FYS 3150 - Project 4

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(Dated: November 20, 2017)

In this project we take into account the Ising model to study which is the most likely state of a lattice at a given temperature T. To perform this we develop a program based on the Monte Carlo method and on the Metropolis algorithm as acceptance rule. Starting from a simple lattice 2×2, we are able to benchmark our numerical results to the theoretical ones. Then we switch to consider a lattice 20×20 to understand how the evolution of mean value of energy and mean value of absolute magnetization is related to the number of Monte Carlo cycles for $T = 1\ k_B\ T\ J^{-1}, T = 2.4\ k_B\ T\ J^{-1}$. Furthermore, in this case, the probability of obtaining an energy is discussed and it is found to be in agreement with the Boltzmann distribution. Eventually, parallelizing our code, we run a simulation with lattices $20 \times 20, 40 \times 40, 60 \times 60, 80 \times 80, 100 \times 100$ and we observe the behaviour of $< E >, < |M| >, C_V, \chi_{abs}$ as functions of temperature, finding various indicators of phase transitions. Through the maxima of C_V and χ_{abs}, we estimate the value of the critical temperature for an infinite lattice finding $T_C = 2.274\ k_B\ T\ J^{-1}$ (from the specific heat) close to the theoretical one found by Onsager. The critical temperature from χ_{abs} is further from the expected value.

- URL to GitHub folder of the code: `https://github.com/DavideSaccardo/Project4_ISING`

I. INTRODUCTION

The Ising model is one of the most studied model in Statistical Mechanics to study phase transitions as it is particularly easy and it's very effective to explain the transition between a ferromagnetic material to a paramagnetic one. In our case, we simplify the model considering the external magnetic field to be null. This yields to an expression of energy as

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

where s_k represents the $k-$th spin in our lattice.

We implement a code based on the Monte Carlo method and on the Metropolis algorithm to accept or not a move. In fact, this algorithm is particularly good to module achievement of an equilibrium for a system. This program is then tested with respect to the theoretical results from a 2×2 lattice finding a good agreement as the number of MC cycles overcomes the million. Therefore, we study the lattice 20×20 for $T = 1\ k_B\ T\ J^{-1}$ and $T = 2.4\ k_B\ T\ J^{-1}$ and for an initial configuration with all the spins up and one with random oriented spins. In particular we consider the mean energy ($< |E| >$), mean absolute magnetization $< |M| >$ and accepted moves as function of MC cycles and we find how many cycles are needed to reach an equilibrium. This result is useful to start the system from the state of equilibrium for further considerations.

At this point, we consider the probability $P(E)$ of obtaining an energy E after the equilibrium state for $T = 1\ k_B\ T\ J^{-1}$ and $T = 2.4\ k_B\ T\ J^{-1}$. Through the variance, we confirm these distributions to be Boltzmann as we expect.

Finally, we parallelize our code to be able to evaluate bigger lattices in reasonable time and with a reasonable amount of data. Using 10^6 MC cycles and 8 processors in the computers of the university, we are able to find the $< E >$, $< |M| >$, the specific heat and the susceptibility (computed with the absolute value of M) as functions of the temperature for lattices of size $L = 20 \times 20, 40 \times 40, 60 \times 60, 80 \times 80, 100 \times 100$. Using these curves we detect the signals of a phase transitions of the second order. Hence, we fit the curves of C_V and χ_{abs} to find the maximum for each lattice declared before. From the maxima, we are able to find the critical temperature for each lattice. Finally, fitting the critical temperature as functions of the inverse of the size dimension $1/L$, we are able to find $T_C(L = \infty)$ from both C_V and χ_{abs}. These values are then compared with the expected one, found by Onsager in 1944.

The report begins with an extensive theoretical part meant to explain a bit more about the Ising model, phase transitions, Metropolis algorithm to the one who are not familiar with these concepts of Statistics and Statistical Physics.

II. METHODS AND ALGORITHMS

The aim of this project it to study which is the most likely configuration (as regards energy $< E >$ and magnetization $< |M| >$) of a lattice at a given temperature T. To accomplish this, we introduce the *Ising model*, which is able to simulate the behaviour

of a magnetic material with respect to thermal energy and external magnetic field. In particular, the Ising model with dimension $D \geq 2$ is able to predict a phase transition of the second order at a certain critical temperature T_C. However, let us first explain the model itself. Here we consider a square lattice Λ of dimension $L = N \times N$, where N is the number of spins. Each domain of the lattice is occupied by an atom with a corresponding magnetic moment, which can be $\uparrow$ or $\downarrow$. The spins are represented by $s_k = \pm 1$, where 1 means that the spin is pointing up and -1 means the opposite. An example of the lattice is showed in Fig. (1). The energy of the sys-

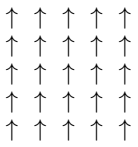


Figure 1: Example of a lattice 5×5, with all the spins up.

tem is given by two contributions: the interaction between neighbouring spins and the action of an external magnetic field to each spin. The first tends to align the spins, therefore we have a favourable configuration (negative energy) when spins are both up or both down, and an unfavourable (positive energy) when a spin is up and a spin is down. As for the external magnetic field, if it points up, it favours the up spins, and vice versa in the other case. With this consideration, the Ising model energy is represented by

$$E = -J \sum_{<kl>}^{N} s_k s_l - h \sum_{k}^{N} s_k \tag{1}$$

where the notation $< kl >$ represents nearest neighbours pair, that is we are summing over nearest neighbours only, L represents the total number of spins, and J is a coupling constant, which represents the strength of the interaction between neighbours spins. As regards the sum over nearest neighbours, there are two possibility to treat the ends of our lattice. One is the so called "free ends", i.e. the contribution from point to the right or left of the endpoints is null. Hence, we have $E = -J \sum_{i,k}^{N-1} s_{i,k} s_{i,k+1} - h \sum_{i,k}^{N} s_{i,k}$. The other possibility is the so called "periodic boundary conditions": the right neighbour of spin s_N assumes the value of the first spin in that line. For example in one dimension, if we consider N spins, we have that the neighbour of the right of s_N is equal to s_1. In the program and in all the calculations, we use periodic boundary condition.

For what it concerns eq. (1), if we consider $J > 0$, as said above, the alignment of spins is energetically favoured. This leads to a spontaneous magnetization at low temperature: interacting with its neighbours, a spin can influence the behaviour of other spins located at macroscopical distance from the first [[1]].

For our interests, we consider no external magnetic field ($h = 0$). Hence the energy of our system is

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

Moreover, fixing temperature, volume, and number of particles, our system can be described as a canonical ensemble. Hence the likelihood probability (P_i) of finding the system i a configuration i is described by Maxwell-Boltmann distribution that is

$$P_i(T) = \frac{e^{-E_i \beta}}{Z} \tag{2}$$

where $\beta = 1/(K_B T)$ ($K_B = 1.38 \times 10^{-23}$ Joule/K is the Boltzmann constant, but we set $K_B = 1$), $Z = \sum_{i=1}^{m} e^{-E_i \beta}$ is the partition function, and m is the total number of microstates. Hence we can define the mean energy and mean magnetization as

$$< E >= \sum_{i=1}^{M} E_i P_i(T) = \frac{\sum_{i=1}^{m} E_i e^{-E_i \beta}}{\sum_{i=1}^{M} e^{-E_i \beta}}$$
$$< M >= \sum_{i=1}^{M} E_i P_i(T) = \frac{\sum_{i=1}^{m} M_i e^{-E_i \beta}}{\sum_{i=1}^{M} e^{-E_i \beta}},$$

and the variance of E and M through the relations

$$\sigma_E^2 =< E^2 > - < E >^2$$
$$\sigma_M^2 =< M^2 > - < M >^2 .$$

At this point, in statistical mechanics we can relate these statistical quantities with macroscopical ones through thermodynamical potentials. Let's introduce the *Helmhotz free energy*:

$$F =< E > -TS, \tag{3}$$

which becomes in the canonical ensemble

$$F = -\underbrace{K_B T}_{1/\beta} \log z \tag{4}$$

where, here and then, as log we mean the natural logarithmic. Eq. (3) and Eq. (4) allow us to relate the mean energy with the entropy of the system: in fact F represents the coexistence between the principle of minimization of energy and of increment of entropy as the temperature increases. At equilibrium, these two principle reach a balance, which is represented by Helmhotz's free energy.

