Project 3.
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Ana Planes Hernandez.
Nikolai Sigersvold.

github.com/fastfirefly

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1 ABSTRACT

The aim of this report is to look into the Ising model, commonly used for solving and understanding the concepts of phase transitions. Markov chains, constructed with the well known Metropolis algorithm for sampling from a probability distribution, will be complemeted with Monte Carlo. Hereby, we will study the behaviour of a thermodynamic system reaching its equilibrium state, testing the efficiency of the implemented algorithms for probability sampling.

2 INTRODUCTION

When dealing with numerical problems in high dimensions, Monte Carlo methods are very efficient and highly convenient to use given their excellent performance. Nonetheless, these approaches are based on probabilistic techniques, handling probability distributions from which sampling can often get very difficult. Markov chains are a fairly common way to statistically model random processes, used in several fields. They are generated by the Metropolis algorithm, which uses a simple technique to accept or reject a proposed move, and is a remarkably effective way to sample from a predetermined probability distribution.

We aspire to study how the binary system described by the Ising model evolves towards the equilibrium state when the temperature is raised, and to determine the time it takes to reach this steady state, and the critical temperature in which the system experiences a phase transition from a magnetic phase to a stage with zero magnetisation, for different dimension lattices using the procedure mentioned prior to this which will be properly described in the upcoming sections.

In the present report, we began by presenting the scheme teorethically. All of the different methods that have been used are expounded subsequently along with a brief guide of how to implement the code to resolve the desired problem. Results are critically discussed for the several subproblems and a conclusion is presented at the end where we offer a summary of the outcomes.

3 THEORY

A ferromagnetic transition takes place when the temperature is raised. At the time the material goes over a critic temperature T_c, also known as Curie Temperature, materials undergo a sharp change in their magnetic properties.
Ferromagnetic materials are made of atoms, or units, which have a magnetic moment that is affected by the electromagnetic field.
When their temperature is less than the critic temperature, these units are alligned, meaning their magnetic moments point to the same direction. When the temperature goes over the Curie point, they will be randomly alligned and the material will lose its magnetisation, and become a paramagnetic material.

The **Ising Model** is a model used to study the behaviour of ferromagnetic materials, which can be solved analitically. In this model, these units can only take two values, spin pointing up or down.
Given N particles in a square, the energy of the system is given by:

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

where the sum only includes the closest neighbours, the spins s_k and s_l can only take values ± 1 and J is a parameter that accounts for the interaction between the spins, and is positive.
When all the spins are in the same direction, the total magnetization will be N, while if we have the same number of particles up and down, the magnetization will be null.

When we are close to the critic temperature, it is possible to approximate physical quantities by a power by law behaviour. The mean magnetisation, specific heat and susceptibility may be written as:

$$\langle M(T) \rangle \sim (T - Tc)^{\beta}$$
$$C_V(T) \sim |T_c - T|^{\alpha}$$
$$\chi(T) \sim |T_c - T|^{\gamma}$$

where the critical exponents are $\beta = 1/8$, $\alpha = 0$,$\gamma = 7/4$. The spins become more correlated as we approach the critic temperature, so we can deifne a correlation length, that will therefore increase close to this value.

$$\xi(T) \sim |T_c - T|^{-\nu}$$

This correlation length is proportional to the size of the lattice. We can approximate the critic temperature as

$$T_c(L) - T_c(L = \infty) = aL^{-1/\nu}$$

Setting $T = T_c$, we obtain

$$\langle M(T) \rangle \sim L^{-\beta/\nu}$$
$$C_V(T) \sim L^{\alpha/\nu}$$
$$\xi(T) \sim L^{\gamma/\nu}$$

Using this, we will estimate the value of the critic temperature T_c

4 METHODS

4.1 Markov Chains

In the own Andrey Markov's words, a Markov chain is a stochastic process containing random variables, transitioning from one state to another depending on certain assumptions and definite probabilistic rules.

