Study of phase transisition in finite size magnetic systems using 2D Ising model

Aram Salihi[1]
[1]Department of Physics, University of Oslo, N-0316 Oslo, Norway

November 22, 2018

Abstract

In this numerical study we are going to use the two dimensional Ising model to investigate how different thermodynamical quantities behave. The main interest and the goal of this study is to look at the behaviour of large system when reaching the Curie temperature, and compare the numerical Curie temperature with the analytical solution found by Onsager [Hjorth-Jensen, 2015]. In this article we have analytically solved the two dimensional Ising for 2×2 lattice, and numerically solved for lattices with spins $L = \{40, 60, 80, 100, 120\}$. The study where successful, and we obtained a estimation of the Curie temperature to be $T_C = 2.24 \pm 0.029$ with a relative error 1.278% which is quite acceptable.

Contents

1 Introduction

The Ising model is a simple but very elegant theory which describes the behaviour of ferro- and anti-ferromagnets in materials, and is widely used in statistical physics to get a better understanding of different thermodynamical quantitites. The model consist of a lattice where each points represent a dipole with configruation $+1, -1$. The energy of the lattice is described by the sum of interal magnetic moment interaction between neighbouring dipoles. This Ising model has analytical solutions for one and two dimensions, but analytical solutions for higher dimensions are yet not been discovered due to complexity which occours in the system. The solution for one dimension were derived by the German physicist Ernst Ising, and also concluded that phase transitions does not exist in the Ising model, he also further concluded that phase transition does not exist for higher dimension. This was later proven to be wrong by the famous Norwegian theoretical physcist and chemist Lars Onsager. He showed that an analytical solution does exist and the Ising model unders goes second order phase transition when approaching the Curie temperature [Mohn and Wohlfarth, 1987] for infintely large lattice. After this critical point, the lattice looses the ability of self magnetize and becomes a paramagnet.

For finite lattice sizes for large system the problem becomes more complex and impossible to find a solution. Since the lattice system described in the Ising model is microcanonical it follows Boltszmann statistics, the problem arises in the partition function. The partition function need all possible configruations of the lattice, which goes as 2^N, in order to calculate the probability function. Since we know that probability distribution do exist, we can use the Metropolis algorithm to solve this problem for finite lattice sizes. The beauty of this algorithm is that its not dependent on the parition function, but only the acceptance ratio from different states calculated by the boltzmann factor. In this project we are going to use the Metropolis algorithm to investigate different thermodynamical quantities and the phase transition in the two dimensional Ising model and try to estimate the Curie temperature. We are going to use this estimation to compare with analytical solution found by Onsager [Hjorth-Jensen, 2015] for inifinetly large lattice.

2 Mathemetical and physical theory

2.1 Ising model

As mentioned in the introduction we will be looking at the so called 2-Dimensional "Ising model". The Idea is pretty simple and straight forward. Imagine having a microcanonical (fixed temperature T) system consisting of a square lattice with dimension $L \times L$. In this lattice, each points corresponds to a particle with a magnetic dipole (which we will call for spin) . We will define the spin confiquration of a invidual particle as

$$s = \{-1, +1\} \tag{1}$$

The particle will either point upwards or downwards. Now each particle internal magnetic field will have the freedom to interact with its surrounding particles. When changing a configuration, i.e changing a arbitrary spin, the hamiltonian of the system will change according to

$$H = -\mathcal{J} \sum_{\langle kl \rangle}^{N} s_k s_l + \mathcal{B} \sum_{k}^{N} s_k \tag{2}$$

Where $\mathcal{J}$ is the coupling constant which expresses the strength of the interaction between neighbouring spins, and $\mathcal{B}$ is a external magnetic field interacting with the current magnetic field of dipole k. A derivation of the hamiltonian can be found at [Hott, 0513]. We will look at a simplified case, where we assume no external fields acting on our system, thus $\mathcal{B} = 0$

$$H = -\mathcal{J} \sum_{\langle kl \rangle}^{N} s_k s_l \tag{3}$$

Notice we have used the symbol $\langle kl \rangle$ to indicate that we only sum over neighbouring spins. The magnetic moment of a certain configuration is then defined as

$$M = \sum_{k}^{N} s_k \tag{4}$$

Since this system is a microcanonical system it can be described perfectly with Boltzmann statistics. For further explaination please consider [Pokrovsky, 2012]

2.2 Boltzmann statistics

Suppose we have system $\mathcal{S}$ with a fixed temperature T and no interaction with its surrounding envirorment, meaning no exchange of heat/energy. The system will keep its shape, number of particle and the total energy is conserved. Thus, in other words we have thermal equilibrium at all time. The probability of a state or configruation i for a given energy configruation E_i (in our case E_i is from equation (3)), the probability distribution function is defined by boltzmann statistics

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

where $\beta = 1/(k_b T)$ and Z is the partion function. The Partition function is easily derived, the total sum of all possible states are 1

$$\sum_{i \leq N} P(E_i) = \sum_{i \leq N} \frac{1}{Z} e^{-\beta E_i} = 1 \tag{6}$$

Solving this with respect to Z, we will achieve

$$Z = \sum_{i \leq N} e^{-\beta E_i} \tag{7}$$

The partion function is a another word for normalization constant. Notice that the sum is over all microstates i, consisting of N states.

2.3 Expectation value

For a given energy confiquration there exist a probability distribution function $P(E_j)$. Now if we let a general variable Ψ^n represent a physical quantity from this system described by $P(E_j)$ there is a expectation value. Using the probability distribution function and discrete points, the expression for expectation value of Ψ^n is then:

$$\langle \Psi^n \rangle = \sum_{j \leq N} \Psi^n P(E_j) = \frac{1}{Z} \sum_{j \leq N} \Psi^n e^{-\beta E_j} \tag{8}$$

This expression will become very handy as we are going to derive analytical expression for important thermodynamical quantities.

2.4 Thermodynamical quantitites

By using the ising model we wish to calculate different thermodynamical quantitites, to see how the system behave for different temperatures, and how the change is from one phase to another. The quantitites we wish to calculate is heat capacity and magnetic Suscepbility.

2.4.1 Heat Capacity

The definition of heat capacity is

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T}\left(\frac{\partial}{\partial \beta} \ln Z\right) \tag{9}$$

For the sake of simplicity in our numerical calculation we will not use the above definition. Since we are using discretized points, we will therefore use the following expression (which is equivalent)

$$C_v = \frac{\mathrm{Var}(E)}{kT^2} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2} \tag{10}$$

Where $\langle E^2 \rangle$ is the expectation value of squared energy and $\langle E \rangle$ is the expectation value of energy. The fully derivation of the heat capacity is given in the appendix (8).