From statistical mechanics, we can also show that

$$< E >= k_B T^2 \Big(\frac{\partial \log z}{\partial z}\Big)_{V,N} = \frac{\partial(\beta F)}{\partial \beta}. \quad (5)$$

We can combine eq. (5) with the definition of specific heat

$$C_V = \Big(\frac{\partial < E >}{\partial T}\Big)_V$$

to get

$$C_V = \frac{1}{k_B T^2}\frac{\partial^2}{\partial \beta^2}\log z \propto \frac{\partial^2 F}{\partial T^2}. \quad (6)$$

However, knowing that $\sigma_E^2 = \partial^2 \log z/\partial\beta^2$, we can also write

$$C_V = \frac{\sigma_E^2}{k_B T^2}.$$

In the same way, we can evaluate the magnetic susceptibility as

$$\chi = \frac{\sigma_M^2}{k_B T}. \quad (7)$$

In some cases it's useful to compute χ as the variance of $|M|$:

$$\chi_{abs} = \frac{< |M|^2 > - < |M| >^2}{k_B T}. \quad (8)$$

The reason for using eq. (8) is that for small lattices like ours and few MC cycles, $< M >$ can give important fluctuation around 0, when we get closer to the critical temperature T_C. Hence, substituting $< M >$ with $< |M| >$ allows to cancel these fluctuations. Anyway, for large lattices (like $L = 1000 \times 1000$), it should be used $< M >$ (i.e. the correct expression), as the fluctuations vanish automatically. We state that from this point to the end of the report we consider mean energy, mean absolute value of magnetization, specific heat and magnetic susceptibility per spin as it's easier to compare different sized lattice in this way.

As for the units of measure, we express the energy is units of J and the temperature in units of $k_B T J^{-1}$. In this way the exponential of the Boltzmann factor ($e^{\beta E}$) is unitless. Therefore, scaling the equations, $< M >$ is unitless, $[C_V] = [k_B]$ and $[\chi] = J^{-1}$.

As regards the theoretical solutions to Ising model, Ising hilmself found the solution to the one dimensional case, which doesn't predict a phase transition. For what it concerns the two-dimensional case, the solution was much harder and it was found by the Norwegian chemist and theoretical physicist, Lars Onsager in 1944. His solution leads to the famous formula for the critical temperature:

$$\frac{k_B T_C}{J} = \frac{2}{\log(1+\sqrt{2})} \simeq 2.269 \quad (9)$$

Here, we are going to show the solution of the two dimensional case with $L = 2 \times 2$, which is easy but it's also useful as benchmark to our program.

A. Lattice 2×2

In this situation, It's easy to find the analytical expression of several quantities which we are interesting with, such as the expectation value of the energy $< E >$, mean absolute value of magnetic moment $< |M| >$, the specific heat C_V and the susceptibility χ. All these quantities are computed as functions of T.

With lattice 2×2, we have a total number of $2^4 = 16$ configurations as we have $L = 4$ spins. If we number our spins as s_1, s_2, s_3, s_4, the energy of one of the configurations (microstates) taken on by our system is $E_i = -J\sum_{<kl>} s_k s_l$ $(i = 1, \ldots, 16)$. If we explicate last expression, we get $E_i = -(s_1 s_2 + s_1 s_3 + s_4 s_2 + s_3 s_4) \cdot 2J$. While the total magnetization for a given configuration i is $M_i = \sum_j^N s_j$. Evaluating the energy and magnetization of each configuration we can construct Tab. (I).

Table I: The table displays number of degeneracies and the respective energy and magnetization per number of spins up.

Number of spins up	Degeneracies	E_i $[J]$	M_i
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

From this table, we can compute the partition function

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 12e^0 + 2e^{-8J\beta} + 2e^{8J\beta} \quad (10)$$

where $\beta = K_B T$. From eq.(10), we can compute the expectation value of energy per spin and mean

absolute value of magnetic moment per spin:

$$E = \frac{\sum_{i=1}^{16} e^{-\beta E_i} E_i}{Z} = \frac{16e^{-8J\beta} - 16e^{8J\beta}}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} J \tag{11}$$

$$|M| = \frac{\sum_{i=1}^{16} e^{-\beta E_i} |M_i|}{Z} = \frac{+8e^{+8J\beta} + 16}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} .. \tag{12}$$

We note that $|M|$ is unitless. From eq. (11), we get the specific heat per spin as

$$C_V = \frac{64}{T^2} \frac{3\cosh 8\beta + 1}{(6 + 2\cosh 8\beta)^2} \frac{1}{k_B}. \tag{13}$$

Instead from eq. (12), we compute the susceptibility (χ_{abs}) per spin as

$$\chi_{abs} = \frac{6e^{8J\beta} + 2e^{-8J\beta} + 6}{T(19 + \cosh(16J\beta) + 12\cosh(8J\beta))} J \tag{14}$$

and

$$\chi = \frac{4}{T} \frac{e^{8J\beta} + 1}{6 + 2\cosh(8J\beta)} J. \tag{15}$$

See Appendix for a complete derivation of the three expressions.

B. Phase transition

As introduced above, the two-dimension Ising model succeeds in predicting the second order phase transition, which occurs between ferromagnetic materials and paramagnetic ones. However, we would like to spend some lines to explain better what happens.

A phase transition happens when there is an abruptly change in the macroscopical quantities of a system. In this picture, it's important to introduce the correlation function, which is a kind of measure of the order of a system. In particular, it describes how much correlated are microscopical quantities (in our case it's the covariance of spins) as function of distance and temperature. Therefore we can define a correlation length ξ, which express the distance at which the fluctuation of microscopic quantities are correlated with each other.

We can distinguish between two types of phase transition: first and second order phase transitions. The first one happens when thermodynamic quantities such as magnetization suddenly jump (discontinuously) as function of other macroscopic thermodynamic quantities (as temperature). In this case the correlation length is finite when the "jump" happens. On the other hand, the second order phase transition are characterized by divergent susceptibility, infinitive correlation length and a scale behaviour of the correlation function around the critical point, which is the point of the phase plan, where the phase transition happens [[2]]. Another way of defining them is in relation with the partition function and free energy: the discontinuity or divergence of the derivative of partition function or free energy is an indicator of phase energy of the order of the derivative. Hence, a first order phase transitions is recognized as a discontinuity of energy (first derivative of F as eq. (5)), while a second order as a discontinuity of specific heat (second derivative of f as eq. (6)). In the Ising model, the heat capacity diverges, thus we have a second order transitions. Also the susceptibility (which it could be demonstrated that is $\chi \propto (\partial^2 F/\partial h^2)_{h\to 0}$, where h is the external magnetic field) diverges: an ulterior confirm of the order (second) of this phase transition.