We define a probability distribution function $\omega_i(t_i)$ as the likelihood of being in a given state i at a time t_i, that is normalised $\sum_i \omega_i(t) = 1$.
The probability of jumping from a state j to a state i is given by the transition probability, $W(j \to i)$, that is time independent and can be written in terms of a stochastic matrix, where all rows and columns sum to 1, and its largest eivenvalue is 1.
Then, a Markov chain is defined as follows.

$$\omega_i(t+\epsilon) = \sum_j W(j \to i)\omega_j(t)$$

When the system evolves, meaning $t \to \infty$, $\omega_i(t \to \infty) = \omega_i$, it will eventually reach the most likely state.
The system stabilises over time, and it will stop depending on time at some point. This steady state corresponds to the eigenvector of the stochastic matrix W with largest eigenvalue, that is to say, the eigenvector with eigenvalue 1.

However, in most cases, the matrix W is either unknown or too complicated. Then, the Metropolis Algorithm is the solution.
We can rewrite the unknown matrix $W(j \to i)$ as:

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

where $T(j \to i)$ is defined as the likelihood of making a transition and $A(j \to i)$ is the likeliness of accepting the transition suggested.
We can bring this new definition of the transition probability to the Markov chain.

$$\omega_i(t+\epsilon) = \sum_j T(j \to i)A(j \to i)\omega_j(t) =$$
$$\sum_j [T(j \to i)A(j \to i)\omega_j(t) + \omega_i T(i \to j)(1 - A(i \to j))]$$

Then,

$$\omega_i(t+\epsilon) - \omega_i = \sum_j [T(j \to i)A(j \to i)\omega_j(t) - \omega_i T(i \to j)A(i \to j)]$$

in the limit when $t \to \infty$, we have that $\omega_i(t+\epsilon) - \omega_i = 0$, meaning that

$$\sum_j [T(j \to i)A(j \to i)\omega_j(t) - \omega_i T(i \to j)A(i \to j)] = 0$$
$$T(j \to i)A(j \to i)\omega_j(t) = \omega_i T(i \to j)A(i \to j)$$

which is known as **detailed balance**, and explains the dynamic between two state systems. It declares that, when in equilibrium, if the probability transition between two states is known, then we also know the probability of the reverse

transition.

Consequently, we have that

$$\frac{\omega_i}{\omega_j} = \frac{T(j \to i)A(j \to i)}{T(i \to j)A(i \to j)}$$

if we make the assumption that $T(j \to i) = T(i \to j)$, then

$$\frac{\omega_i}{\omega_j} = \frac{A(j \to i)}{A(i \to j)}$$

4.2 Metropolis Algorithm

The Metropolis Algorithm is a sampling rule for accepting or rejecting a suggested configuration according to some conditions. It is widely used due to the balance between efficiency and simplicity of it when having to deal with probability distributions from which sampling can be somewhat difficult.

Going back to what we had in the previous subsection, the quantity

$$\frac{A(j \to i)}{A(i \to j)}$$

is what we will call the **acceptance ratio**.

When generating a random number r from the probability distribution function we are considering, the Metropolis algorithm will either accept or reject the move by comparing this number to the acceptance ratio.
If

$$r \leqslant \frac{A(j \to i)}{A(i \to j)}$$

we accept the proposed configuration.
In the following subsection, we discuss how this method is applied to the specific model we are concerned about in this project.

4.3 Implementation

In order to implement these algorithms in our code, the first things that needs to be done is initialise the system, in other words, set the initial and final temperatures, the steps in between, dimension of the spin matrix and number of Monte Carlo cycles.
Then, the metripolis algorithm gets started. The energy differences are found and, according to an ordered or random starting configuration (with all the spins pointing in the same direction or them being incoherently ordered), the energy, spin matrix and magnetisation are activated.
Next, for each Monte Carlo iteration, the program picks a random spin and calculates its acceptance ratio, which is given by

$$\frac{A(j \to i)}{A(i \to j)} = \frac{\frac{e^{-\beta E_i}}{Z}}{\frac{e^{-\beta E_j}}{Z}} = e^{-\beta(E_i - E_j)}$$

since our probability distribution correspons to the Boltzmann distribution, which gives the probability that a system will be in a certain state as a function of that state's energy and the temperature of the system.
The probability of the system being in a state i is proportional to