2.4.2 Magnetic susceptbility

The definition of magnetic susceptbility is

$$M = \frac{\partial \langle M \rangle}{\partial B} = \frac{1}{\beta}\frac{\partial}{\partial B}\left(\frac{\partial}{\partial \beta} \ln Z\right) \tag{11}$$

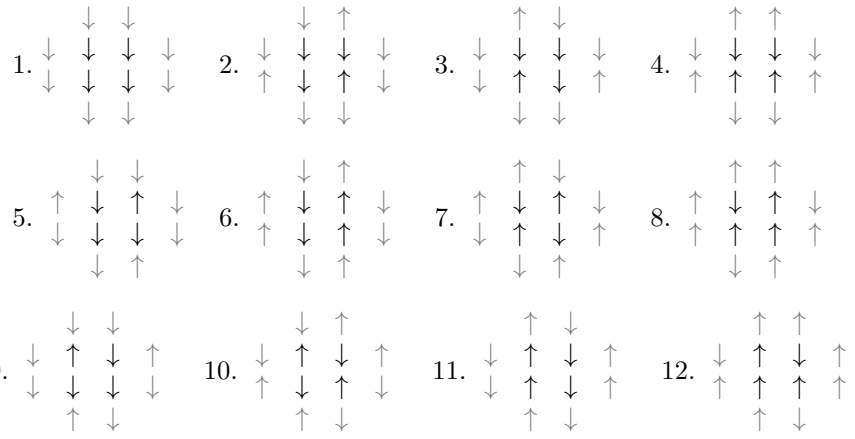
Where B is the magnetic field strength of spin i. It is crucical to not mix β and B, β represent unit of energy per kelvin and B is magnetic field stength in teslas T. Again for the sake of simplicity we will not choose to use the above expression, we will therefore derive another expression which is equivalent to the expression above. Consider the following

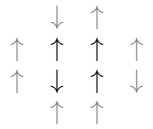
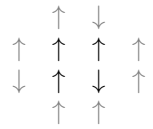
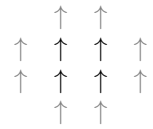
$$\chi = \frac{\mathrm{Var}(M)}{kT} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT} \tag{12}$$

The fully derivation of this expression is given in the appendix (9).

2.5 Analytical solution for 2×2 lattice

Assume a system with number of spins equal to $L = 2$ in a 2×2 square lattice. We have total of four spins, where each spin have two spin orientation, $\{+1, -1\}$. Meaning we have $2^4 = 16$ lattice configruations. Using periodic boundary conditions we will obtain these lattice configruations states



13.  14.  15.  16. 

Using the energy given in (3) in section (2.1) the lattice system will have these five possible energy states

Number of ↑	Multiplicity	Energy	Magnetic moment
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4

The partition function for these configruations becomes

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 2e^{8\beta J} + 2e^{-8\beta J} + 12 = 4\cosh(8\beta J) + 12 \tag{13}$$

The probability distribution function for this system becomes for a lattice in state j with energy E_j

$$P(E_j) = \frac{e^{-\beta E_j}}{4\cosh(8\beta J) + 12} \tag{14}$$

Now that we have an analytical expression for the partition for all possible configurations of the lattice, we can now derive analytical expression for C_v, $\langle |M| \rangle$ and χ.

2.5.1 Heat capacity

In order to calculate the heat capacity we need the mean expaction value, $\langle E \rangle$, and the expectation value of sqaured energy, $\langle E^2 \rangle$. Using the general expression for expectation value (8), thus

$$\langle E \rangle = \frac{1}{Z} \sum_{i}^{16} E_i P(E_i) = -\frac{8J \sinh(8\beta J)}{\cosh(8\beta J) + 3} \tag{15}$$

and the squared energy

$$\langle E^2 \rangle = \frac{1}{Z} \sum_{i}^{16} E_i^2 P(E_i) = \frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3} \tag{16}$$

Using the analytical expression (8) presented in previous section, the solution of the heat capacity becomes

$$C_V = \frac{\mathrm{Var}(E)}{kT^2} = \frac{1}{kT^2} \left(\frac{256J^2 \cosh(8\beta J)}{4\cosh(8\beta J) + 12} - \left(\frac{8J \sinh(8\beta J)}{4\cosh(8\beta J) + 12} \right)^2 \right) \tag{17}$$

2.5.2 Magnetic susceptibility

Again using the same approach as previous, the partition function still remains the same. The expectation value of the magnetic moment is given as

$$\langle M \rangle = \frac{1}{Z} \sum_{i}^{16} M_i P(E_i) = 0 \tag{18}$$

and the squared magnetic moment

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{i}^{16} M_i^2 P(E_i) = \frac{8e^{8\beta J} + 8}{3\cosh(8\beta J) + 3} \tag{19}$$

Using this and the analytical expression from (12), the magnetic susceptibility becomes

$$\chi = \frac{\mathrm{Var}(M)}{kT} = \frac{1}{KT} \frac{8e^{8\beta J} + 8}{3\cosh(8\beta J) + 3} \tag{20}$$

2.5.3 Expectation value of absolute magnetic moment

Recall from previous that the expectation value for M were zero. We are now interest if $|M|$ has a explicit expression. As before using the definition of the expectation value, the expectation value of absolute magnetic moment is given as

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i}^{16} |M|_i P(E_i) = \frac{2e^{8\beta J} + 4}{3\cosh(8\beta J) + 3} \tag{21}$$

2.6 Phase transisition

As explained in [Sen. P. K, 1993] there is no phase transitions in the one dimensional ising model since due to never achieving a ordered confiquration of the system. This means that the lattice remains as a ferromagnetic system for β. As proven later by the famous Norwegian theoretical physcisit and chemist, Lars Onsager, proved that there exist phase transitions (for second order phase transition please check [Mnyukh, 2013]) in two dimensional Ising model when reaching the curie tempeature [Hjorth-Jensen, 2015]. Meaning that for a random confiqurated square lattice (with no external magnetic field exterted on it) for low temperatures the system will be in a ferromagnetic state until it has reached the curie temperature where it undergoes a second order phase transition and become paramagnet where it looses its ability to self magnetize. Near this critical or so called curie temperature, T_C, we can use simple power law approximation to show how different thermodynamical quantities behave. Consider the following mean expressions

2.6.1 mean magnetization

$$\langle M(T) \rangle \sim |T_C - T|^{\beta} \tag{22}$$

Where $\beta = 1/8$. A similar relation can applies also for the heat capacity and magnetic susceptbility