In our case (2D Ising model, with external magnetic field $h = 0$), hence, we have a second order phase transition. This is represented by a spontaneous magnetization $< M > \neq 0$ for $T < T_C$, where T_C is the critical temperature, where we have the transition. On the other hand, for T above the critical temperature, the mean magnetization vanishes. It's useful to note that $< M >$ approaches T_C with infinitive slope: it's a signal of a critical phenomenon, which is marked by a particular thermodynamical variable, which vanish at T_C, the "order parameter". In this situation, the order parameter is the mean magnetization. As we can't consider infinitive lattice, but just finite ones, we won't see a divergence in the heat capacity or susceptibility. Instead, we'll see a swelling for both the functions in correspondence of the T_C.

Near T_C, using mean field theory, one could demonstrate that thermodynamical quantities have a power law behaviour:

$$\begin{aligned} &< M(T) > \sim (T - T_C)^{\beta} \\ &C_V(T) \sim |T_C - T|^{-\alpha} \\ &\chi(T) \sim |T_C - T|^{\gamma} \end{aligned} \tag{16}$$

where $\beta = 1/8,\ \alpha = 0,\ \gamma = -7/4$. As regards the correlation length behaviour, we have the following

$$\xi(T) \sim |T_C - T|^{-\nu}, \tag{17}$$

i.e. ξ is infinitive in $T = T_C$ and dies exponentially for $T \neq T_C$ Eq. (17) can be motivated qualitatively with the following picture.

- $T \gg T_C$: we are in the regime where the entropy is the most important term, the system is disordered, hence the spin fluctuations aren't correlated as we don't have an alignment between neighbours spins.

- $T \to T_C^+$: progressively domains of order grow in the lattice among the field of disorder, thus the local alignment improves and also the correlation length.

- $0 < T < T_C$: in this regime the principle of minimization of energy dominates causing the spins to align globally. The fluctuation of a spin doesn't affect the others, because there is an infinite number of ordered spins, which counters massively.

- $T \to T_C^-$: here, domains of disorder grow in the field of order, decreasing the pressure to align globally and increasing the correlation length.

As the correlation length could be seen as a measure of the length of the order and disorder domain in the two cases above respectively, when $T = T_C$ we have a good coexistence between order and disorder (our lattice is half ordered and half disordered).

In our computations, we are limited to finite dimension Ising model. However, we could use the scaling eq. (16) to relate a finite lattice with one in the thermodynamical limit and we could find the scaling of the critical temperature

$$T_C(L) - T_C(L = \infty) \propto \alpha L^{-1/\nu}, \tag{18}$$

where a is a constant. In our case, having $\nu = 1$, we compute the specific heat and susceptibility for $L = 40 \times 40, 60 \times 60, 80 \times 80, 100 \times 100$, we fit the expressions and we extract the maximum. Though that, we find the critical temperature for each size, and extending to 0 the fitting line of T_C as function of $1/L$, we get $T_C(L = \infty)$.

It's important to state briefly that there is another way of seeing a phase transition: symmetry breaking. For $T > T_C$ the system stay the same if we flip all the spins (the mean magnetization is null and the material is ferromagnetic), i.e.

$$s_k \to -s_k.$$

However, when the system is cooled below T_C, it's forced to chose a particular alignment (all spins up or all spins down), leading to a spontaneous magnetization, which makes the material ferromagnetic.

C. Algorithm

To compute various thermodynamical quantities such as mean energy, mean magnetization, specific heat and susceptibility we write a code based on the Monte Carlo, which is a way of obtaining results performing repeated random samplings.

Essentially our code is based on three functions: initializeLattice, MCcomputation, writeResultstofile. After having defined the initial and final temperature, the temperature step, the number of spins and number of Monte Carlo cycles desired, the first function provides to create the lattice with $L =$ numberOfSpins $\times$ numberOfSpins and to fill it with spins. This could be done in two way depending on how we define flag:

- flag = 1: it fills randomly the lattice with spins up $+1$ or down -1 using a random number generator, which is the Mersenne-Twister' one;

- flag = 0: it fills the lattice with all the spins up.

Moreover, the function computes the initial energy with periodic boundary conditions and the initial magnetization. As regards *MCcomputation*, it contains the loop over the number of MC cycles decided before. For each cycle, the code loops over all the spins in the lattice matrix and the proposoal of flipping a random spin is made (still using RNG Mersenne-Twister). Whether the prososal is accepted or not is regulated by the selection rule built using *the Metropolis algorithm*. Finally, it updates the expectation values, which are later printed to file. The printing function is writeResultstofile, which also normalizes all the expectation values with respect to the number of MC cycles. In this way, we are assuming that

$$< E >= \frac{\sum_{i=1}^{m} E_i e^{-E_i \beta}}{\sum_{i=1}^{M} e^{-E_i \beta}} \simeq \frac{\sum_i E_i}{\text{MCcyles}}. \tag{19}$$

Furthermore, the function computes all the thermodynamical quantities of interest ($C_V, \chi, < E >, < |M| >$) per spin, which allows us to compare the values with lattice of different size.

This setup is used for small lattices. For bigger lattices (such as the ones used to find the critical temperature), the code is parallelized using the library OpenMPI. With this implementation, we are able to perform Number of processors $\times$ *MCcycles* experiments in the same time as just one *MCcycles* without parallelization. This allows us to collect more data and to have a better statistics. The data originated from each processor are collected all together using MPI_Reduce and they are normalized by the Number of processors $\times$ *MCcycles* by writeResultstofile.

a. Metropolis' algorithm In a Monte Carlo simulation, the strategy is to chose a selection of random states according to a probability distribution, which in our case is the Boltzamann distribution (eq. (2)). This could be implemented straightforward using the Boltzmann distribution as acceptance rule. However, this is highly inefficient as we would have to compute the partition function (it's a sum

over microstates, with 2^L terms, for good size lattice $L \sim 100 \times 100$ it's impossible to compute). Therefore, we avoid this and we base of MC on Markov processes (random walks with selected probability for making a new move) to accept or not a new state. Markov processes allows our system to reach the most likely state of the system (in thermodynamics this means to reach an equilibrium) starting from a random state, when we run the system for long time. In this picture, it is inserted the Metropolis algo, which as it is based on a Markov chains has to obey the condition of ergodicity and detailed balance.

We want to understand what is the PDF $w(t)$ after a time ϵ, i.e.

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

where w_i represents the probability of being in a state i at a time $t+\epsilon$ and $W(j\to i)$ is the transition probability to move from state j to the state i. W can be written as a matrix. It's important to note that W, w represent probabilities, indeed they have to satisfy

$$\sum_j w_j(t) = 1$$
$$\sum_j W(j\to i) = 1$$

at each time t.

In a Markov chain process, usually, W is unknown. In this situation, the Metropolis algo steps out on the stage.

