FYS3150/4150 Project 4

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Abstract

We studied a second order phase transition in a two-dimensional binary spin lattice. We used the Ising model in order to describe the lattice, where the probability for each state of the system was given by the Boltzmann distribution. We simulated the evolution of the system with the Markov chain Monte Carlo method, where the criterion to accept a new configuration was given by the Metropolis algorithm. The first results we found were the mean energy $\langle E \rangle$, the mean absolute value of the magnetic moment $\langle |\mathscr{M}| \rangle$, the susceptibility χ and the heat capacity C_V for a 2x2 lattice. With 10^6 Monte Carlo cycles all the results coincides with the expected values up to the second decimal digit. The second result we found, is that in order to reach the steady state for a 20x20 lattice we need to run at least 10^4 Monte Carlo cycles. In the end we simulated phase transitions for $20x20$, $40x40$, $80x80$ and $100x100$ lattices. The computed critical temperature is $k_B T_C/J = 2.263 \pm 0.008$ where J is a constant, which is compatible with the expected value.

All programs used to produce and plot these results, as well as output files containing the results referred to in this text, can be seen at `https://github.com/Krissvang/Computational-Physics-group`.

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1 Introduction

The aim of this project is to simulate the evolution of a system by using a Markov chain Monte Carlo method. Markov chain Monte Carlo simulations are widely used in physics in order to study different systems, it is therefore important to be able to simulate in a reliable way the evolution of a system. This project looks at the study of phase transitions in a two dimensional lattice. The system we are going to study is a binary system that simulates spins lattice. The spins can point either up or down in this model, and each spin can only interact with its neighbours. This model is called the Ising model. The transitions we are going to study is the one from a magnetic phase (where the system has a finite magnetic moment) to a phase with zero magnetization. This transition happens because the ground state is an ordered state with all the spins assuming the same value, in this case the system got a finite magnetic moment. As the temperature increases the most probable configuration for the system becomes a less ordered one in which half of the spins has got one value and half the other. As a consequence the total magnetic moment becomes null. The Markov chain is used to make the system evolve in time, we will simulate a random walk with a selected probability of making a move, where

every new move is independent from the history of the system. The criterion to accept a move is given by the Metropolis algorithm. This method allows the system to evolve as statistical mechanics requires it to [1]. Any state that has a probability different from zero could be explored by the system [2]. These laws must not be violated by the statistical simulation.

In this text we first describe general Markov chains and the Metropolis algorithm, and how these can be applied to the Ising model. We then find theoretical results for a simple 2×2 lattice of spins, and use these as a benchmark to test our program. Finally, we give numerical results for larger lattices.

2 Methods

In this section are described the methods used in this project: Markov chains, the Metropolis algorithm and the Ising model. The Ising model is really useful to model a two spin system. A Markow chain allows us to simulate the evolution of the system and the Metropilis algorithm makes the system evolve coherently with the probability distribution of the states. Here we also explain what we expect to get during the phase transition and which are the theoretical results for a 2x2 lattice. We also explain what types of unit tests we have done.

2.1 Markow chains

A Markow chain is a stochastic model where we start with a probability distribution function (PDF) $w_i(x_0,t_0)$, and after a given number of time steps we obtain a steady state, i.e. the system reaches equilibrium. The transition probability from state j to state i, for some small time step ε, is given by $W_{ij} = W(j \to i)$, thus $w_i(\varepsilon) = \sum_j W_{ij} w_j(0)$. Note that since w_i and W_{ij} represent probabilities, we have that

$$\sum_i w_i = 1$$

and

$$\sum_j W_{ij} = 1$$

We then have that at a time $t_n = n\varepsilon$ that the PDF is given by

$$w_i(t_n) = \sum_j W_{ij}^n w_i(0) \quad \Longleftrightarrow \quad \hat{w}(t_n) = \hat{W}^n \hat{w}(0) \tag{1}$$

Where $\hat{w}(t)$ is the vector with entries $w_i(t)$ and $\hat{W}$ is the matrix with entries W_{ij}. The problems we now face is the fact that the transition probability W_{ij} is not known or too complicated, this is solved by the Metropolis algorithm.

2.2 Metropolis algorithm

Since W_{ij} is unknown, we let $W_{ij} = W(j \to i) = A(j \to i)T(j \to i) = A_{ij}T_{ij}$ where $A(j \to i)$ is the acceptance probability and $T(j \to i)$ is the probability for making the transition to the state i being in the state j. This is

the idea of the Metropolis algorithm, we suggest a move to a new state j from a state i with some transition probability $T(j \to i)$, we accept the move with a probability $A(j \to i)$ and use the new state as our next starting state, or refuce the move with a probability $1 - A(j \to i)$ and use the original state again. In order to write the Markow chain using A and T we assume that they are time independent and we use that we accept a move with probability A_{ij} and reject a move with probability $1 - A_{ij}$. Thus we get the equation

$$w_i(\varepsilon) = \sum_j [T_{ij}A_{ij}w_j(0) + w_i(0)T_{ji}(1 - A_{ji})] = w_i(0) + \sum_j [T_{ij}A_{ij}w_j(0) - w_i(0)T_{ji}A_{ji}] \tag{2}$$

Using that $\sum_j T_{ij} = 1$. We see that this equation is similar to the so calles master equation given by

$$\frac{dw_i(t)}{dt} = \sum_j [W_{ij}w_j - W_{ji}w_i] \tag{3}$$

This implies that equilibrium is reached when $\frac{dw_i(t)}{dt} = 0$. Thus we have that

$$\frac{W_{ij}}{W_{ji}} = \frac{T_{ij}A_{ij}}{T_{ji}A_{ji}} = \frac{w_i}{w_j} \tag{4}$$

If we assume that the probability to transition from state i to j is symmetric, i.e. $T_{ij} = T_{ji}$, we get that

$$\frac{A_{ij}}{A_{ji}} = \frac{w_i}{w_j} = R \tag{5}$$

In statistical mechanics it is natural to use the Boltzmann distribution for w, we will now implement this algorithm in the Ising model.