$$P_i \propto e^{-\beta E_i}$$

Consequently, the condition to accept the proposed move is

$$r \leqslant e^{-\beta \Delta E}$$

where r is a random number between 0 and 1.
If the move is accepted, it flips the spin, adds the energy and magnetic moment to their total.
Then, the program updates the values of the energy E_i, the magnetisation M_i, and their squares, E^2, M^2, adding it to the previous ones.
Lastly, the code is set to compute the total averages, given by

$$\langle E \rangle = \frac{1}{MC} \sum_{i=1}^{MC} E_i$$

$$\langle |M| \rangle = \frac{1}{MC} \sum_{i=1}^{MC} M_i$$

It is fair to justify why we flip one spin at a time instead of running through them all and flip them randomly. If we did the latter, we would have to calculate all of the energies, wich would increasy significantly the amount of CPU time, while if we limit the change to one single spin, only the energy difference from one configuration to another needs to be calculated, resulting in a way more efficient algorithm.

5 RESULTS

5.1 Two spins

For a 2x2 lattice, the possible spin arrangements are shown in the adjacent table. Thus, we are able to calculate the analytical values for the expectation value of the energy, the mean absolute value of the magnetic moment, the specific heat, and the susceptibility in an analytical manner.

Table 1: Different arrangements for a 2x2 lattice

Number of spins up	Number of configurations	E	M
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	+8J	0
1	4	0	-2
0	1	-8J	-4

The partition function Z is given by

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

where N is the dimension of the lattice, in this case 4.
The expectation value for the energy is given by the expression

$$\langle E(T)\rangle = \frac{1}{Z}\sum E_i e^{-\beta E_i} = \frac{-\partial}{\partial\beta} lnZ = -8J\frac{\sinh(8J\beta))}{\cosh(8J\beta)+3}$$

Similarly, the mean magnetisation is

$$\langle M(T)\rangle = \frac{1}{Z}\sum M_i e^{-\beta E_i} = \frac{1}{Z}(-4e^{8J\beta} + 4e^{8J\beta} - 8e^0 + 8e^0) = 0$$

But the absolute mean magnetisation is

$$\langle |M(T)|\rangle = \frac{4 + 2e^{8J\beta}}{\cosh(8J\beta)+3}$$

The specific heat can be written in terms of the energy variance as follows

$$C_V(T) = \frac{\sigma_E^2}{K_B T^2} = \frac{1}{k_B T}\frac{64J^2}{\cosh(8J\beta)+3}(\cosh(8J\beta) - \frac{\sinh^2(8J\beta)}{\cosh(8J\beta)+3})$$

And, lastly, the susceptibility, in terms of the magnetisation variance

$$\chi(T) = \frac{\sigma_M^2}{K_B T^2} = \frac{1}{k_B T}\frac{8(e^{8J\beta}+1)}{\cosh(8J\beta)+3}$$

In the next table we present the results got computing the Ising model for T=1 and 10^6 Monte Carlo cycles, and the analytical results from the previous expressions, setting the same value for the temperature.
We know that, when we are in a very small temperature, the system is intended to have all the spins oriented in the same direction, so the mean magnetisation is supposed to be the unit, analitically.

Table 2: Analytical and numerical values for a 2x2 lattice

	$\langle E\rangle$	$\lvert M\rvert$	C_V	χ
Numerical	-1.996002	0.99862	0.03192	0.00398
Analytical	-1.995981	1	0.03219	0.00401

Next, we present the mean energy as a function of the number of Monte Carlo cycles, so as to estimate the equilibrium value and number of cycles that are needed in order to achieve a good agreement.

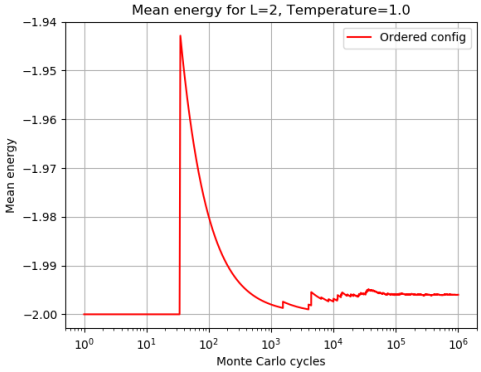

Figure 1: Plot showing the mean energy with respect to the number of Monte Carlo cycles.