As W is unknown, we model it as a product of two probabilities: $A(j\to i)$, probability for accepting a proposed move from j to i and $T(j\to i)$, probability for making a transition. Hence, we have

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

At this point, we want to understand the processes that leads to equilibrium. To do this, we have to investigate the PDF after a time ϵ. From a dynamical point of view, to move from j to i, we can just accept the transition from j to i, or if we are already in i, we reject the move. Considering T, A time independent, we can express the last reasoning as

$$w_i(t+\epsilon) = \sum_j [w_j(t)T_{j\to i}A_{j\to i} + w_i(t)T_{i\to j}(1-A_{i\to j})]. \tag{20}$$

Since $\sum_j T_{j\to i} = 1$ (normalization condition), we can rewrite eq. (20) as

$$w_i(t+\epsilon) - w_i(t) = \sum_j [w_j(t)T_{j\to i}A_{j\to i} - w_i(t)T_{i\to j}A_{i\to j}].$$

At the steady state (equilibrium, most likely state), we have

$$w_i(t+\epsilon) - w_i(t) = 0 \tag{21}$$

i.e. the state becomes time-independent. Using eq. (21), in the limit $t\to\infty$, the system has to reach equilibrium. Therefore, we get the expression

$$\sum_j w_j(t)T_{j\to i}A_{j\to i} = \sum_j w_i(t)T_{i\to j}A_{i\to j}. \tag{22}$$

However, eq. (22) is not sufficient to guarantee the generation of the correct distribution after many interactions. To avoid to run into cyclic solutions,w e introduce the detailed balance condition, which guarantees to reach the most likely state:

$$w_j(t)T_{j\to i}A_{j\to i} = w_i(t)T_{i\to j}A_{i\to j}.$$

We still have this unknown quantity (the transition probability). Anyway, we can take the ratio and we obtain

$$\frac{w_j}{w_i} = \frac{T_{i\to j}A_{i\to j}}{T_{j\to i}A_{j\to i}}.$$

In our case $w_i = w^{-\beta E_i}$, hence we have a model for w_j/w_i, which is

$$\frac{w_i}{w_j} = e^{-\beta(E_j - E_i)} = e^{-\beta\Delta E},$$

and using uniform PDF for N spins ("brute force Metropolis"), the probability of picking a given spin is

$$T_{i\to j} = T_{j\to i} = \frac{1}{N},$$

which leads to

$$\frac{w_j}{w_i} = e^{-\beta\Delta E} = \frac{A_{i\to j}}{A_{j\to i}}.$$

If $w_j/w_i > 1$, we have $E_j < E_i$, viz we are moving to a state with lower energy, and hence, we set $A_{i\to j} = 1$, which is the largest acceptance probability, to be sure to accept this move. However, this can't be the only possibility, because we would violate the ergodic hypothesis and this would lead to a biased statistical averages. This hypothesis states that every possible state of the system can be reached by any Markov process from any starting point, if we tun the simulation for enough time. Practically, to avoid this, we accept a move to a state with higher energy than the state when we are, if random number $r \in [0,1]$ is bigger than the ratio w_j/w_i, i.e. than the exponential $e^{-\beta\Delta E}$. On the contrary, we refuse the move. In the code this is implemented with the condition

```
deltaE<=0||RandomNumberGenerator(gen)<=
        differenceOfEnergy[deltaE/4+2].
```

In fact, this condition is redundant, because if $\Delta E \leq 0$, as differenceOfEnergy $= e^{-\beta\Delta E}$, obviously $RandomNumberGenerator(gen) \leq differenceOfEnergy$. However, this redundant condition allows us to skip the generation of a random number, which is a quite slow process and it leads to a faster code.

Moreover we note that using Metropolis we avoid the computation of Z as it vanishes when we take the ratio w_i/w_j.

Now, we just need an efficient way to compute the differences of energy. There are two ways of accomplishing it. One it to flip all the spins, to compute the total energy of the system and to perform Metropolis at the end of each MC cycle. The other is to loop over all the spins, but when we have to flip one of them, we immediately compute the energy and we perform Metropolis. These two are mathematically equivalent. However we choose the second as it is computational more efficient than the other. In fact, to compute the energy in the first case we need roughly $\sim L^2$ FLOPS, where L is the total number of spins, whereas in the second we just need ~ 4 FLOPS. Furthermore in the Ising model there are only 5 different cases of difference of energy, hence we can pre-calculate them and we can save a lot of CPU time.

III. OUR RESULTS

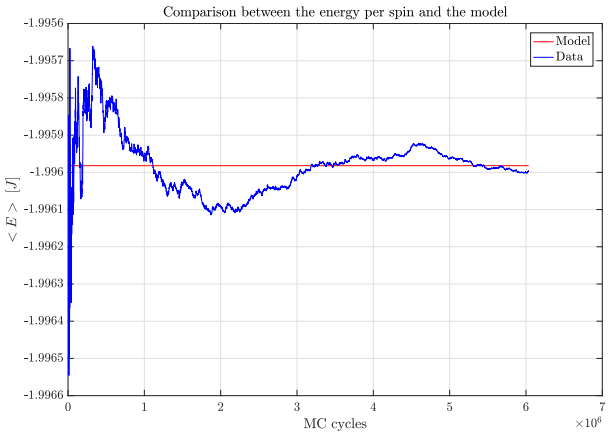
A. Lattice 2×2

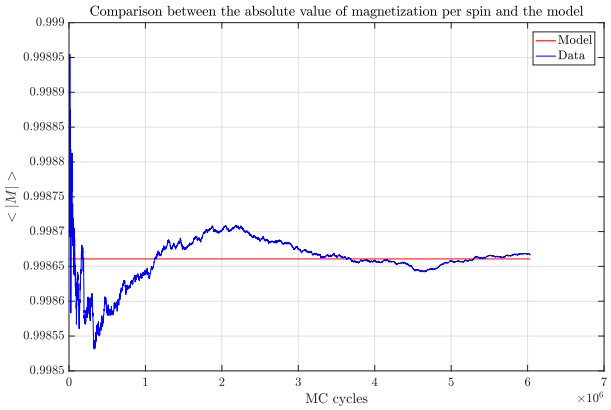
Firstly we run a simulation over a Lattice of dimension $L = 2 \times 2$ initialized with all the spins up. This is useful to benchmark our numerical results to the theoretical ones stated in the paragraph (II A), to understand if our code is correct and how many MC cycles are needed to reach a successful agreement. We run our code with $T = 1.0 \mathrm{k_B T J^{-1}}$ and we watch the progress of the quantities E, $|M|$, C_V, χ with respect to the theoretical expectation at that temperature (Fig. (2)) as we increase MC cycles from 10^4 to $6 \cdot 10^6$ with a step of 1000. From the figure, we can see a good agreement when we overcome the millions of MC cycles. Moreover, we see that our code is correct as the numerical values approach the theoretical ones even better as we increase the number of MC cycles. As regards χ and χ_{abs}, we note that the first is more stable than the second. However, this is not in contrast with what is written in the section above, as the strong fluctuations of χ happens at $T \sim T_C$ for such small lattices, while here we consider $T \ll T_C$.