2.3 The Ising model

The goal of this project is to study the properties of an $L \times L$ lattice of spins, where the energy of a particular spin configuration (microstate) is given by [3]

$$E = -J \sum_{i=0}^{L} \sum_{j=0}^{L} s_{i,j} \left(s_{i,j-1} + s_{i-1,j} \right) \tag{6}$$

where J is a parameter and $s_{i,j} = \pm 1$ is the spin in the i'th row and j'th column of the lattice. In this project the system is considered to be ferromagnetic, thus $J > 0$. Note that we are using periodic boundary conditions (effectively, this can be seen as surrounding the lattice with "copies" of itself), so that $s_{-1,j} \equiv s_{L-1,j}$, $s_{i,-1} \equiv s_{i,L-1}$, $s_{L,j} \equiv s_{0,j}$, and $s_{i,L} \equiv s_{i,0}$. This is implemented by representing the indices as $i \to (L+i)\%L$. In this way the index -1 will become $L-1$, etc.

Ideally, to calculate the expectation value for the energy, heat capacity, etc. of the system one would use The Boltzmann distribution, which gives the probability of being in a particular microstate i as [3]

$$P_i = \frac{e^{-\beta E_i}}{Z} \tag{7}$$

where E_i is the energy given by (6), $\beta \equiv (k_B T)^{-1}$ (k_B is the Boltzmann constant), and $Z \equiv \sum_i e^{-\beta E_i}$ is called the partition function. For large systems this quickly becomes problematic, however; the system contains L^2 spins which can each have the values ± 1, which means that there are 2^{L^2} accessible microstates. Thus the partition function quickly becomes practically impossible to calculate.

Instead, we let the system start in some initial state and then let it evolve over some number of Monte Carlo cycles [4]. For each cycle the configuration is changed, and new values for the energy, magnetization (equal to the sum of the spins), etc. are calculated and in the end averaged [5]. The state was changed by flipping one random spin in the lattice, as this makes the new energy very simple to calculate; only four terms in (6) change, namely those that involve the spin which is being flipped. The effect of this change is that these four terms change sign, which means that the energy change is given by (here the ij'th spin is being flipped)

$$\Delta E = 2J s_{i,j} \left(s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1} \right) \tag{8}$$

(here $s_{i,j}$ refers to the spin before flipping) The possible values for ΔE are $-8J$, $-4J$, 0, $4J$, and $8J$ [3]. The change in magnetization is $\Delta \mathscr{M} = -2 s_{i,j}$. The new energy and magnetization are then obtained by simply adding these changes.

Not all of these changes can be accepted, however; to ensure that the system behaves according to (7), one must use a sampling rule to determine whether the change is accepted or not. Here we used the Metropolis algorithm [3], which depends on the ratio between the probabilities of the new and the previous states, given by $R \equiv e^{-\beta \Delta E}$ (here one can see another advantage of only flipping one spin at a time; ΔE can only have five different values, as mentioned above, so these factors can be pre-calculated, thus greatly reducing the number of operations). If $R \geq 1$, the new state is more probable than the previous one, so the move is always accepted. If $R < 1$, the probability for accepting the move is equal to R. In practice this is implemented by using a random number generator to pick a number between 0 and 1 from a uniform distribution. If this number is smaller than R the move is accepted; if not, it is rejected.

This procedure is repeated L^2 times for each Monte Carlo cycle. For each cycle, new values of E, $\mathscr{M}$ (magnetization), E^2, $\mathscr{M}^2$ and $|\mathscr{M}|$ are collected. The heat capacity and magnetic susceptibility can then be found by [3]

$$C_V = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{9}$$

$$\chi = \frac{1}{k_B T} \left(\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2 \right) \tag{10}$$

2.4 Analytical solutions for a 2x2 lattice

The simplest case that the Ising model can describe is a two-dimensional spin system with $L = 2$. This means that there are two spins in each dimension. The partition function Z for this system with periodic boundary condition is

$$Z = \sum_{i=0}^{16} e^{-\beta E_i} = 12 + 2e^{8\beta J} + 2e^{-8\beta J} \,. \tag{11}$$

Indeed in this case we have 16 different states. The expectation value for the energy E is

$$E = \langle E(T) \rangle = \sum_{i=0}^{16} \frac{E_i e^{-\beta E_i}}{Z} = -\frac{\partial \ln Z}{\partial \beta} = \frac{16 J e^{-8\beta J} - 16 J e^{8\beta J}}{Z} \,. \tag{12}$$

The mean magnetization $|\mathscr{M}|$ is

$$|\mathscr{M}| = \langle|\mathscr{M}(T)|\rangle = \sum_{i=0}^{16} \frac{|\mathscr{M}_i| e^{-\beta E_i}}{Z} = \frac{8e^{8\beta J} + 16}{Z}. \tag{13}$$