2.6.2 Heat capacity

$$C_V \sim |T - T_C|^{\alpha} \tag{23}$$

Where $\alpha = 0$

2.6.3 Heat capacity

$$\chi \sim |T - T_C|^{\gamma} \tag{24}$$

$\gamma = 7/4$. The exponent α, β, γ are the so-called critical exponents. The Curie temperature is heavily depended on the lattice size i.e number of spins/particles, when increasing the the number of spins L and the curie temperature T_C converges to a certain value when $L \to \infty$. Ideally this is imposible to achieve numerically since our computational capacity is up to $L = 140$, but have chosen only do simulations from $L = 2$ to $L = 100$ to save time. The beauty is that we can estimate the Curie temperature through so-called finite scale sizing relations it is possible to relate the behaviour of finite and infintely large lattice. The Curie temperature scales then as

$$T_C(L) - T_C(L \to \infty) = aL^{-1/\nu} \tag{25}$$

Where ν can be calculated from $\xi \sim |T_c - T|^{-\nu}$ and a is some constant. In order to find a estimate for $T_C(L)$ we must find out what the constant a is, to do so we can look at the difference for two lattices L_1 and L_2. Consider

$$aL_1^{-1/\nu} - aL_2^{-1/\nu} = (T_C(L_1) - T_C(L_1 \to \infty)) - (T_C(L_2) - T_C(L_2 \to \infty)) \tag{26}$$

Notice when $L_1, L_2 \to \infty$ there basicly identical, thus $T_C(L_1 \to \infty) = T_C(L_2 \to \infty)$. This will cancel each other out. Solving with respect to a, we will obtain the following expression

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} \tag{27}$$

Using this expression for a in (25), and solve it for $L(L \to \infty)$

$$T_C(L \to \infty) = T_C(L) - \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} L^{-1/\nu} \tag{28}$$

The Curie temperature can be observed when we observe a breaking point. The second order phase transition are characterized by a divergent magnetic susceptibility and heat capacity. A analytical solution has been achieved for ν by Lars Onsager, for further explaination please read [**?**] The analytical solution Lars Onsager found is on the form:

$$T_C(L \to \infty) = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.269 \tag{29}$$

2.7 Periodic boundary condition

To avoid problems at the boundary we will assume that we have a crystal which is infinitely large, but in reality there is no such things. So in order to bring out this affect we let particles on the boundary interfere with particle on the oposite end, we will then achieve a continous force/field exchange and avoid discontinuities. In this project we will be only looking at a slice of this crystal with dimension $L \times L$ as mentioned previously sections. A expression for this is derived and illustraded in section (3.1)

2.8 Metropolis algorithm

Suppose having a system in a random spin confiquration i and we wish to find out it evovles with time and how it reaches steady state. The problem is we do not how we can oriante the different spins to reach equilibrium, thus the system is not deterministisc. The positivie thing is that the system can be described with a probability density function $P(E_i)$ for configruation i. Using the probabilistic nature of this system, we can use Monte Carlo simulation to see how the system evovles with time. Once the probability density function is known we can take random samples

from it and proceed the simulation.

Many simulation are then performed until a desired result is found. The solution of the problem will then be the result found normalized according to number Monte Carlo used. Now Monte Carlo simulation is not a specific algorithm, but rather a set of algorithm which uses this idea. For further detailed explaination please consider [Hjorth-Jensen, 2015]. The downfall is that we cannot choose all Monte carlo methods for this project, because computing the partion function Z for large system is quite impossible. It is not possible to calculate all spin oriations for large system. We must then develop a algorithm which bypasses this problem. One of the Monte Carlo methods bypasses this problem. The beauty of the Metropolis algorithm is that we only look at the probability ratio of two different energy states, the so called acceptance ratio, dentoed as $A_{i\to j}$. Meaning we are looking at a lattice in some state jumping to another state, by flipping a random spin $\mathcal{S}$. Thus

$$A_{i\to j} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j/Z}}{e^{-\beta E_i/Z}} = e^{-\beta(E_j - E_i)} = e^{-\beta \Delta E} \tag{30}$$

As we see the partion function cancels out, thus we bypass this problem we initially had. In order to accept this jump and update the thermodynamical quantitites, the acceptance ratio $A_{i\to j}$ must be lower than a random number ζ

$$\zeta \leq e^{-\beta \Delta E} \tag{31}$$

This number is defined by a uniformal random distribution in the interval $[0, 1]$. If

$$\zeta > e^{-\beta \Delta E} \tag{32}$$

Then we cannot accept the change of state, and we must continue to choose a random spin and flip it, and then again check if the new configruation satisfies (31). How this algorithm is implemented and simplified is explained in section (3.3).

2.9 Thermodynamical equilibrium for the lattice system

Since we are dealing with probalistic system, a fundemental theorem probability theory states that [Sen. P. K, 1993]; Performing the same experiment for a large amount of cycles, the deviation will after a while die out and the system and the average of the result normalized will tend to the expectation value, and converge to it if sufficiently amount cycles is provided. Meaning if we find the number of Monte Carlo cycles, 10^N, needed to achieve equilibrium. This value can be found when simulating for small lattice system and see when the different quantities converge. We can use this value at all time when running simulations for larger systems. This will save a tremendious amount of time, since we are reducing the computational time and calculations by some factors at the same time achieving good precision for different thermodynamical quantities.

3 Method

In this section, we will explain how the theory is implented and used as method in the project. The theory behind these method are explained in the previous section. (2)

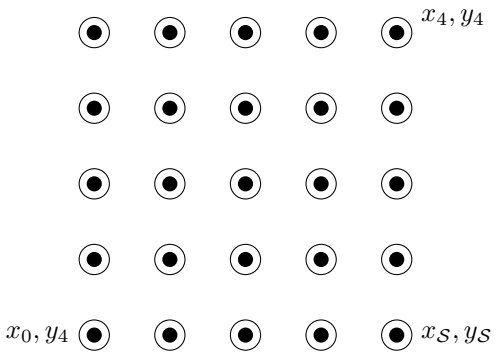
3.1 Periodic boundary

Using the knowledge from section (2.7) we can easily derive a expression the boundary condition by using modular division. Choose a random spin $\mathcal{S}$ which has a position at (x_i,y_i). We know that this spin will be affected by neighbouring spin at position (x_{i+1},y_{i+1}) and (x_{i-1},y_{i-1}). However, if this spinn, $\mathcal{S}$, has the position ($x_{boundary}$,$y_{boundary}$), it will be affected by the spin on the opposite of the lattice as explained previously. Meaning either left or right most or top or bottom most

particle. Using this intuition we can derive a simple and elegent expression which finds the particle that affects spinn $\mathcal{S}$, thus

$$i = (i + N + \xi) \mathrm{mod} N \tag{33}$$

Where i is the current index position of $\mathcal{S}$, N is the number of spins (not total) and ξ chooses direction (left,right, up or down) we want to look at. Notice if $i = N$ then $i_{new} = 0$, which means that spin $\mathcal{S}$ with index $i = N$ is affected by another particle with index position $i_{new} = 0$. Using this we will have no problem computing the new confiquration energy when flipping spin $\mathcal{S}$. A diagram of this idea is shown down below.



Notice that $\mathcal{S}$ is on the bottom right boundary, the spins which will affect $\mathcal{S}$ have the coordinates x_0, y_4 and x_4, y_4. The computation of the energy difference from one state to another will be explained in the next section.