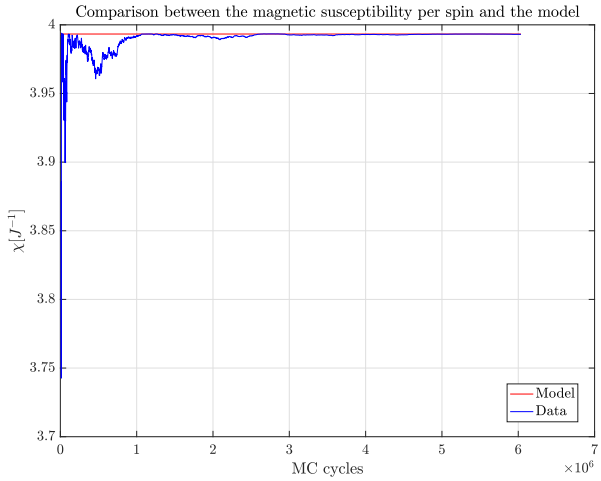
B. Lattice 20×20

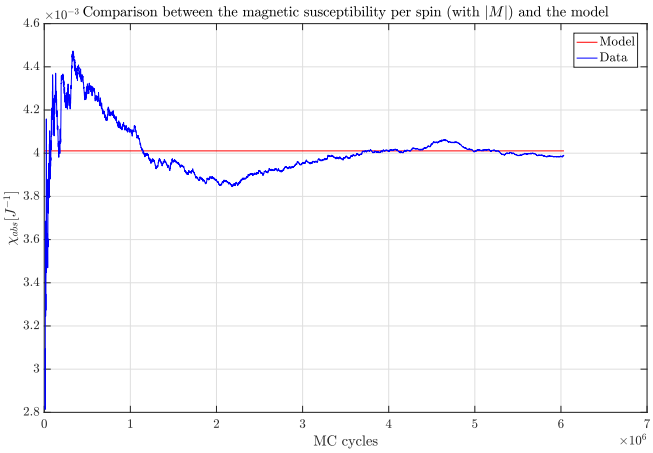
At this point, we move our analysis to consider a lattice of dimension $L = 20 \times 20$. We run a simulation with 10^6 MC cycles and we want to see the "story" of the energy E and the absolute magnetization $|M|$ as function of MC cycles (actually, we interpret the number of Monte Carlo cycles as time). We perform this computation for both $T = 1.0 \mathrm{k_B}$ T $\mathrm{J^{-1}}$, $T = 2.4 \mathrm{k_B}$ T $\mathrm{J^{-1}}$ and for both the initial configurations with all the spins up and random spins. With the initial configuration with all the spins up (Fig. 3), for both temperatures the energy starts with it's lowest values and it approaches the mean value by below as expected: the configuration with all the spins in the same direction is the one with lowest energy. As we can see, for low temperature, the energy and the magnetization approach rather quickly the mean value, while for the higher temperature it takes a bit longer and they fluctuate more around the mean values. These are direct consequences of the Boltzmann distribution: with higher temperature, the Boltzmann factor allows the system to access more states, indeed there are more fluctuations around the mean value. Instead, with low temperature, the most likely state is the ground state and the Boltzmann factors give a low likelihood of moving out. At high temperature, our system enters a regime of disorder, which shows itself with a lower magnetization and a mean energy that is far from the lowest value with respect to $T = 1 \mathrm{k_B}$ T $\mathrm{J^{-1}}$. In fact, increasing the temperature will lead to a magnetization of zero after the transition phase as the spins of the system will become completely disordered. However we can consider the equilibrium to be reached after $\sim 5 \cdot 10^4$ MC cycles, which is thus our equilibration time. As regards the accepted choices, we can see that when we increase the temperature the number of accepted moves increase of a factor bigger than 10. This is still due to the fact that at higher temperature, the system can access to more states, which represent more moves.

For what it concerns the initial configuration with random spins (Fig. (4)), we can see that the energies approach the mean value from above for both the temperatures. This is what we expect as with this initial configuration the initial energy would be higher than the energy at the equilibrium. Moreover, the behaviour of the curve of energy with low temperature is really smooth due to the fact that at $T = 1 \mathrm{k_B}$ T $\mathrm{J^{-1}}$, the most likely state chosen is the ground state and there is not much possibility of going out of that. Therefore, fluctuations are nearly zero around the mean energy. On the other hand, at higher temperature the system can access more states and thus we have more fluctuations around









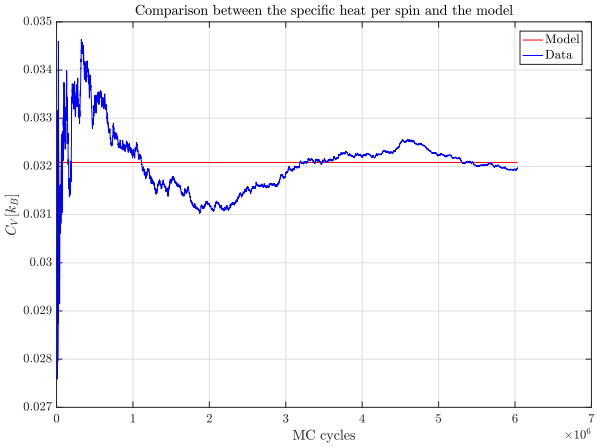


Figure 2: In these figures we compare the theoretical values of quantities such as $< E >, < |M| >, C_V, \chi_{abs}, \chi$ with the ones obtained numerically for $T = 1.0 \mathrm{k_B TJ^{-1}}$ for MC cycles $\in [10^4, 6 \cdot 10^6]$. As we can see to obtain a good agreement we have to overcome the millions of MC cycles.

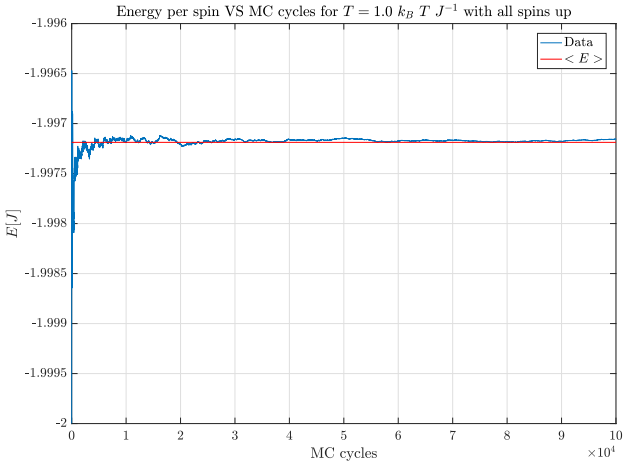
the mean value as we can see from the Fig. (4). Furthermore, at higher temperatures, the entropy dominates producing a lower value of magnetization and mean energy with respect to low temperature. However, the "velocity" of the curves to reach the mean value is nearly the same between the two different initial configurations. Therefore, even in this case, we can state that the equilibrium state is reached in about $\sim 5 \cdot 10^4$ MC cycles. As regards the accepted moves, while in Fig. (3), the two lines start far from the beginning and they keep a nearly constant distance, here the two curves start really close. This is due to the fact that the random initial configuration makes the the difference of the energy of the system in the two different temperatures to be much smaller than in the other configuration. Hence, at the beginning, at both temperatures we have a high entropy and the system can access a number of states at $T = 1\mathrm{k_B\ T\ J^{-1}}$, which is comparable to the number of states at $T = 2.4\mathrm{k_B\ T\ J^{-1}}$. These many states reflect themselves on an important number of accepted moves at the beginning. However, as we increase the cycles, for the low temperature, the principle of minimization of energy kicks in and the energy is lowered more than in the case of high temperature. Therefore, the Boltzmann factor gives low states to access and the possibility to escape from the ground state becomes close to zero.