It is useful to calculate the mean absolute value of the magnetic moment because the mean magnetic moment is always equal to zero (since for every state there is a state with the opposite magnetization and the same energy, given by flipping every spin in the lattice). The heat capacity is

$$C_V = \frac{1}{k_B T^2} \frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{1}{k_B T^2} \frac{64J^2(1 + 3\cosh(8\beta J))}{(3 + \cosh(8\beta J))^2}. \tag{14}$$

The susceptibility χ is

$$\chi = \frac{1}{k_B T} \left(\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2 \right) = \frac{1}{k_B T} \frac{32e^{8\beta J} + 32}{Z}. \tag{15}$$

2.5 Phase transition

A phase transition consists in a abrupt change of macroscopic properties of the system, as external parameters are changed, such as temperature or pressure. The Ising model in two dimensions undergoes a phase transition. This means that below a critical temperature, this model exhibits a mean magnetization $|\mathscr{M}| \neq 0$. Above the critical temperature the mean magnetization is equal to zero. This happens because at a low temperature the most likely state is the ground state that in this case corresponds with an ordered state. All the spins assume the same value, this results in a macroscopic mean magnetization. When the temperature increases the spins starts to became more disordered. At a certain point the most disordered state becomes the most likely states. In this state half of the spins assume one value and the second half the opposite one. As a result the mean magnetization vanish. At the critical temperature, the heat capacity C_V and the susceptibility χ are discontinuous or diverge with an infinitely large lattice (thermodynamic limit). This means that the variance in energy and magnetization are discontinuous or diverge.

With a finite lattice we are only approximating an infinite lattice (a real system will practically be "infinite," as its size will typically be of order $\sim 10^{23}$) and the variance of the simulation will always be proportional to $1/\sqrt{M}$ [4], where M is the number of configurations which in our case is proportional with N, the lattice size [3]. Since our lattices will always be of a finite dimensions, the computed C_V or χ will not exhibit a diverging behavior. We will however notice a broad maximum. This maximum becomes sharper and sharper as M and L are increased. The correlation length ξ is an important quantity in studies of phase transitions. For the Ising model the correlation length is related to the spin-correlation function, which again defines the magnetic susceptibility. This quantity defines the distance over which the fluctuations of the microscopic degrees of freedom are significantly correlated with each other. It depends from external conditions such as temperature. Second order transitions are defined as processes in which the correlation length diverges at the critical point. The phase transition we are studying is a classical second order phase transition. In our calculations with the Ising model, we are however always limited to a finite lattice and ξ will be proportional to the size of the lattice at the critical point. Could be demonstrated that the critical temperature T_C scales as

$$T_C(N) - T_C(N \to \infty) = aN^{-\frac{1}{\nu}}, \tag{16}$$

where a is a constant and in this case $\nu = 1$. This makes it possible to extract the "actual" critical temperature from experiments with finite lattice sizes; using linear regression with N^{-1} as "x" and $T_C(N)$ (the temperature

where the heat capacity has its maximum for a given lattice size $N \times N$ as "y"; the intercept of the fitted line is then the critical temperature for an infinite lattice. With $\nu = 1$ the theoretical value for the critical temperature is (in units where $k_B = J = 1$) $T_C = 2/\ln(1+\sqrt{2}) \approx 2.269$ [6].

2.6 Unit tests

To ensure that the algorithms described above works as intended, and have been implemented correctly, we made several unit tests that the programs had to pass. All the tests for this program has been made on a 2x2 lattice because it is the simplest case. The system is randomly initialized with values that must be $+1$ or -1 for each position of the lattice. Thus, we have checked that after the initialization the sum of the elements of the spin lattice matrix was included in the interval $[-4;4]$ and that all the elements were different from zero. By knowing that all the elements are integers and they are all initialized in the same way is easy to conclude that the initialization was correct. We have also tested that the energy of the system was equal to the expected one after the initialization. In order to test the Metropolis algorithm we have checked (in the same way as before) that the spin matrix was still composed by element equal to $+1$ or -1 after the application of the algorithm. We have also verified that the number of changed configuration of the system for one run of the algorithm was included in the interval $[0;4]$. We expect this as explained in the section 2.3. To test to whole algorithm we have checked that the computed mean energy, heat capacity, susceptibility, mean absolute value of the magnetic moment and mean magnetic moment were compatible with the ones that we expect [1] after 10^6 Monte Carlo cycles. The theoretical values were computed by using the equations shown in section 2.4.

3 Results

The obtained results are discussed in this section. We start from the simplest case of a 2x2 lattice. Then are shown the results for a 20x20 lattice. In the end of the section are visible the output we get for the simulation of the phase transition. This has been done with lattices of different size. We note that we have used the common convention of setting $J = k_B = 1$.

3.1 2x2 lattice

The first result we achieved was useful to check that the program was working properly. We studied the evolution of a 2x2 system and we computed the mean energy, the mean magnetization $|\mathscr{M}|$, the specific heat C_V and the susceptibility χ for $T = 1.0$ (in units of kT/J). We compared the obtained results with the theoretical ones we get in section 2.4. The comparison has been done for both a random initialization of the system and an ordered initialization with all the spins equal to one. the results are shown in table 1.