We can see that the plot above reproduces the result that were expected. For a small number of Monte Carlo cycles, the results for the mean energy oscillate, not giving a clear result. However, as they are increased, the values will eventually start converging towards a value of the mean energy, corresponding to the steady state. For an approximate number of 10^6 cycles, we are able to obtain a good agreement, as it can be observed in the plot.

5.2 Twenty spins

In this case, we consider a 20x20 lattice, where the dimension is 400.
In order to study carefully the time needed to reach the equilibrium situation, we examine how the mean energy and magnetisation behave as functions of the number of Monte Carlo cycles for two different temperatures: T=1 and T=2.4. We also look upon two starting configurations, one in which the spins are equally oriented, and one in which they have a random orientation. Like this, it is possible to estimate the time the system takes to reach the steady state.

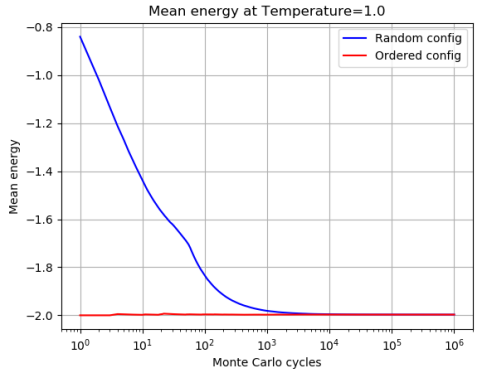

Figure 2: Plot showing the mean energy with respect to the number of Monte Carlo cycles for T=1 for a random and ordered configuration

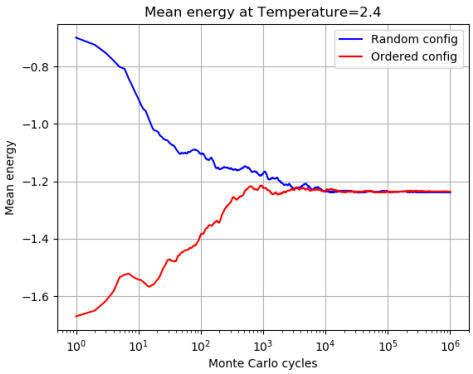

Figure 3: Plot showing the mean energy with respect to the number of Monte Carlo cycles for T=2.4 for a random and ordered configuration

The two plots above show the mean energy as a function of the number of Monte Carlo cycles for both temperatures and starting configurations.
In the first plot, it can be seen how, for an ordered configuration, the system will start at a very low energy, as it is to be expected for low temperatures. On the other hand, the random configuration starts in a completely random mean energy. In both cases, the values for the mean energy will oscillate, the oscillations being larger in the case of the random configuration as it can be observed in the plot where they are both compared, and eventually reach equilibrium.
In the second plot, corresponding to a slightly higher temperature, we observe a similar behaviour, except for the fact that, for the ordered configuration, the mean energy starts in a small value and converges to the steady state, which is a little bit higher.
In both cases, for an approximate number of 10^4 cycles, the equilibrium state will be reached.

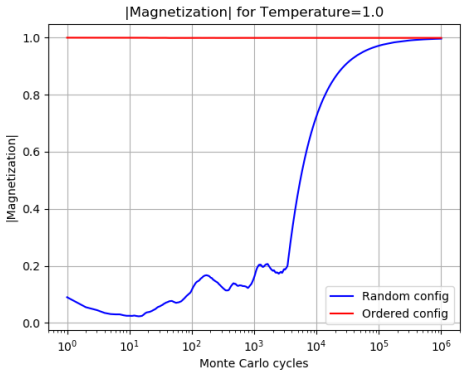

Figure 4: Plot showing the mean magnetisation with respect to the number of Monte Carlo cycles for T=1 for a random and ordered configuration