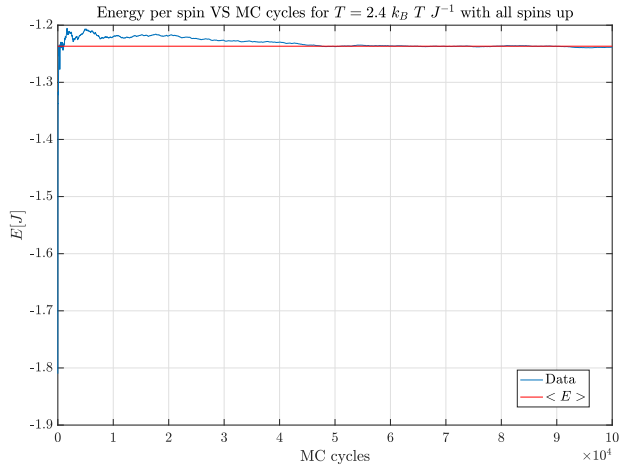
We want to investigate deeper the Boltzmann distribution. Thus we compute the probability $P(E)$ of obtaining the allowed values of energy for the lattice $L = 20 \times 20$ for both $T = 1.0\mathrm{k_B\ T\ J^{-1}}$ and $T = 2.4\mathrm{k_B\ T\ J^{-1}}$. To do this, we consider the system after it is arrived to the steady states, i.e. after $5 \cdot 10^4$ MC cycles as found before. As we can see from Fig. (5), the two probabilities show clearly the aspect of a Boltzmann distribution. For $T = 1.0\mathrm{k_B\ T\ J^{-1}}$, the principle of minimization of energy dominates, hence the system has nearly 0 likelihood to escape from the ground state and other states don't influence the mean value $< E >= -1.997J$. From this observation, it derives the highly picked behaviour the distribution and the 90% of probability of finding a state with energy $\sim -2J$. On the other hand, for $T = 2.4\mathrm{k_B\ T\ J^{-1}}$, the entropy dominates and the Boltzmann factor gives an higher likelihood of finding new states Indeed the distribution is more widespread and the mean value is $< E >= -1.237J$. Moreover if we consider the variances computed for both temperature, we find $\sigma_E^2(T = 1.0) = 0.0372$ and $\sigma_E^2(T = 2.4) = 8.154$. As the variance gives information about the spread of the data around the mean value, it's normal to have a bigger spread for higher temperature.

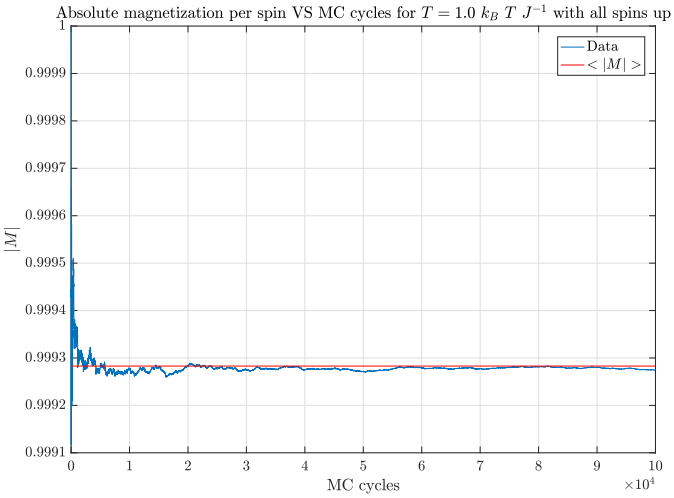
C. Lattice $40 \times 40, 60 \times 60, 80 \times 80, 100 \times 100$ and critical temperature

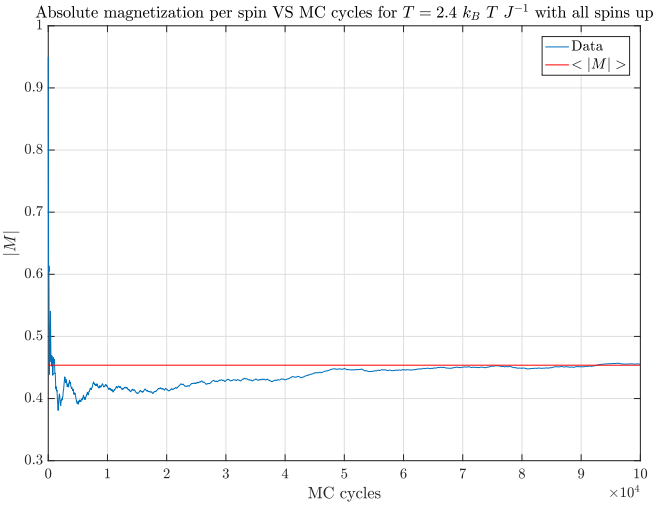
At this point, we want to study bigger lattices in order to find the critical temperature, i.e. when the phase transitions occur. However, firstly, we compare the mean energy, mean absolute magnetization, specific heat and susceptibility (computed with $|M|$) for the different lattices as functions of temperature (Fig. (6)). To perform these calculations, we parallelize our code and we let it run in the university laboratory using 8 processor in parallel. In this ways, we perform 8 times the MC cycles just declared, in the same time or even less that would occur to perform just one. To show this fact, for example, we run a 20×20 lattice with $T \in [2.1, 2.5]$, temperature step $0.005\mathrm{k_B\ T\ J^{-1}}$ and 10^6 MC cycles in our computer and in the computer of the laboratory using 8 processors in parallel and we compare the run time. Our computer takes 3638.42s to finish the computation, while computers of the university in parallel takes 1862.3s. Anyway the number of MC cycles chosen is 10^6 and the step size of temperature is $0.005\ \mathrm{k_B\ T\ J^{-1}}$. Furthermore, we don't consider the data of the firsts $5 \cdot 10^4$ MC cycles, as the system hasn't reached the equilibrium.

From Fig. (6), we can note that as we can increase the lattice size, the energy becomes a steeper function in correspondence of the critical temperature, which is located around $\sim 2.269\mathrm{k_B\ T\ J^1}$. However the energy is still a smooth function, thus we don't find any signal of a phase transition of the first order (as motivated in paragraph (II B)). As regards to the absolute value of magnetization, we note that the curve becomes stepper as we increase the lattice size meaning that we move from a state where all the spins are up (net magnetization nearly 1) to a state where all the spin as are disordered (net magnetization 0). This could be a signal of phase transition. As regards, the other quantities, C_V and χ_{abs}, they show a maximum, which is an indicator of a phase transition: as the size of the lattice is increases, the maximum becomes stepper, if we could consider an infinite lattice, the two functions would diverge in that point. As motivated in paragraph (II B), the divergence of specific heat and susceptibility is a signal of a phase transition of the second order, which happens above the critical temperature. Therefore, we fit each curve for every different lattice size with CFTOOL (MATLAB) to find each maximum. From the maxima, we go back to the critical temperatures at which the phase transitions happens at that lattice size. Then, following eq. (18), we plot these critical temperatures as function of $1/L$, where $L = 40^2, 60^2, 80^2, 100^2$, and we fit the data. The fit line is thus prolonged to meet the $y - axis$. The









