribution of the energy for temperature $T = 1.0$ for a random $L = 20$ lattice.

Figure 13 shows the probability distribution of energy for the temperature $T = 1.0$. This corresponds to he very low standard deviation, which means that the distance between the mean energy and the other energies are small. Almost every state is in the ground state at low temperature and thus the energy spread must be small. For the temperature $T = 2.4$ (Figure 14 and Figure 15) we see that the probability have shifted to a higher temperature, the energy peaks around $E = -1.2$. It means that the system is fluctuating around a higher energy when the temperature is higher. The plot for higher temperature resembles a Gaussian distribution. With an increasing number of lattice sites we should expect an Gaussian distribution. We have observed that the system behaves as expected. The system reaches the equilibrium state and oscillate around it. The probability as a function of energy appears to be as expected for higher and low energies. We can therefor assume that the implementation of the algorithm is correct.

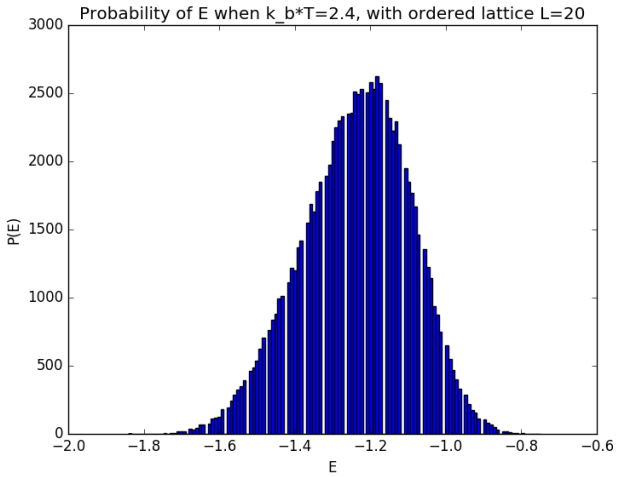

Figure 14: The probability distribution of the energy for temperature $T = 2.4$ for an ordered $L = 20$ lattice.

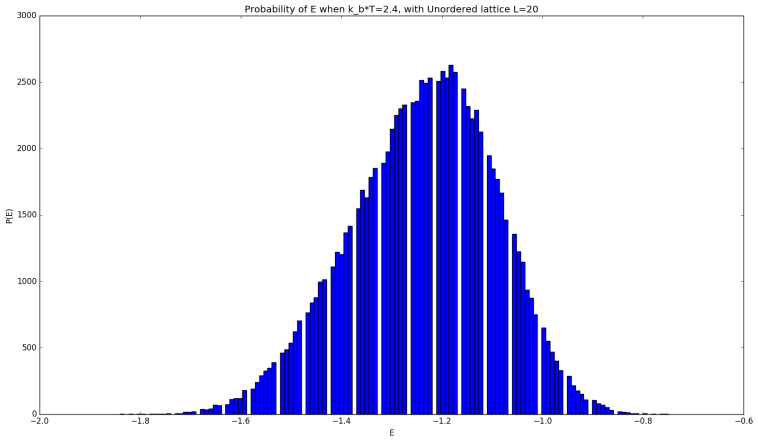

Figure 15: The probability distribution of the energy for temperature $T = 2.4$ for a random $L = 20$ lattice. .

4.4 Numerical studies of phase transitions

In this subsection we will use our algorithm to study the behavior of the Ising model in 2 dimensions close to the critical temperature as a function of the lattice size $L \times L$. We will plot the expectation value for the energy, the absolute magnetization, the heat capacity and the susceptibility as a function of temperature for four different values of the lattice $L \in [40, 60, 100, 140]$ and for $T \in [2.0, 2.3]$ with a step in temperature $\Delta T = 0.05$ or smaller. We will then try to see if we can see a phase transition and from this calculate the critical temperature for which the phase transition occurs.

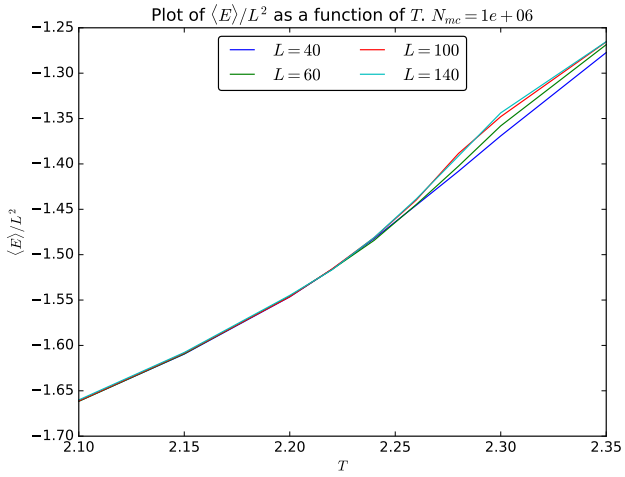

Figure 16: The expectation values for $\langle E \rangle$ as function of T.

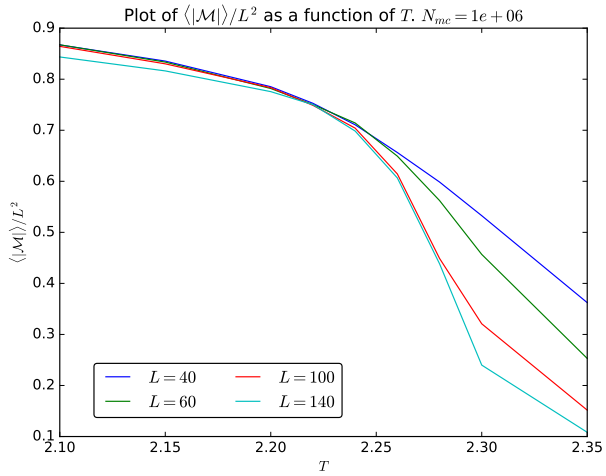

Figure 17: The expectation values for $\langle |M| \rangle$ as function of T.