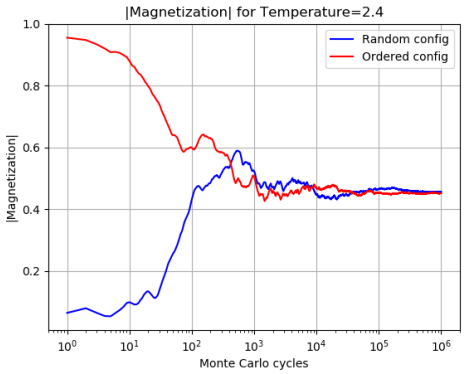

Figure 5: Plot showing the mean magnetisation with respect to the number of Monte Carlo cycles for T=2.4 for a random and ordered configuration

The two plots above show the magnetisation as a function of Monte Carlo cycles now, where we can observe the expected behaviour.
For the plot corresponding to the lower temperature, the ordered configuration will start at a value 1, and oscillate slightly in comparison to the random configuration, which will get started at an arbitraty value of the absolute magnetisation and soon converge towards the most likely state.
The second plot, corresponding to T=2.4 shows a similar behaviour. In this case, both configurations will oscillate and end up settling onto the equilibrium state. The magnetisation will then require around 10^6 cycles to reach this steady state.

Next, the number of accepted configurations as a function of Monte Carlo cycles are presented for both starting configurations and temperature. We can observe how the number of accepted configurations increases if we consider the random starting arrangement, since it does start in a higher energy and accepts a larger number of configurations, and will eventually converge towards the most likely state, accepting at some point as many microstates as the ordered one. For the smallest temperature, the ordered case barely varies in comparison with the other, always staying close to the ground state where it starts from. For the slightly higher temperature, however, it will accept a few more configurations as time goes by.

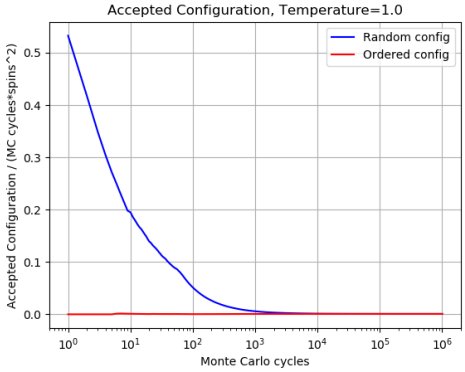

Figure 6: Plots showing the number of accepted configurations as a function of Monte Carlo cycles for T=1 for a random and ordered configuration

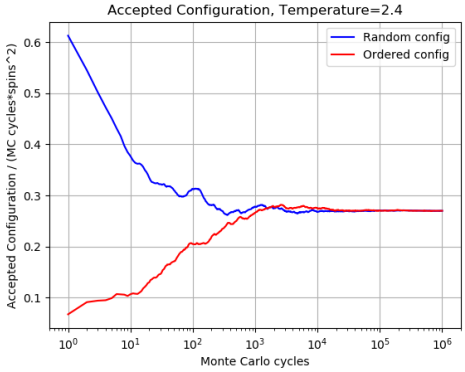

Figure 7: Plots showing the number of accepted configurations as a function of Monte Carlo cycles for T=2.4 for a random and ordered configuration

The probability distribution of the energy for the different energy levels, $P(E)$ is analised next. The following histograms show the behaviour of the probability for the two different temperatures. When it is small, the plot looks thinner and longer, and the most likely value turns out to be the initial value. When T is large, on the other hand, the histogram looks broader and shorter, because the probability is distibuted in more energy levels. It is worth mentioning how the probability distribution looks like a gaussian, just as it was expected.