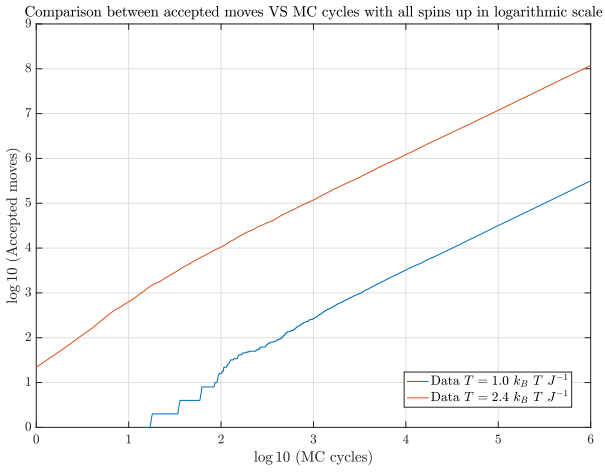
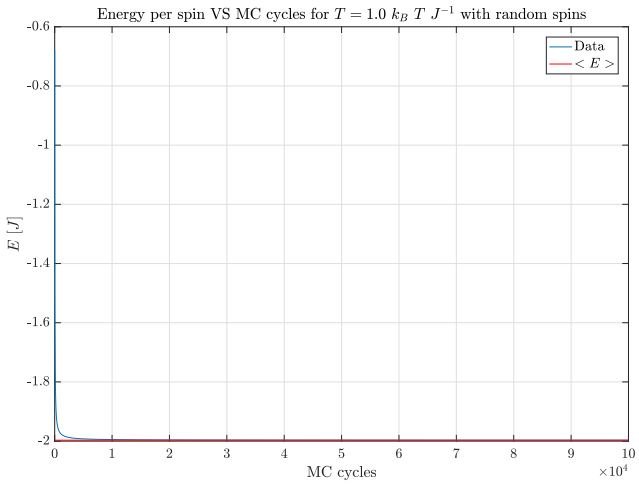
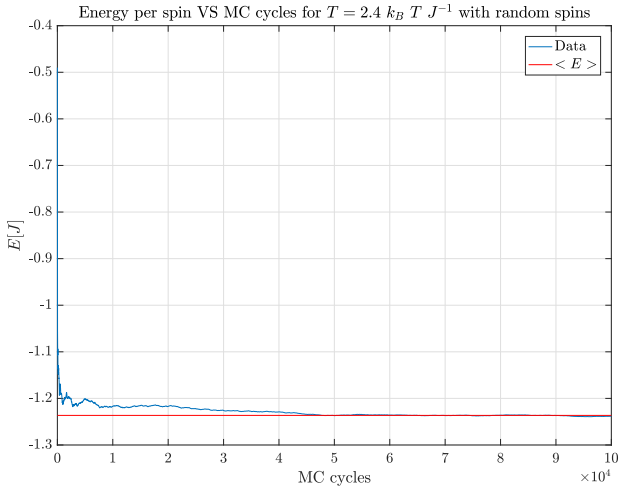
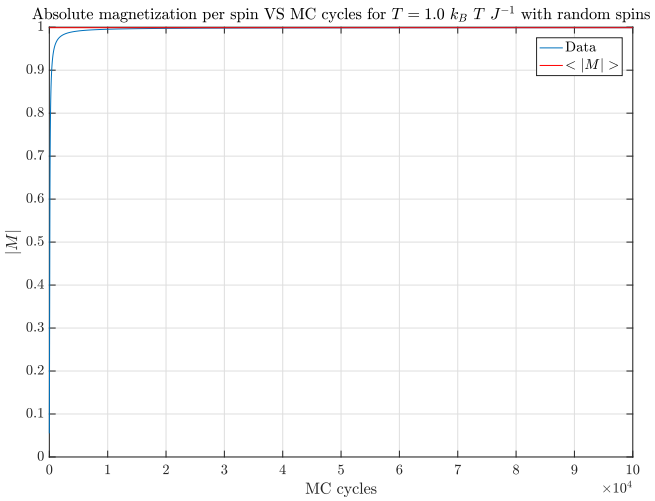
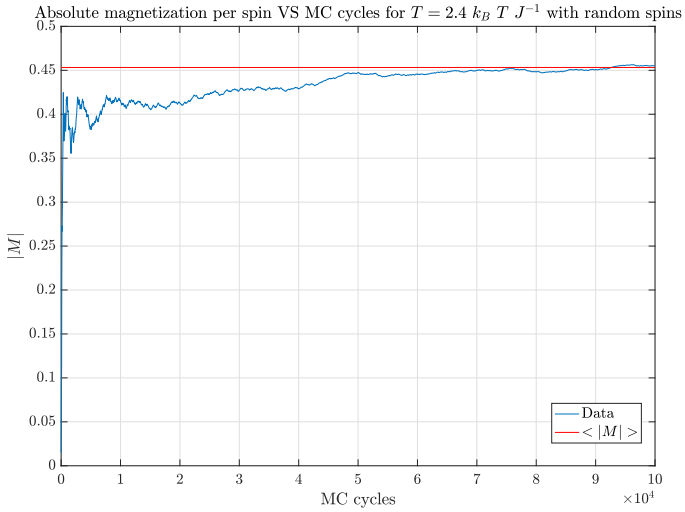


Figure 3: In these figures we compare the values of energy, absolute magnetization and number of accepted moves as function of MC cycles for $T = 1.0 \mathrm{k_B TJ^{-1}}$ and $T = 2.4 \mathrm{k_B TJ^{-1}}$ with the initial configuration of all spins up. The number of MC cycles performed is up to 10^6, but we narrow the $x - range$ up to 10^5, without this choice it would be impossible to see the initial behaviour. As we can see, the equilibrium can be considered reached after $\sim 5 \cdot 10^4$ cycles.









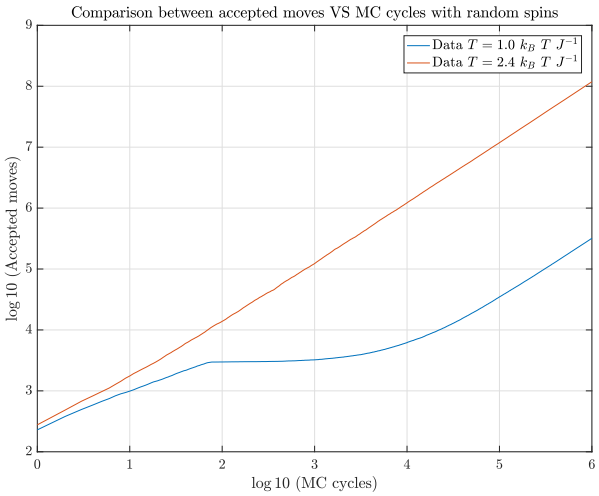


Figure 4: In these figures we compare the values of energy, absolute magnetization and number of accepted moves as function of MC cycles for $T = 1.0 \mathrm{k_B TJ^{-1}}$ and $T = 2.4 \mathrm{k_B TJ^{-1}}$ with the initial configuration of random spins. Even in this case the number of MC cycles performed is up to 10^6, but we narrow the $x - range$ up to 10^5, without this choice it would be impossible to see the initial behaviour. As it is possible to see, the fluctuations of the values decreases around $\sim 5 \cdot 10^4$ MC cycles, which can be considered the equilibration time even here.