3.2 Energy in the system

From subsection (2.1) the hamiltonian for some random lattice confiquration in the ising are described as the interaction between four nearest neighbours. Now the beauty of this theory is: when flipping a random spin, the energy difference from the old to new confiquration is always limited to some values due to same amount of neighbours. This means we can precalculate the acceptance ratio (31). The possible value for ΔE is

$$\Delta E = \{-8J, -4J, 0, 4J, 8J\} \tag{34}$$

and the acceptance ratio

$$A_{i \to j} = e^{-\beta \Delta E} \tag{35}$$

Note that $A_{i \to j}$ have also five values depending on the temperature the lattice experiences, but this is precalculated before the monte carlo simulation starts. This means for every cycle in the metropolis algorithm, we can simply pick a random spin and then check which configruation the neighbouring spin are in, thereafter assigning ΔE to $A_{i \to j}$. This precomputation of the acceptance ratio will reduce the computational time to some extent.

3.3 Metroplis algorithm

Since we have a probability distribution function, we can therefore use Metropolis algorithm. The acceptance ratio from state i to j are expressed as

$$A_{i \to j} = e^{-\beta \Delta E} \tag{36}$$

Where the energy difference ΔE from configruation i to j. Even though we know what ΔE is limited to some values, we must still compute it for every monte carlo and lattice sweep to find

$A_{i\to j}$ when flipping a random spin. We must now choose a random spin $\mathcal{S}$ in the lattice and check the change in energy the lattice experiences, to do so Consider the energy the old and new confiquration experiences

$$\Delta E = E_j - E_i = -J\sum_k^4 s_j s_k + J\sum_k^4 s_i s_k = J\sum_k^4 s_k \underbrace{(s_i - s_j)}_{s_j} = 2Js_j\sum_k^4 s_k \tag{37}$$

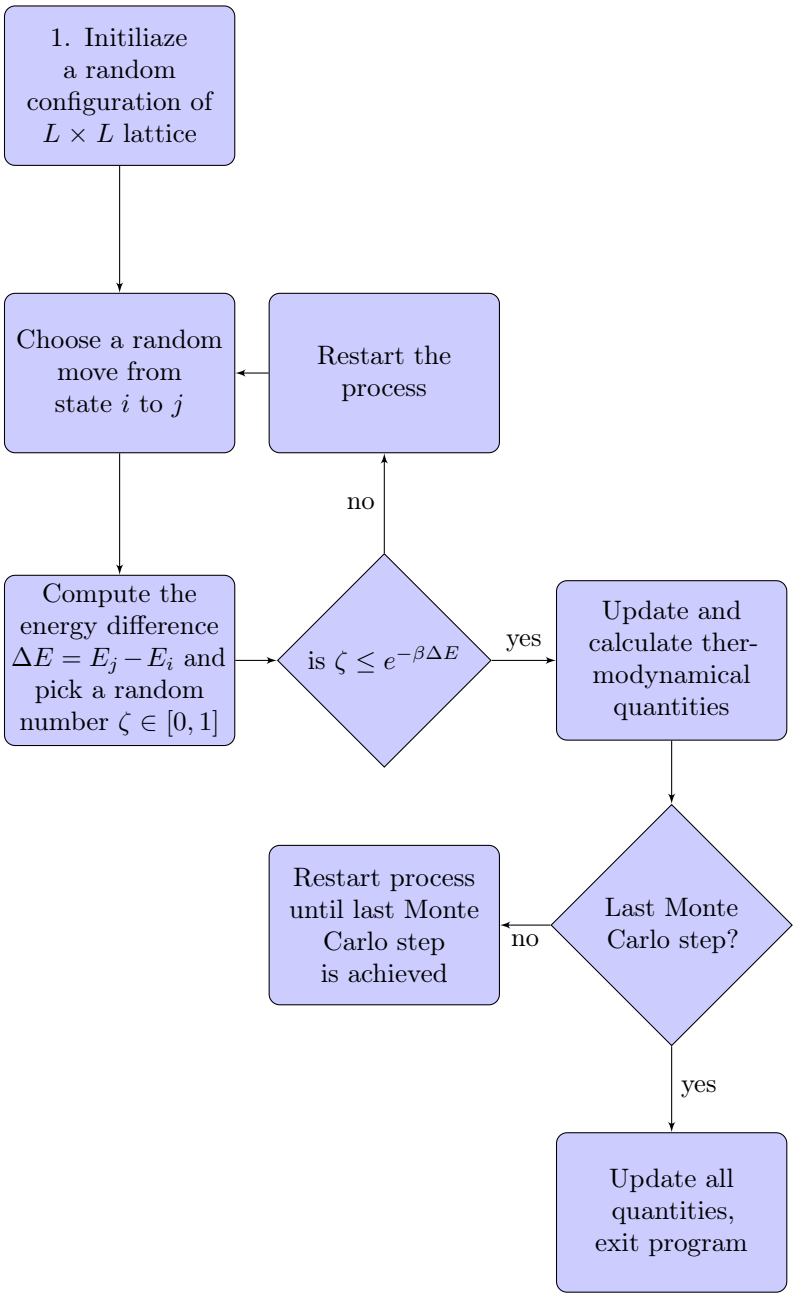
Since $s_i - s_j$ is either 1 or -1 we will just redefine it to $2s_j$, thus

$$\Delta E = E_{i\to j} = 2s_j J\sum_k^4 s_k \tag{38}$$

This sum runs over all neighbouring spin k's. Now the energy difference is calculated, just assign it to a function where $A_{i\to j}$ is precalculated and check:

$$\zeta \leq e^{-\beta\Delta E} = A_{i\to j} \tag{39}$$

The implentation of this is quite easy and can be explained as an floatchart:



3.4 Number of monte carlo cycles in order achieve steady-state

There is two way to find out how many Monte Carlo cycles we need to achieve steady state.

- Plotting the different thermodynamical quantities as function of Monte Carlo cycles and analyze it and check when large deviation dies out.
- Count how many times you get accepted spins flipps and plot it as a function Monte Carlo cycles. When the number of accepted spin flipps get steady and coverges to a certain value. When this happens, it means that for each Monte Carlo cycle after it has converged it doesnt matter how many cycle you use it will always flipp that amount of spins.

4 Implentation of the Ising model and the structure in C++

In this section we will briefly explain the structure and the technicalities behind the program. The program which simulates the Ising model consist of four classes and a main class.