We notice the the computed results are more reliable when we initialize the system randomly. This can be explained by the Boltzmann distribution, (7); here the temperature is relatively low, so the states with higher energies than the lowest are heavily suppressed. Thus when the ground state is reached it is unlikely that the system will "escape" it again, especially for a low number of Monte Carlo cycles. This means that if the initial state is ordered (i.e. the lowest-energy state) there is a chance that very few energies that are not equal to the

ground state energy are collected. Also, we are collecting data before the steady state is reached, which may give unreliable results. Anyway the fact that we do not wait for the system to reach the most likely state does not affect our result too much because we have a small system in this case. For 10^6 Monte Carlo cycles we get results that are equal to the expected ones up to two or three leading digits for all the quantities for a random initialization.

Expected values	-7.9839	0.12833	3.9946	15.9732	
Monte Carlo cycles	**E**	C_V	$\|\mathscr{M}\|$	χ	**Initialization**
10^3	-7.936	0.5079	3.978	1.345	random
10^3	-7.992	0.0639	3.998	0.036	all spins =1
10^4	-7.978	0.1723	3.993	15.497	random
10^4	-7.990	0.0831	3.997	15.087	all spins =1
10^5	-7.981	0.1513	3.993	15.927	random
10^5	-7.983	0.1335	3.994	15.785	all spins =1
10^6	-7.984	0.1230	3.995	15.960	random
10^6	-7.984	0.1271	3.996	15.951	all spins =1
10^7	-7.984	0.1278	3.995	15.970	random
10^7	-7.984	0.1297	3.994	15.967	all spins =1

Table 1. In this table are displayed the results we get for a 2x2 lattice together with the expected values, for $T = 1$.

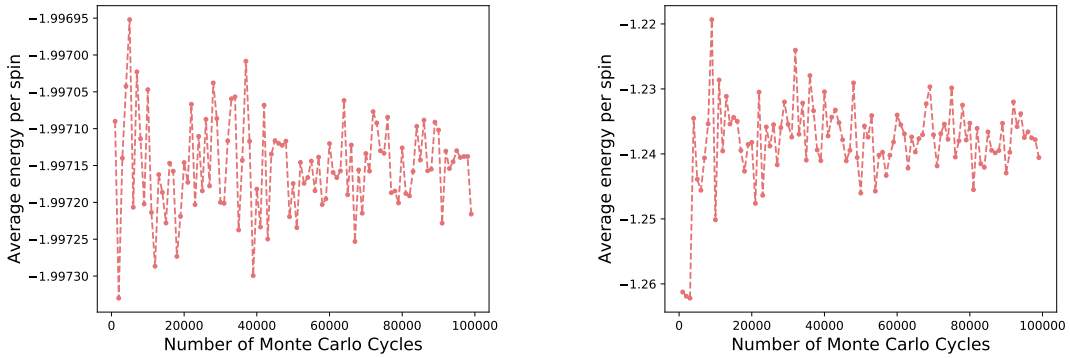
3.2 20x20 lattice

In the previous calculation we did not studied carefully how many Monte Carlo cycles were required in order to reach the most likely state. In this section we want to perform a study of the number of cycles one needs before to reach the equilibrium state and to start computing the various expectations values. The number of Monte Carlo cycles here represents time. The easier way to do this is the graphical one. We plot the mean energy and magnetization as function of the number of cycles. We have have done this for a 20x20 lattice with temperature equal to 1.0 and 2.4 (in units of kT/J) for both a random and ordered initialization.

In figures 1a and 1b are visible the results for the average energy per spin sating with an ordered configuration for the two different temperatures. In figures 2a and 2b we have the same as before, starting with a random configuration. We notice that for $T = 2.4$ the plots are similar, for $T = 1$ they differs. This because in the first case the temperature is relatively low, so when the ground state is reached it is unlikely that the system will ”escape” it again. This is visible if we compare figure 5a with figure 6a. Indeed, the number of accepted configuration when we start from an ordered state is on average much smaller than the number of accepted configuration with an initial random state. This means that if we start from a ordered state, that corresponds with the ground state here, the mean energy of the system will have only small fluctuations with magnitude about 0.15% from the measured value. When we start from a random state, this can be really far in energy from the ground state. Thus the oscillations in the average energy before the ground state is reached can be bigger than the ones in the previous case. For instance the oscillation’s magnitude is about 13% from the measured value for the data in figure 2a. This happens only for a small numbers of Monte Carlo cycles. In this case we can approximate that number with 10^4 cycles. We notice that in the graph with $T = 2.4$ too, i.e. figure 2b, the oscillations begins to stabilize around 10^4 Monte Carlo cycles. The number of accepted configurations