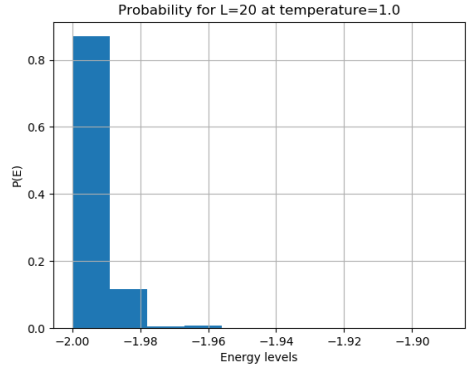

Figure 8: Plot showing the probability as a function of the energy levels for T=1

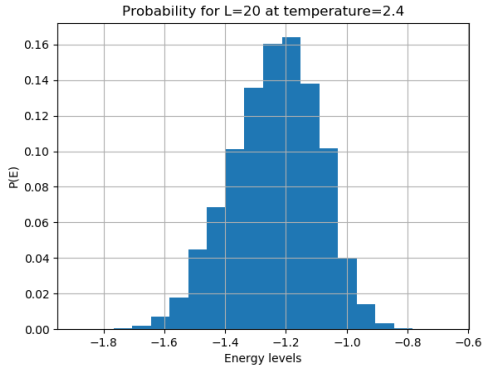

Figure 9: Plot showing the probability as a function of the energy levels for T=2.4

For temperature T=1, we get a value for the variance of **0.023403**, which is the same value we get for the specific heat. The reason is that the specific heat is defined as $C_V = \sigma_E^2/K_B T^2$, and since $K_B T^2 = 1$, $C_V = \sigma_E^2$.
For temperature T=2.4, however, this does not happen. We get a fairly bigger value for the variance, **8.08414** which is to expect, due to the fact that, for a higher T, we have a bigger amount of accepted configurations, meaning the energy values will differ more.

5.3 Phase Transitions

In the present subsection, we focus our attention on the magnetic transition of the system, that is to say, its behaviour when it is close to the critial temperarure in which we know that it will experience the change, losing its magnetisation completely due to the random allignation of the spins.
We consider bigger dimension lattices for this, L=40, 60, 80 and 100 to obtain a better approximation and a small temperature domain, T$\in [2.0, 2.3]$, with a

step of $\Delta T = 0.01$ in order to be able to observe the phase transition.

The following plots show the expected values for E, $|M|$, C_V and χ as a function of the temperature for the selected domain.

As it can be seen in the plot below, the enegy increases with the temperature, almost identically for all of the different dimension lattices, reaching a point in which they will begin to drift apart, corresponding to an inflection point, which is the critical temperature T_C. As the lattice size is increased, the slope at this point increases. This illustrates a phase transition.
At sufficiently high temperatures we would expect the spins to be truly random. In this limit the average energy should approach zero, as each spin would have two spins aligned and two mis-aligned. If we considered a broader domain for the temperature, we would be able to observe this behaviour.

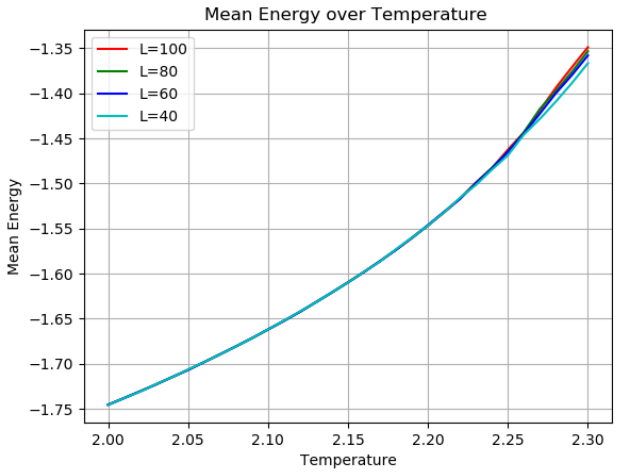

Figure 10: Plot showing the mean energy as a function of T

The next plot shows the mean absolute value of the magnetisation as a function of temperature. The behaviour is expected as, when reaching the critical temperature, this value will drop down to zero, indicating the moment when the phase transition for the material occurs, and all the spins are oppositely oriented. The values corresponding to the largest lattice are the ones approximating the best, as it can be observed how it drops down quicker than the other lattices when reaching the limit.