4.1 Main.cpp

This class takes in 11 input arguments. The arguments are listed in a chronologically order

- argv[1]: type string. Name of the text file that is going to be generated when the program is executed. When the program exit, all thermodynamical quantities are saved into this .txt file.
- argv[2]: type int. Number of spins L.
- argv[3]: type int. Number of Monte Carlo Cycles.
- argv[4]: type double. T_i, Initial temperature the lattice experiences.
- argv[5]: type double. T_f, Final temperature the lattice experiences.
- argv[6]: type double. The stepsize, ΔT, when going trough the interval $T_i \leq T \leq T_f$.
- argv[7]: type string. Three possible string values. Up; initializes the lattice with all spins pointing upwards. Down; initializes a lattice where all spins pointing downwards. Random; All spins are randomly configruated, they either point up or down.
- argv[8]: type string. Two possible string values, ordered or dis_ordered, this arguments are added to the end of file of argv[1] when saving for each step when running the Monte Carlo simulations.
- argv[9]: type bool: two possible value 0 or 1. 0 indicates false, when 0 is used the program only saves the last step when executed. 1 indicates true, the program will save each step when executed.
- argv[10]: type bool: two possible value 0 or 1. 1 indicates true, when executed the program will calculates χ with $\langle |M| \rangle$ instead of $\langle M \rangle$. This is due to avoid fast and alot oscillations when increasing L. When 0 is used, the program calculates χ with $\langle M \rangle$.
- argv[11]: type bool: two possible value 0 or 1. If 1, when the program is executed the simulation result are saved into a pointer array when the system reaches equilibrium/steady state. When 0, the program will save every quantities to the pointer array independently if the system has reached or not reached steady state.

4.2 quantities.cpp

This class consist of four methods. These methods initializes the lattice confiquration when the spin configuration argument is given in Main. This class also initializes precalculates the acceptance ratio $A_{i \to j}$ used in the Metropolis, the initial energy and magnetic moment of the system.

4.3 solver.cpp

This class consists of two methods. The first method is called "calculate_nabo_spin" which calculates the neighbouring spins when looking at the energy difference. The second method is called metropolis which is the method where the metropolis algorithm is implemented.

4.4 Execute_solve.cpp

This class consist of one main method which takes all the input arguments from main.cpp and gives to the MPI and then executes the solver class for desired input from main.cpp.

4.5 dumpfiles.cpp

As the name says, this is the class where all values are dumped into. This class consist of three methods: save_each_step is a method used to save each value from solver.cpp into pointer arrays. Thereafter is this send to another method called save_each_file_step where the result is normalized and different qauntites are calculated and saved to a file with .txt exstension. The last method is called save_last_step, this method as the name says saves the quantities at the end of the Monte Carlo cycle and then saved.

4.6 Parallelization with MPI

The C++ program is entirely parallelized but not perfectly optimized, this is done in order to reduce computational time. The C++ program uses the latest MPI version. The program is mainly executed on macbook pro with two i5 cores.

5 Result

In this section we will present the result produced from the Monte Carlo simulation. We will also give necessary information about parameters in order to produced the same result with same precision. **All results are normalized with respect to total number of spins and monte carlo cycles. Thus we are looking at per spin and total spin, we can interpret this as looking at individual spin.**

5.1 2×2 Lattice

The Monte Carlo simulation used $L = 2$ with different Monte Carlo cycle in the range $N = \{10^2, 10^7\}$ to show convergence towards the analytical solution derived in section (2.5). Note that the result are functions of temperature with unit kT/J. This were done for temperatures in the range $kT/J = \{0.9, 1.9\}$ with $\Delta T = 1e - 3$ stepsize.

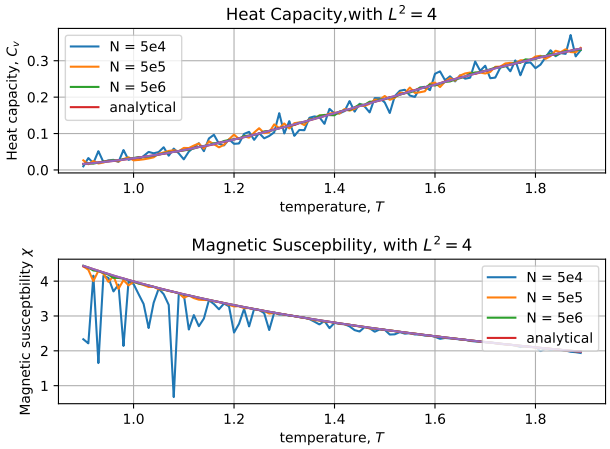


Figure 1: The diagram on the top shows the heat capacity as a function of the temperature for $L \times L = 4$, and the diagram down below is the magnetic susceptibility as function of temperature. Notice that these are plotted against the analytical solution.

We have also plotted the numerical solutions of the expectation value of the energy and absolute magnetization against their analytical solution.

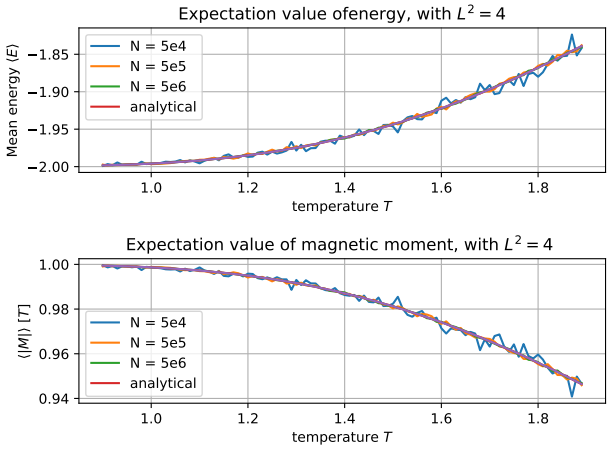


Figure 2: The diagram on the top shows the expectation value of energy as a function of the temperature for $L \times L = 4$, and the diagram down below is the expectation value for absolute magnetic moment as function of temperature.

5.2 Number of Monte Carlo needed to achieve equilibrium for 20×20 lattice

In this section we are going to present result when steady/equilibrium in our Monte Carlo simulations are achieved, this is done for different number of Monte Carlo iteration, but also different spin configruations. We have a chaotic disordered lattice state and one ordered. Please consider the following.

5.2.1 $kT/J = 1$ for 20×20 lattice

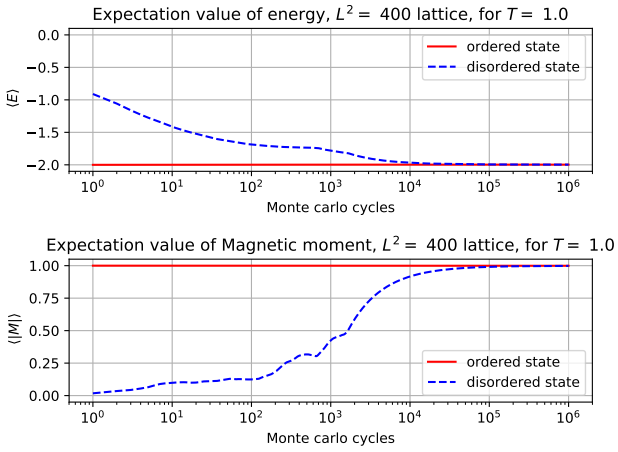


Figure 3: The simulation has been done for from 10^0 to 10^6 Monte Carlo cycles. This has been done for a ordered and disorded spin system for 20×20 lattice. Steady state is achieved at 10^4 for temperature $kT/J = 1.0$. When steady state is achieved the expectation values converges to $\langle E \rangle = -2$ and for absolute magnetic moment $\langle |M| \rangle = 1$.