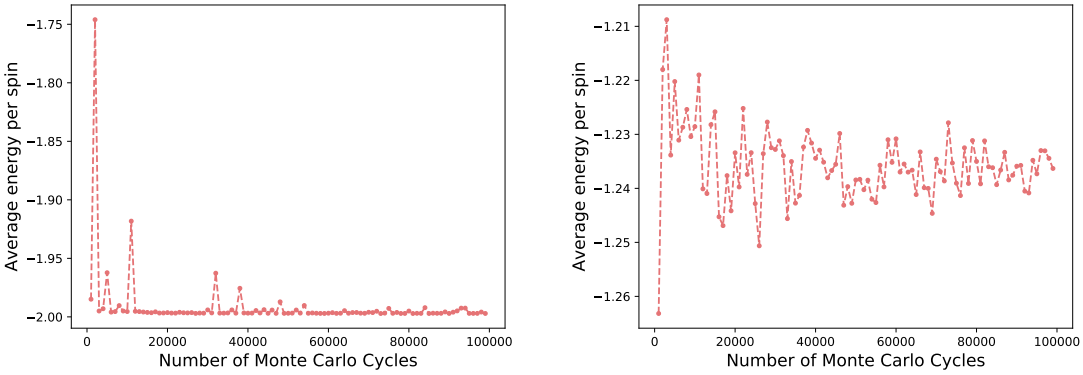
is approximately the same in this case for a random and ordered initial state. This number increases with the temperature if the initial configuration is a ordered state. This because as the temperature increases we have to move from the ground state to a higher-energy state. This passage is statistically favorite by the Boltzmann distribution, thus an increasing number of configurations are accepted as the temperature increases if the initial state is the ordered one. If we start from a random state the number of accepted configuration could increase or decrease with the temperature too. It depends from the initial state.

The same considerations we have made for the mean energy are true for the average absolute value of the magnetization. The plots in this case are displayed in figure 3a, 3b for an ordered initial state and in figure 4a, 4b for a random initial state.



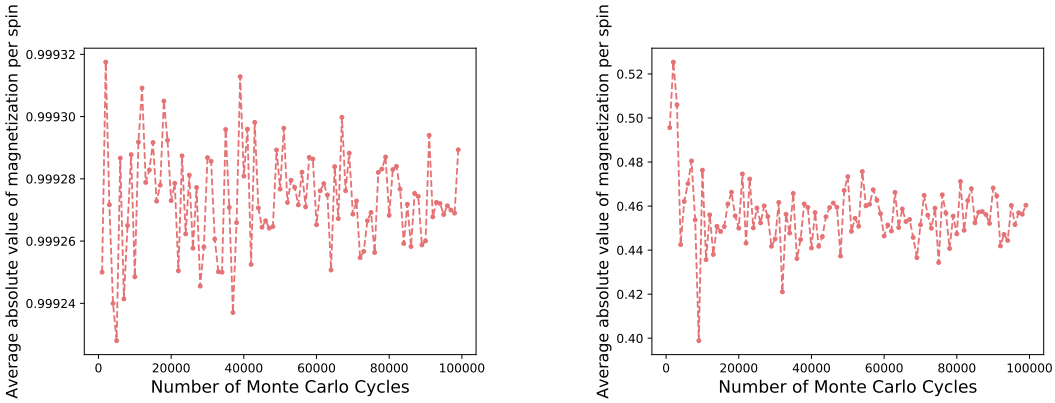
(a) $T = 1$ **(b)** $T = 2.4$

Fig. 1. Average energy as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a ordered configuration. Run with lattice size 20×20. Spacing is 1000.



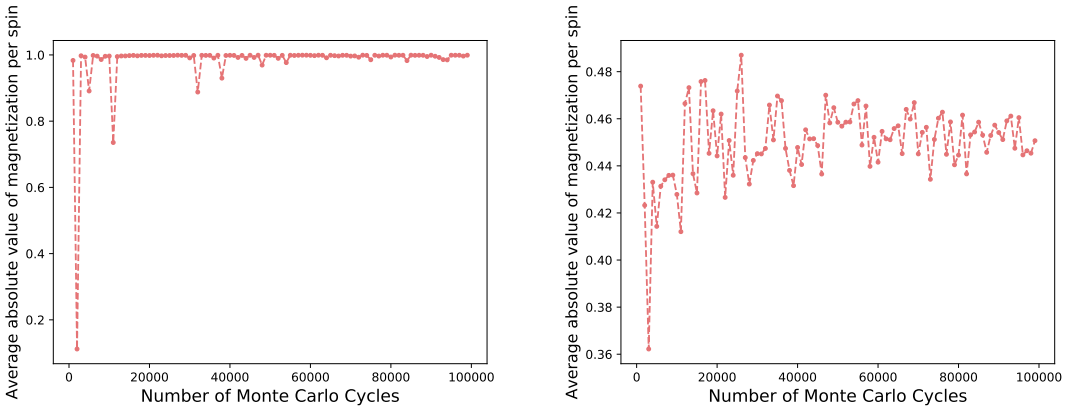
(a) $T = 1$ **(b)** $T = 2.4$

Fig. 2. Average energy as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a random configuration. Run with lattice size 20×20. Spacing is 1000.



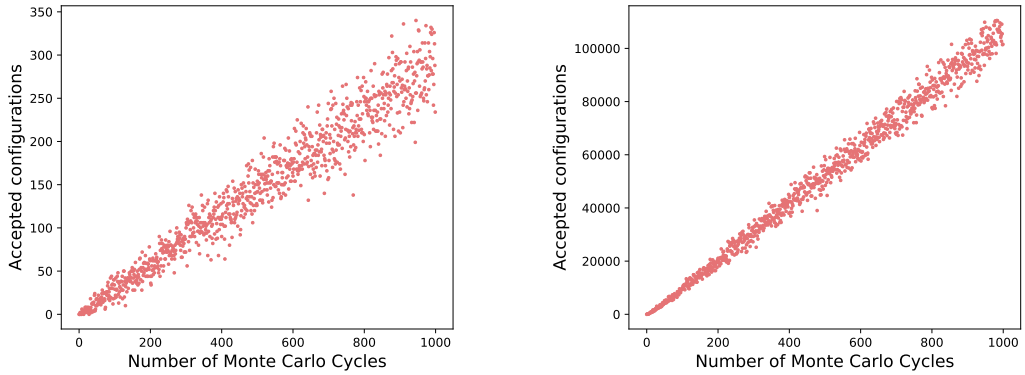
(a) $T = 1$ **(b)** $T = 2.4$

Fig. 3. Average magnetization as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a ordered configuration. Run with lattice size 20×20. Spacing is 1000.