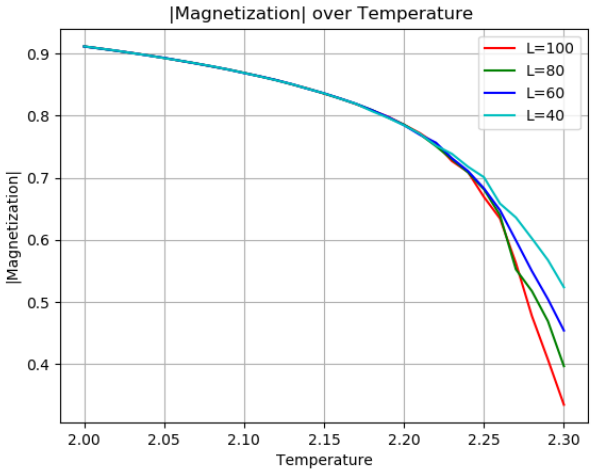

Figure 11: Plot showing the mean magnetisation absolute value as a function of T

The specific value is giving the slope of the mean energy, since

$$C_V(T) = \left(\frac{\partial \langle E(T) \rangle}{\partial T} \right)_V$$

Then, the maximum points in the following plot corresponds to the minimum of the mean energy, that is, when the phase transition occurs. We get different curves for the different dimension lattices, but the one corresponding to the bigest dimmension lattice is giving the best approximation.

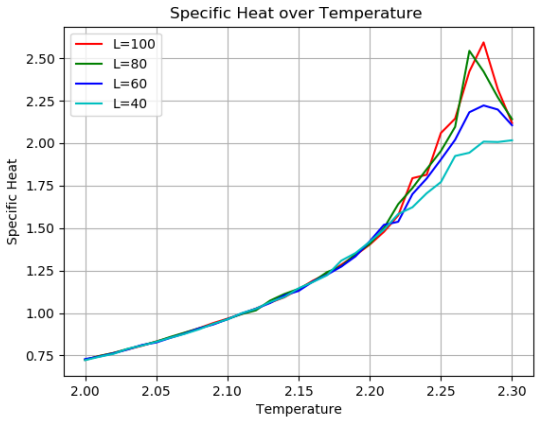

Figure 12: Plot showing the specific heat as a function of T

Similarly, the maximums which can be observed in the plot for the susceptibility correspond to the temperature in which the phase transition occurs, for the different dimension lattices.

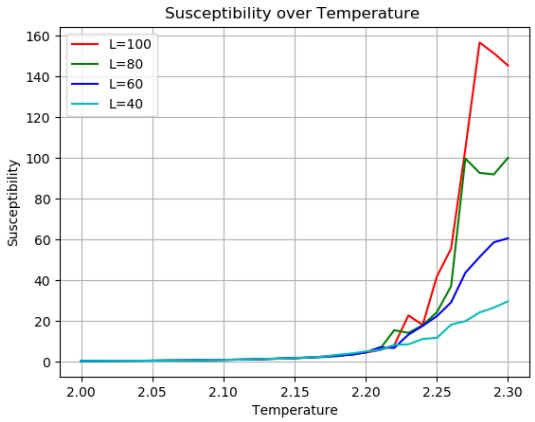

Figure 13: Plot showing the susceptibility as a function of T

When the lattice size approaches a very big number, the critical temperature can be found using the equation

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

The largest lattice dimension that was considered in this report was 100×100, giving an estimated value for the Curie temperature of **2.28**, which is fairly close to the exact value found by Lars Onsager of $kT_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ for $\nu = 1$.

6 CONCLUSION

Using the Monte Carlo Markov Chain method with the Metropolis Algorithm allowed us to simulate the well known Ising model for a magnetic phase transition, studying it both for small and large dimension lattices. The results obtained strongly concur with the theory, enabling us to represent the magnetic transition in reasonably accurate curves, where we obtained a better approximation for the largest dimension lattice. The Curie temperature was roughly obtained for the latter, giving a highly precise value. Consequently, it is possible to state these methods are very effective, and the Ising model can not only be applied to physics, but to a wide range of otherdel fields.

7 REFERENCES

(1) Hjorth-Jensen, M. *Computational Physics. Lecture Notes 2015.* University of Oslo, 2015.
(2) Hastings, W.K. *Monte Carlo Sampling Methods Using Markov Chains and Their Applications* Univeristy of Toronto, 1970.