5.2.2 $kT/J = 2.4$ for 20×20 lattice

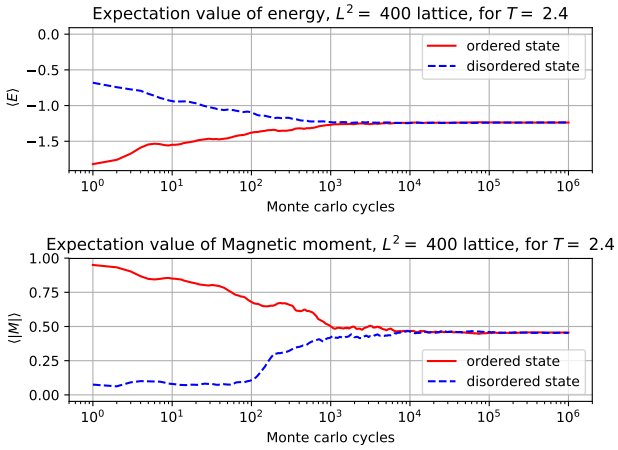


Figure 4: The simulation has been done for from 10^0 to 10^6 Monte Carlo cycles. This has been done for a ordered and disorded spin system for 20×20 lattice. Steady state is achieved in the domain 10^4 to 10^5 for temperature $kT/J = 2.4$. When steady state is achieved the expectation values converges to $\langle E \rangle \approx -1.25$ and for absolute magnetic moment $\langle |M| \rangle \approx 0.47$.

5.2.3 Accepted spin flipps for $T = 1.0$ and $T = 2.4$

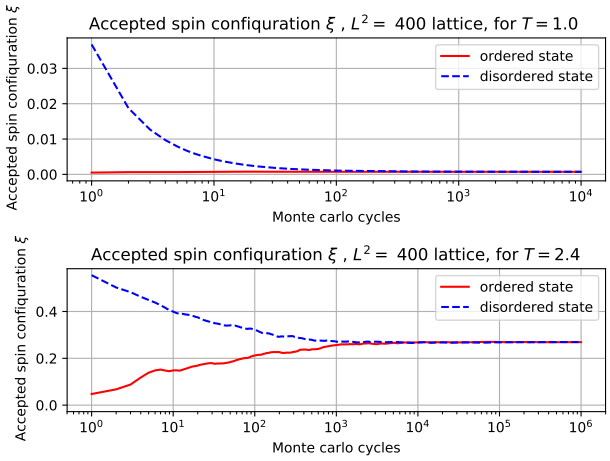


Figure 5: A graph showing how number of accepted flips behave when number of Monte Carlo cycles increases. This is done for dis- and ordered system for temperature $kT/J = \{1.0, 2.4\}$. The system achieves steady state at 10^4 for $kT/J = 2.4$ and 10^3 for $kT/J = 1.0$

5.2.4 Probability density for $kT/J = 1.0$ and $kT/J = 2.4$ for disordered system

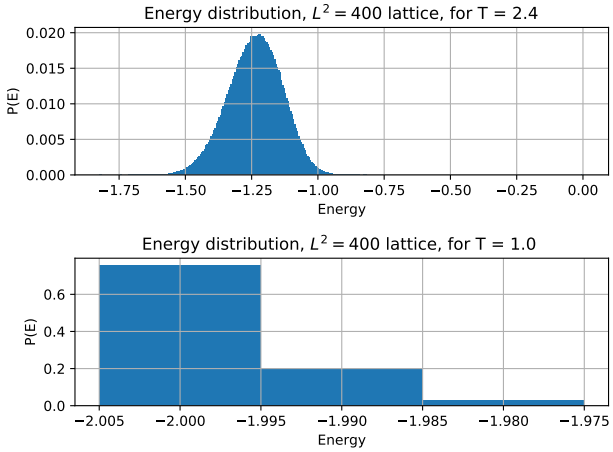


Figure 6: The probability distribution of the energy for a disordered system. As described in the title, this has been done for the temperature $kT/J = \{1.0, 2.4\}$.

5.3 Phase transition for chaotic system for larger lattices

In this subsection we are going to present the result when analyzing how a disordered system behaves after achieving steady state near the Curie temperature for different lattice sizes. We used $L = \{40, 60, 80, 100, 120\}$. These simulations has been done on one node on the supercomputer "Abel" at the university of oslo. We used 16 cores in total with 64GB ram and executed $2e5$ Monte Carlo cycles per cores (in total $3.2e6$ Monte carlo cycles) with a temeprature step $\Delta T = 0.01$ in the interval $kT/J = \{2.20, 2.36\}$. Keep in mind that we have removed 625 Monte Carlo cycles for each core, this is due to that the system achieves steady after 625 cycles (per core) and the real simulation starts after this point.

5.3.1 Heat capacity and Magnetic susceptbility near Curie temperature

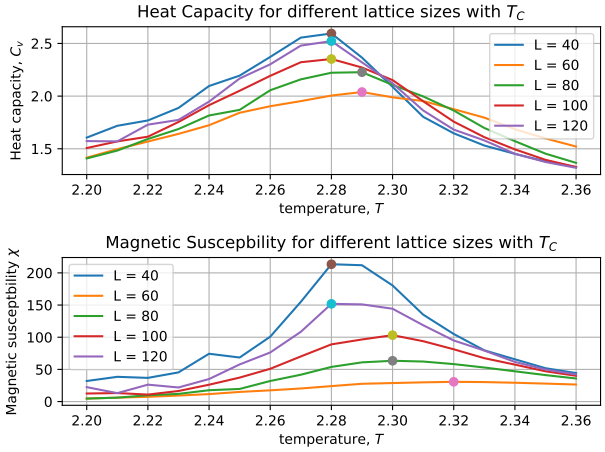


Figure 7: The behaviour of the heat capacity and magnetic susceptibility for different lattice sizes. Notice that the color points indicates where the Curie temperature occours for different lattice sizes.