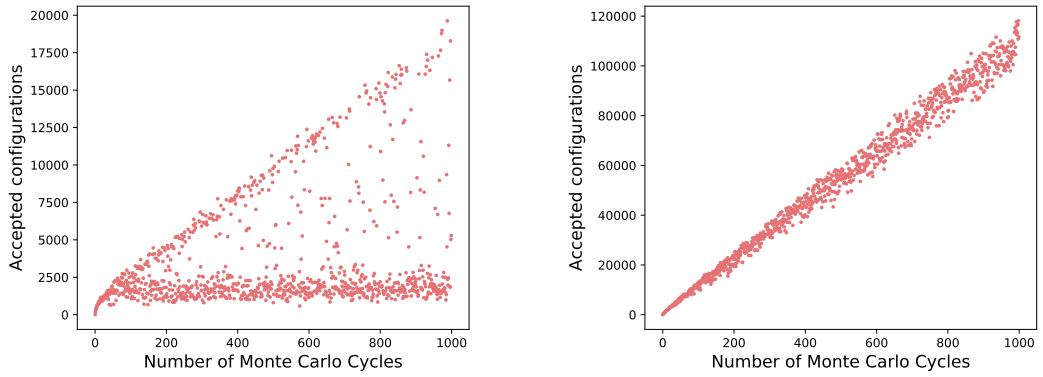
(a) $T = 1$ **(b)** $T = 2.4$

Fig. 4. Average magnetization as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a random configuration. Run with lattice size 20×20. Spacing is 1000.



(a) $T = 1$ **(b)** $T = 2.4$

Fig. 5. Number of accepted configurations as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a ordered configuration. Run with lattice size 20×20.

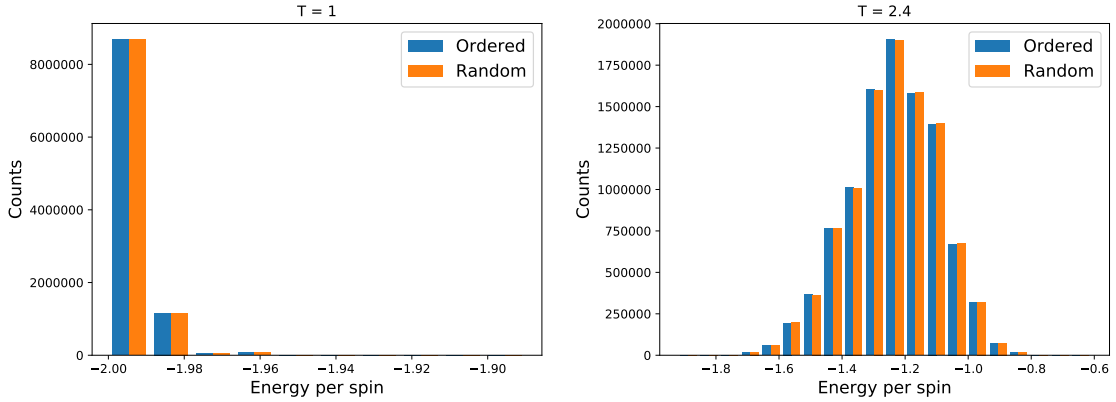


(a) $T = 1$ **(b)** $T = 2.4$

Fig. 6. Number of accepted configurations as a function of number of Monte Carlo cycles at temperature $T = 1$ and $T = 2.4$, given a random configuration. Run with lattice size 20×20.

3.2.1 Energy distribution

To examine the energy distributions for different temperatures, we counted the number of times each energy appeared (after the system had stabilized) for a 20×20 lattice with the temperatures $T = 1$ and $T = 2.4$, and both random and ordered (all spins equal to $+1$) initial states. These results are shown in figure 7.



(a) $T = 1$ **(b)** $T = 2.4$

Fig. 7. Number of counts per energy for temperatures $T = 1$ and $T = 2.4$, with 10^7 Monte Carlo cycles (data were collected after the first 10000 cycles), for both ordered and random initial states.