From figure

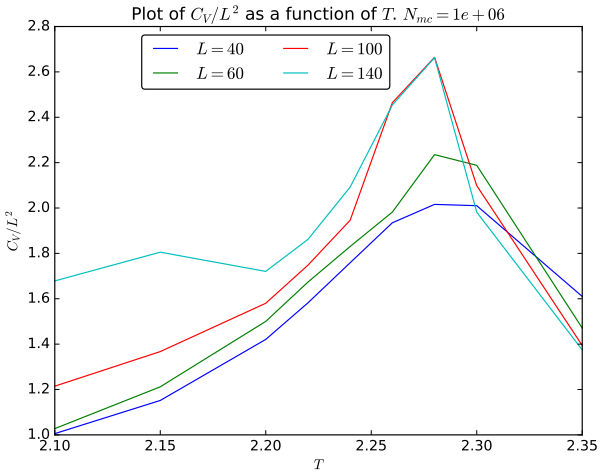

Figure 18: The specific heat capacity as function of T.

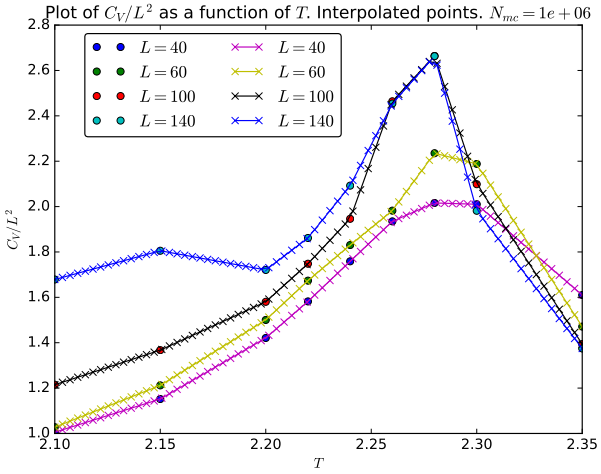

Figure 19: The specific heat capacity as function of T.

Figure 16 shows the expectation values of energies as function of T for all lattice sizes, $L \in [40, 60, 100, 140]$. We see increasing energies as function of temperature . From figure 17 we see that the absolute magnetization for all different lattice sizes decreases, and lies in domain $0.8 - 0.9$. This is natural as the syetem is close to ground state with either spin ($\uparrow$) or spin ($\downarrow$), resulting $|M| = 1$. On the other hand for higher temperature the system is in a more random state with as many spins ($\uparrow$) and ($\downarrow$) so it is reasonable that the magnetization approaches zero for higher temperature. An indication of a phase transition. From figure 18 and 19 we observe a maximum at same temperature, which indicates a phase transition.

4.5 Extracting the critical temperature

From figures 18 we can read the critical temperature values. See table below

L	$T_C(C_V)$
20	2.32
40	2.29
60	2.28
80	2.27

Table 5: Table of the values for the critical temperature red from figure 18; from the plot the heat capacity.

We calculate the estimate for the critical temperature and compare with the theoretical value $T_c = 2.269$. We have done this with the help of python program `finding_T_c.py`

$MeanValue$	$Finitescalingapproxof T_c)$	$Relativeerror$
-0.000406944444444	2.27000290675	0.000442003854575

Table 6: Table of the values for the critical temperature read from the plot the heat capacity.

4.6 parallelization

By using *MPI* we have manged to keep the elapsed time as small as possible, which helped us to run multiple simulation simultaneously, giving us a much faster code in result. Even with *MPI* it took us quite a long time doing all the operations. For the lower temperature the simulation time was longer then for the higher temperature for different matrices. This also proven that the parallelization is a necessary process in order to run algorithm for different temperatures for bigger matrices such as 80×80 or for higher dimensions than $80 - dim$. Why is parallelization important? The answer to this question is to consider the configuration space. The total number of configurations of the system is enormous even for a small numbers of spins. Consider our "favorite" $L = 20$ system, when $L = 20$, it means $N_s = 20^2 = 400$, and number of configurations $= 2^{N_s} = 2^400 = 2.58 \times 10^{120}$. If we tried to enumerate the configurations at a billion per seconds on a very fast computer, it would take us 2.58×10^{120} seconds which corresponds to 8.8×10^{103} years to compute the average magnetization.

5 Conclusions

At last we can conclude following: It is obvious that the metropolis algorithm is a reliable simulation for a spin lattice experiencing a second order phase transition describe by Ising model. The phase transition and critical temperature is discovered. The results between the results from the numerical integration and statistical physics used in this project matches very well, and we also got very good results for the critical temperature, $T_c = 2.27000290675$, which only deviates from the result from statistical physics in the thermodynamic limit with a relative error 0.0004.

6 References

[1] Github address : `https://github.com/sarahbra/Project4/tree/master/Project4/Project4A`
[2] Github address : `https://github.com/AnisaYn/Project4`
[3] M. Hjort-Jensen. Computational physics, lecture notes fall 2015. Department of Physics, University of Oslo, 2015
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[6] *http* : $//www.ww.amc12.org/sites/default/files/pdf/upload_library/22/Hasse/00029890.di991727.99p0087h.pdf$

*I have used **Alex Ho's** figures(8,9,10,12,16,17,18,19), because I was unable to plot the rest of results and also because I was not able to contact other students I have been working with. Since I was unable to contact **Andrea** i could not provide the github address where all the other programs are located*