5.3.2 Expectation value of absolute magnetic momenet and energy under phase transition

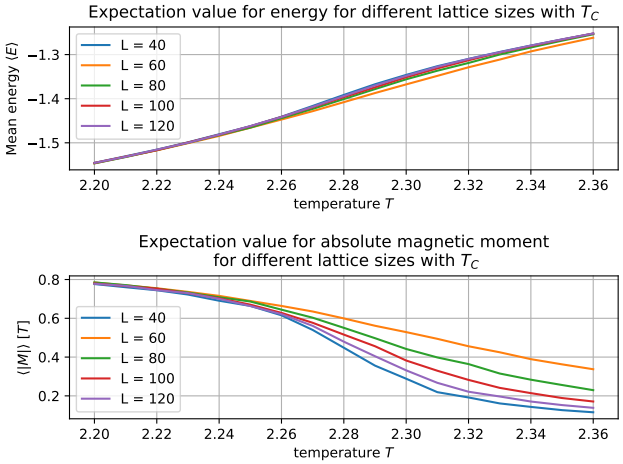


Figure 8: The behaviour of the expected energy and absolute magnetic moment when the system undergoes a second phase transition

6 Discussion

6.1 2×2 lattice, analytical vs numerical solution

Analyzing the result from 2×2 lattice from subsection (5.1), there was no suprise that the numerical solution when increasing the number Monte Carlo cycle will converge towards the analytical solution found in subsection (2.5). This is a consequence of law of large number as explained in subsection (2.9). Notice when analyzing figure (1) and (2), that after $N = 1e6$ (where $5e5$ Monte Carlo cycles were distributed equaly between two cores) we do get pretty good and accurate results. This result gives us an good indication on how many Monte Carlo cycles it is needed to produce results with good precision. For larger systems than 20×20 using $5e6$ per cores (if using two cores) the computational time increases significantly, and therefore using $1e6$ total Monte Carlo cycles enough in order to save computational time.

6.2 Time required to achieve steady-state

In this numerical study we refer time to number of Monte Carlo cycles needed to acheive stability. As mentioned previous, we are heavily interested in how larger systems behave when increasing the lattice size. When increasing the lattice size, we also increase the computational time, so therefore having a good knowledge on how the system behaves for different spin configuration and parameters is crucial.

When analyzing figure (3), we notice that for a ordered spin oriented lattice (all spins points upward or downwars) $\langle E \rangle$ starts very close to the expected value, the same goes with absolute magnetic moment. The explaination of this is that lattice is already in the lowest possible state and therefore flipping spins is not required to achieve lower states. This observation and explaination is supported by the first figure in (5). Analyzing this figure we notice that almost no spins are flipped. Looking at the energy distribution for this system we notice that the lowest possible energy is around ≈ -1.9999 with a probability of ≈ 0.80. Thus we obtain stability and steady state after $N = 10^2$ Monte Carlo cycles if using a ordered system. Meaning when calculating for large systems we can exclude the first 100 steps if using ordered orientation, and then look at the behaviour of the system.

Analyzing the result further, we clearly notice there is a big difference between ordered and disordered spin states (all spins has randomly oriented orientation). The explaination behind this behaviour: is that the lattice wants to achieve a stable spin orientation, thus the result will be either all spin pointing upwards or downwars. When achieving this stable spin orientation, the lattice will be in the lowest possible state for $kT/J = 1$. A particle or a system of several particles always want to tend to the lowest possible energy state. In this case the lowest possible energy is $\langle E \rangle \approx -1.9999$.

Increasing the temperature to $kT/J = 2.4$ we get some interesting results, see figure (4). When analyzing for the ordered lattice state, where each spin points upwards. The system does not start as close to the expected energy $\langle E \rangle \approx -1.2486$, but starts at a lower energy state ≈ -1.5897. Which is relatively close, but not as close for the case with $kT/J = 1.0$. From here the system take approximately $N = 10^4$ Monte Carlo cycles in order to achieve lowest possible state and stability. The number of accepted spin flipps has also significantly increased when analyzing (5) and the number of accepted spin stabilizes around 10^4.

Notice that the magnetic moment of the system also decreases observed in figure (8). This obersvation is in depth explained in subsection (6.4). The explaination of this is that we will approach a configruation where almost half of the spins are either oriented up, and the other half oriented down. In this case we have some presentage of random oriented spin left, thus resulting in a lower magnetic moment.

When looking at the disordered system, a very interesting sight occours when looking at the magnetic moment in figure (8). It appears it is almost zero, it appears that we are more stable system. Meaning a large amount of spins starts in a configruation where almost half of the spins are pointing up and the other pointing down. Notice that magnetic moment is not zero, but very close. After few Monte Carlo cycles, 10^2, the system is forced to approach another configruation in order to achieve stability. It wants to balace out a state with lower energy and a state with higher entropy. This is a consequence of Helmholtz free energy, thus the system wants to minimize this quantity. As we see the system then equilibriate itself and find steady state after 10^4 Monte Carlo cycles. Looking at the probability distribution for this temperature and a disordered configuration in the lattice, we will observe that the most likely energy is at ≈ -1.23475. Which is actually the energy the lattice wants to end up in. All in all for both temperatures is 10^5 a very good amount of Monte Carlo cycles to simulate since all quantitites are stabilized after 10^4.

6.3 Probability distribution

Recall from figure (6), we see that probability distribution for the energy varies for different temperatures. For $kT/J = 1$ the most desired state is when the expected energy is around ≈ -1.999, this is the state where all spins point in the same direction. The result of this that the expected magnetic moment is ≈ 0.9999. For $kT/J = 2.4$ We get a spread, where the probability density is a almost gaussian distributed. The highest and the most desired energy is ≈ -1.23548 for this case, but still there spins with higher and lower energy than this. This is due to not all of the spins are aligned in the same direction. There a few of them still randomly oriented. The variance for $kT/J = 1.0$ is:

$$\sigma^2_{kT/J=1} \approx 0.004220 \tag{40}$$

and for $kT/J = 2.4$

$$\sigma^2_{kT/J=2.4} \approx 0.001567 \tag{41}$$

The standard deviation does not make sense for the case with $kT/J = 1.0$, and thus were ignored. For the case $kT/J = 2.4$ the standard deviation were $\sigma \approx 0.03958$.

6.4 Phase transition

In this study we have analyzed the phase transition for five different lattices sizes. As mentioned in subsection (2.6) when the system gets closer to the Curie temperature, it undergoes a second phase transition. Where thermodynamical quantities such as heat capacity and magnetic susceptibility is discontinous at T_c. This behaviour is observed in figure (7). After this point the system goes from a ferromagnet to paramagnet, i.e looses its ability to self mangetize which can be oberserved in figure (8). As you can see the magnetic moment tends to lower values, and becomes zero for some temperature values, $T >> T_c$. The convergence is heavily dependent on the lattice size. The bigger lattice the faster the magnetic moment converges towards zero. As consequence of this, the energy of the system increases because after a while when system stabilizes half of the spins is oriented up and the other half pointing down. This gives a higher energy, and the magnetic moment dies out for large temperatures. Thus becoming a paramegnet. The estimated Curie temperature for these five lattices are given in the table down below

L	T_C	C_v	χ
40	2.28	2.60	213.43944
60	2.32	1.88	30.675726
80	2.30	2.11	63.38758
100	2.30	2.20	103.19285
120	2.28	2.52	151.86274

Table 1: This table list the value of the heat capacity and magnetic susceptbility at T_c for different lattice sizes with spin L. There is a minimal difference in T_c for the heat capacity and magnetic susceptbility where the discontinuity occours