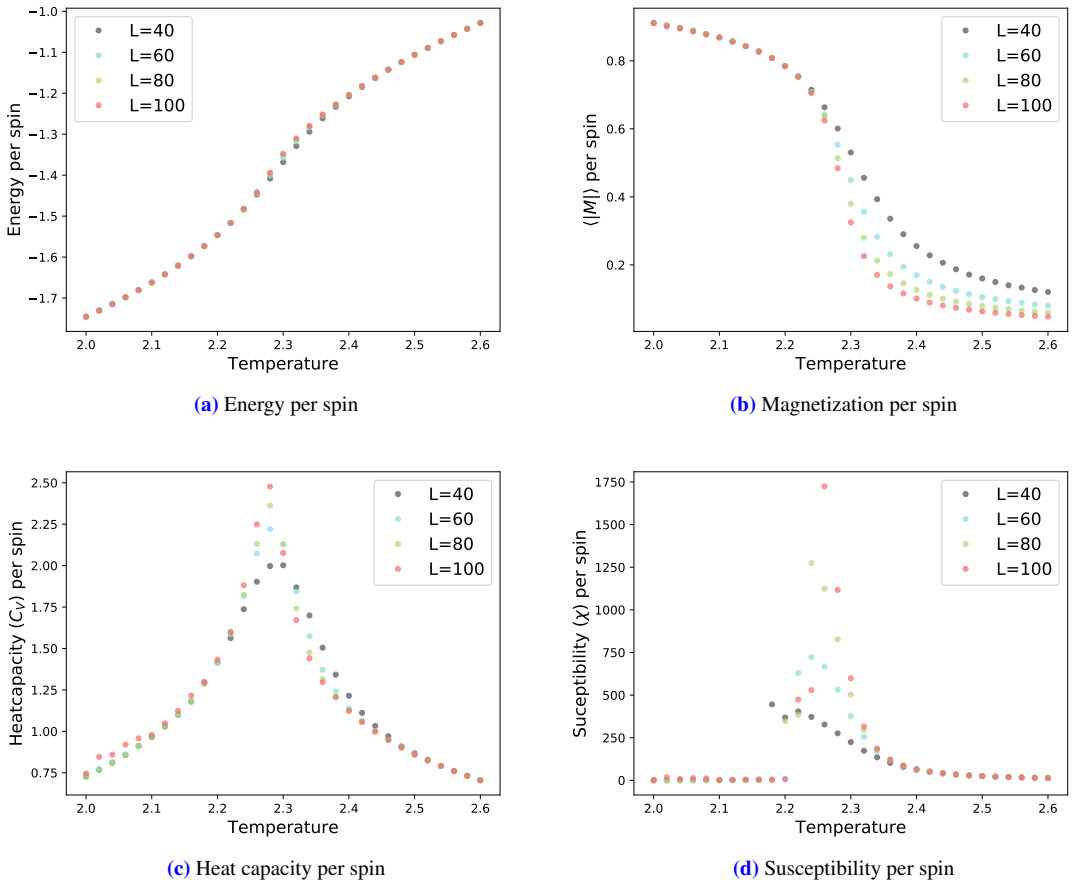
The distributions are essentially independent of the initial state, which is as expected since we allowed the system to equilibrate before collecting data; thus the state as we started collecting data is approximately the same, regardless of the initial state. However, the distributions for the two temperatures are very different; for $T = 1$ the system is almost exclusively in its ground state (all spins aligned), with a standard deviation of $\sigma_E \approx 0.008$ (calculated using (9), so that $\sigma_E = \sqrt{k_B T^2 C_V}$), while for $T = 2.4$ the distribution is much wider ($\sigma_E \approx 0.14$, which fits with the observed distribution; it is a little over half its maximum value at one standard deviation away from the mean, as it should in the case of a normal distribution), and the ground state is not the most likely state. This can be understood from the Boltzmann distribution, (7); the lower the temperature is,

the quicker the distribution drops to zero for increasing energies. Thus, for low temperatures, the system will remain in, or close to, its ground state, while the distribution gets wider for increasing temperatures.

This also explains why the most likely state changes with the temperature. For very high temperatures the distribution is approximately independent of energy (until we reach a phase transition); instead, the multiplicities of the different energies (the number of accessible microstates with a given energy) dominate the distribution, and the most likely energy is the one with the highest multiplicity. In this case the ground state is very unlikely, as there are only two possible states with the lowest energy (all spins aligned in either direction) Then, as the temperature decreases, high energies will become more and more suppressed by the Boltzmann distribution, and the energy of the most likely state decreases, until it reaches the low-temperature limit where all states except the ground state are heavily suppressed.

3.3 Phase transition

in this section we shown our results regarding the behaviour of the Ising model in two dimensions near to the critical temperature as function of the lattice size N. We have considered L= 40, 60, 80 and 100. The temperature interval have studied is $T \in [2.0, 2.6]$. The temperature step ΔT is equal to $\Delta T = 0.05$. We computed the mean energy $\langle E \rangle$ per spin, the mean magnetization $\langle |\mathscr{M}| \rangle$ per spin, the heat capacity C_V per spin and the susceptibility χ per spin. The results are displayed in figure 8a, 8b, 8c and 8d. As we expect in a phase transition as the one that we have studied, C_V exhibits a broad maximum for a certain temperature. In the thermodynamic limit this should be a divergence point but with the experiment we get only an approximation of this behaviour because of the limited extension of our lattice as explained in section 2.5. For this reason as the size of the lattice is increased we get a sharper peak. The value of $|\mathscr{M}|$ is different from zero at low temperatures and goes to zero as the temperature increases. This is a symptom of a transition from a ferromagnetic phase (for $T < T_C$) to a paramagnetic phase (for $T > T_C$). The curve does not exhibit a discontinuity in the first derivative, as we expect for a second order phase transition. Anyway as we increase the lattice size the curve becomes steeper. This because of the same reason as before. The susceptibility χ shown a discontinuity point near to the critical temperature. The mean energy E increases as the temperature rises. The function seems to be linear for $T \ll T_C$ and for $T \gg T_C$. in correspondence of the critical temperature we have different behaviour of the function that manifests the phase transition. The Susceptibility χ exhibits a sharper peak as the lattice size increases.