The main goal of this numerical study where to estimate the Curie temperature and to get a better understanding of the phenomena , using the produced result and recall the constant a in (27)

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} \tag{42}$$

Using $L = 120$ and $L = 60$ with $\nu = 1$, we can estimate this constant to be

$$a \approx 4.8 \tag{43}$$

And using (25) for $L = 120$, we get that

$$T_C(L \to \infty) = 2.28 - \frac{4.8}{120} \approx 2.24 \tag{44}$$

The theoretical predicted by Onsager is ≈ 2.269. Using this we can calculate the relative error is

$$\epsilon_{rel} = 100\% \frac{|2.269 - 2.24|}{2.269} \approx 1.278\% \tag{45}$$

Which is acceptable. We could have achieved quite significantly much better T_C result if we choose to use smaller than $\Delta T = 0.01$. The problem is we need to increase the number of Monte Carlo cyclus, thus the computational time increases significantly. For this run, we runned 16 cores on one node on the super computer ABEL. We used in total $3.2e6$ Monte Carlo cycles, where each core took $2e5$ cycles. All in all the acceptable result is

$$T_C(L \to \infty) \approx 2.24 \pm 0.029 \tag{46}$$

7 Conclusion

Our goal of this numerical study was to get a better understanding of what happens with our system when it nears the Curie temperature. As it turns out the system after T_C the system magnetic moment converges toward zero for large temperature. Thus resulting in higher energy states which also approach zero for higher temperatures. This is due to that the material has spins where half of the spins are pointing upwards and the other half down, this result in increase of energy for individual spin, resulting a higher energy state for the lattice. The conclusion is that the system goes from a ferromagnetic system to paramagnetic system.

In general we have found out that in order to achieve a stable and steady state system, we only require to perform $N = 10^4$ Monte Carlo cyclus. For larger system the computational time increases significantly since we need to go through every spin particles in the lattice, therefore it is crucial to have good understanding of how the different type of thermodynamical quantities converges. It is good to use 10^5 Monte Carlo cycles for large system, eventhough we used $3.2e6$, but this was due to accessbility on a better computer, and we took the chance to improve our data. Further, we also found the analytical solution of 2×2 lattice.

References

[Hjorth-Jensen, 2015] Hjorth-Jensen, M. (Fall 2015). Computational physics fys3150/fys4150, lecture notes.

[Hott, 0513] Hott, M. (08.05.13). The solution of the 2d ising model.

[Mnyukh, 2013] Mnyukh, Y. (2013). Second-order phase transitions, l. landau and his successors. *American Journal of Condensed Matter Physics*, 3(2): 25-30.

[Mohn and Wohlfarth, 1987] Mohn, P. and Wohlfarth, E. P. (1987). The curie temperature of the ferromagnetic transition metals and their compounds. *Journal of Physics F: Metal Physics*, 17(12):2421.

[Pokrovsky, 2012] Pokrovsky, V. (March 27, 2012). Basic statistical models part i ising model.

[Sen. P. K, 1993] Sen. P. K, S. J. M. (1993). Large sample methods in statistics. *Springer*.

8 Appendix A: Derivation of heat capacity

In this section we are going to derive the relation:

$$C_v = \frac{\mathrm{Var}(E)}{kT^2} \tag{47}$$

Consider the following mathematical definition of heat capacity

$$C_v = \frac{\partial \langle E \rangle}{\partial T} \tag{48}$$

Before we start to derive this equation it is useful to derive the expectation values of energy and energy squared. Consider

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = -\frac{\partial}{\partial \beta} \ln Z \tag{49}$$

and

$$\langle E^2 \rangle = \frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i} \tag{50}$$

Notice that the parition function is $Z = \sum_i e^{-\beta E_i}$, meaning if we differentiate Z with respect to the boltzman factor β, we will obtain (49) times the inverse of Z. If we second differentiate Z with respect to the boltzman factor, we will acieve (50) times the inverse of Z. Thus we can write

$$\langle E \rangle = \frac{1}{Z} \frac{\partial Z}{\partial \beta} \tag{51}$$

And

$$\langle E^2 \rangle = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} \tag{52}$$

Going back to the definition of heat capacity, and use the expectationv value of the energy, we can write

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = -\frac{\partial}{\partial T} \frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial T} \left(\frac{1}{Z} \sum_i E_i e^{-\beta E_i} \right) \tag{53}$$

Differentiating this and performing the chain rule

$$C_v = -\frac{1}{Z^2} \sum_i E_i e^{-\beta E_i} \frac{\partial Z}{\partial T} + \frac{1}{Z} \sum_i \frac{E^2}{kT^2} e^{-\beta E_i} \tag{54}$$

The term

$$\frac{\partial Z}{\partial T} = \sum_i \frac{E_i}{kT^2} e^{-\beta E_i} \tag{55}$$

Using this in our expression, we have

$$C_v = -\frac{1}{kT^2} \left(\frac{1}{Z^2} \sum_i E_i e^{-\beta E_i} \right)^2 + \frac{1}{kT^2} \left(\frac{1}{Z} \sum_i e^{-\beta E_i} \right) \tag{56}$$

Notice that first term is just sqaured expectation value of the energy, and the second term is just expectation value of the energy squared. Thus

$$C_v = \frac{1}{kT^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{\mathrm{Var}(E)}{kT^2} \tag{57}$$

9 Appendix B: Derivation of Magnetic susceptibility

In this section we are going derive the relation between magnetic susceptbility and the variance of the magnetic moment. Consider the definiton of magnetic susceptibility

$$\chi = \frac{\partial \langle M \rangle}{\partial B} \tag{58}$$

Where B is the magnetic field strength. Using the definition of expectation value on the magnetic moment, we can write this as:

$$\chi = \frac{\partial}{\partial B}\left(\frac{1}{Z}\sum_i M_i e^{-\beta E_i}\right) \tag{59}$$

If we assume the general case where the energy states can be written as

$$E_i = \epsilon_i - M_i B \tag{60}$$

Where ϵ is the energy from (3) and M_i is the magnetic moment. Thus

$$\chi = \frac{\partial}{\partial B}\left(\frac{1}{Z}\sum_i M_i e^{-\beta(\epsilon_i - M_i B)}\right) \tag{61}$$

Now differentiating this with respect to the magnetic field strength B by using the product and chain rule, we will achieve the following

$$\chi = \underbrace{-\frac{\beta}{Z^2}\sum_i M_i^2 e^{-\beta(\epsilon_i - M_i B)}}_{\langle M \rangle^2} + \underbrace{\frac{\beta}{Z}\sum_i M_i^2 e^{-\beta(\epsilon_i - M_i B)}}_{\langle M^2 \rangle} \tag{62}$$

This is just

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT} = \frac{\mathrm{Var}(M)}{kT} \tag{63}$$

Which another expression for the magnetic susceptibility.