(a) Energy per spin

(b) Magnetization per spin

(c) Heat capacity per spin

(d) Susceptibility per spin

Fig. 8. Energy-, magnetization-, heat capacity- and susceptibility per spin as a function of temperature for different lattice sizes $L \times L$. Run with 10^7 Monte Carlo cycles starting with a random configuration.

In order to get the last results has been useful to parallelize the code. To achieve this we used MPI. One can see from table 2 that running the program with four parallel processes decreases the CPU time by a factor between three and four. One would expect an improvement of a factor four in The computational time. It does not happen however; this might be due to a bottleneck of the CPU that was used or the extra time required to call the additional functions necessary for parallelization (e.g. adding the contributions from each process). If that is the case, one might expect the computational time to approximately become inversely proportional to the number of processes when this number gets larger. This would be interesting to look further into in the future.

k_BT/J	**Computation time without parallelization [s]**	**Computational time with parallelization [s]**
2	806.33	246.6
2.2	822.83	252.1
2.4	837.2	256.3

Table 2. Comparison between the computational time required to run the code with and without parallelization. Both codes has been optimized with the compiler flag -O3.

By using equation (16) and the data shown in figure 8c has been possible to estimate the critical temperature in

the thermodynamic limit i.e. for $L \to \infty$. We have fitted the T_C value we get from the simulations for different values of L with the expression (16) as is shown in figure 9. The expected result for the critical temperature [6] is

$$\frac{k_B T_C}{J} \approx 2.269\,. \tag{17}$$

The result we get is

$$\frac{k_B T_C}{J} = 2.263 \pm 0.008\,. \tag{18}$$

This result is compatible with the expected one because the difference between the estimated and theoretical values is $0.006 \in [-0.008, +0.008]$.

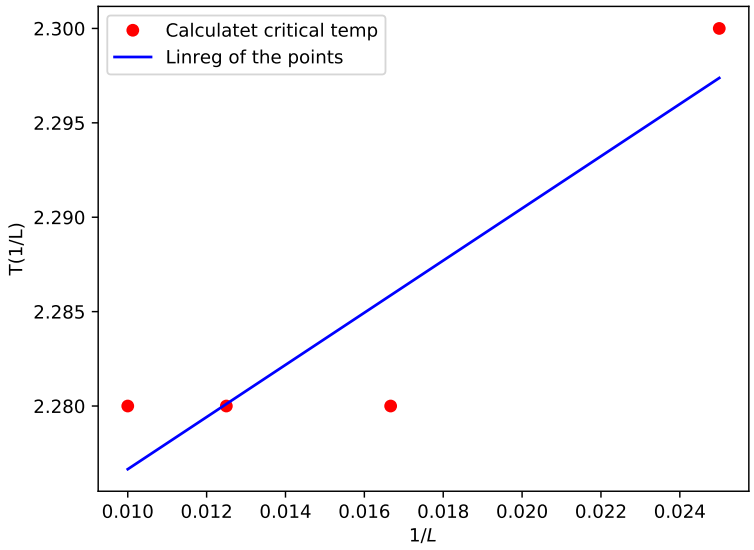


Fig. 9. In this plot the red points are the critical temperature values taken from the data in figure 8c. The blue line is the linear fit on this points. The law for the fit is given by equation (16).

4 Conclusion

The first results we get is the mean energy $\langle E \rangle$, the mean absolute value of the magnetic moment $\langle |\mathscr{M}| \rangle$, the susceptibility χ and the heat capacity C_V for a 2x2 lattice with 10^6 Monte Carlo cycles, all coincides with the expected values at least up to the second decimal digit. This results are useful in order to check that the program is working properly. The second result we get is that in order to reach the steady state for a 20x20 lattice we need to run at least 10^4 Monte Carlo cycles, it is important to note that the numbers of cycles could vary based on which configuration we start from and the temperature of the system. 10^4 is a value that worked for our experiments. The third result is that in a 20X20 lattice when $T = 1$ the system is almost exclusively in its ground state and the standard deviation on the energy is $\sigma_E \approx 0.008$. When $T = 2.4$ the distribution is wider $\sigma_E \approx 0.14$ and the ground state is not the most likely state. This happens because the probability of each configuration for a given temperature is described by the Boltzmann distribution. In the end we simulated phase transitions for $20x20$, $40x40$, $80x80$ and $100x100$ lattices. The theory tells us that this is a second order phase transition, thus the derivative of the mean magnetization should diverge at the critical point and the specific

heat should exhibit a divergence point. Our results does not show discontinuity because of the limited size of our lattice. To see the divergence we should run the experiment with a much bigger lattice. Our measurement of the critical temperature is affected by the limited size of the lattice as well. From the previous results is possible to estimate the value in the thermodynamic limit. The result we get is $k_B T_C/J = 2.263 \pm 0.008$ where J is a constant, which is compatible with the exact value. It is worth noting that this result is not very reliable because we have done the fit with only four points. Moreover, these points do not seems to follow a linear trend. We could get a more reliable estimation for the value of T_C with simulations with smaller temperature-steps and for more lattice sizes L. The greatest limitation of the algorithm is that we are using a binary model. In the classical theory almost no observable can assume only two values. Another limitation regards our computational power. Due to our machines we are able to simulate only low dimensional lattices. For this reason a three dimensional simulation is almost impossible to run. One way to make the simulation more effective is to use the Potts model [3], which is not a binary model. In this case the spins can take more than two possible values. We could also use more computational power to run a three-dimensional model instead of a two dimensional one. With this model we will get a more reliable simulation of a solid material.

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