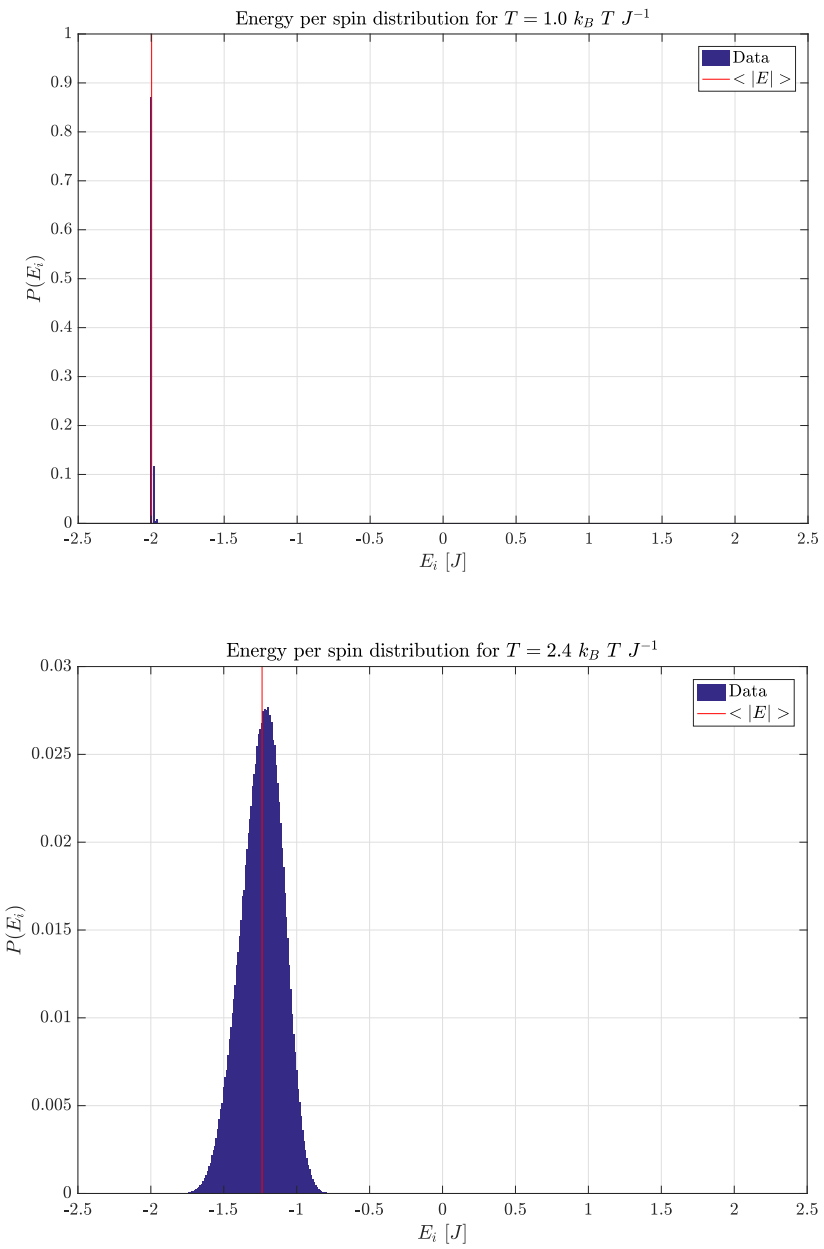


Figure 5: In these figures are shown the distribution of probability for $T = 1\mathrm{k_B}$ T J^{-1} (above) and $T = 2.4\mathrm{k_B}$ T J^{-1} below. As we can see the data in the second one are more spread than the first one as in the high temperature regime, the entropy dominates and the system has access to more states than it would have at low temperature.

point of intersection gives us the critical temperature at $L = \infty$ (Fig. (7)). The results are summed in Tab. (II). As we can see from the table, the value of critical temperature obtained from χ_{abs} is really far from the theoretical one. This could be explained as the maximum of χ_{abs} is less determined and the curve fluctuates more on that than with respect to the maximum of C_V. On the other hand, the value given by C_V is quite close to the Onsager's T_C. If we could consider the uncertainties, we would probably find an agreement: in fact using CFTOOL we can obtain the uncertainties of the maxima, which are of the order of ~ 0.01, but these have to be propagated along to find the ones of the critical temperatures and it's quite difficult. However, we should also take into account the correlation errors due to

Table II: In this table is shown the comparison between the value of critical temperature found by Onsager (2.269) and the ones find from fit of the critical temperatures from C_V and χ_{abs}.

	Model	From C_V	From χ_{abs}
T_C $[k_B\ T\ J^{-1}]$	2.269	2.274	2.287

the RNG, which is a pseudo random number generator and hence as we generate tons of numbers, our data would be also correlate. Anyway, if we consider bigger lattice and many more MC cycles we would find a better value of critical temperature and mainly a better agreement of the results of C_V and χ_{abs}. Moreover, it's important to stress again that here we use χ_{abs} as our lattices are small, increasing the lattice dimensions would allow us to use χ and also this could improve our results.

IV. CONCLUSION

Through an analysis of the Ising model , we were able to see how it is effective in predicting a phase transition from the ferromagnetic to the paramagnetic materials. Thus the determination of the critical temperature became the mainly aim of the project.

The test on the code using the theoretical results of the lattice 2×2 has shown a good agreement when the number of Monte Carlo cycles overcomes the million.

As regards the lattice 20×20, the equilibrium time for $< E >$ and $< |M| >$ to reach equilibrium for both the temperatures of $T = 1.0\mathrm{k_B\ T\ J^{-1}}$ and $T = 2.4\mathrm{k_B\ T\ J^{-1}}$ and for both the initial configuration with all the spins up and with random oriented spins is shown to be $\sim 5\cdot10^4$ MC cycles. Furthermore, these quantities and the number of accepted moves behave with respect to the temperature as we expect from the Boltzmann distribution. Moreover at the equilibrium, the probability of finding an energy E_i is studied for both the temperatures declared above. Even in this case the results are demonstrated to be compatible with a Boltzmann distribution through the use of the variance of energy.

Then, we consider lattices with dimensions $L = 20\times20, 40\times40, 60\times60, 80\times80, 100\times100$ and we study the behaviour of the mean energy, mean absolute value of magnetization, specific heat and magnetic susceptibility (calculated with $|M|$) as functions of T for each lattice. In these curves we found the indicators of a phase transitions of the second order such as the maximum of C_V and χ_{abs}. Finally taking advantage of the maximum of C_V and χ_{abs}, which are located on the critical temperature, we were able to find T_C per each lattice. From these, we were able to estimate the T_C with a lattice with infinite dimension for both the C_V and χ_{abs} finding

$$T_C(L=\infty) = 2.274\ \mathrm{k_B\ T\ J^{-1}} \quad \text{from the specific heat}$$
$$T_C(L=\infty) = 2.287\ \mathrm{k_B\ T\ J^{-1}} \quad \text{from the susceptibility.}$$

As these values are far from the exact one of $2.269\mathrm{k_B\ T\ J^{-1}}$, we try to give an explanation of this distance and also on the motif of the discrepancy between the critical temperature from specific heat and susceptibility as they should be close with each other.

V. APPENDIX

a. Derivation of C_V lattice 2×2

$$\begin{aligned}
C_V &= -\frac{1}{L}\frac{1}{T^2}\frac{\partial^2 \log Z}{\partial\beta^2}\frac{1}{k_B} = \\
&= 16\frac{1}{LT^2}\frac{8(e^{8\beta}+e^{-8\beta})(12+2e^{-8\beta}+2e^{8\beta})-16(e^{8\beta}-e^{-8\beta})^2}{(12+2e^{-8\beta}+2e^{8\beta})^2} = \\
&= 4\cdot16\frac{1}{LT^2}\frac{(e^{8\beta}+e^{-8\beta})(6+e^{-8\beta}+e^{8\beta})-(e^{8\beta}-e^{-8\beta})^2}{(6+e^{-8\beta}+e^{8\beta})^2} = \\
&= 64\frac{1}{LT^2}\frac{(2\cosh 8\beta)(6+2\cosh 8\beta)-4\sinh^2 8\beta}{(6+2\cosh 8\beta)^2} = \\
&= 64\frac{1}{LT^2}\frac{12\cosh 8\beta+4}{(6+2\cosh 8\beta)^2} = \\
&= \frac{64}{T^2}\frac{3\cosh 8\beta+1}{(6+2\cosh 8\beta)^2}\frac{1}{k_B}
\end{aligned} \tag{23}$$

b. Derivation of χ_{abs} lattice 2×2

$$\begin{aligned}
\chi_{abs} &= \frac{1}{L}\frac{< M^2 > - < |M| >^2}{T}\frac{1}{J} \\
&= \left(\frac{32e^{8J\beta}+32}{12+2e^{-8J\beta}+2e^{8J\beta}} - \frac{+256+256e^{8J\beta}+64e^{16J\beta}}{(12+2e^{-8J\beta}+2e^{8J\beta})^2}\right)\frac{1}{L}\frac{1}{T}\frac{1}{J} \\
&= \frac{6e^{8J\beta}+2e^{-8J\beta}+6}{T(19+\cosh(16J\beta)+12\cosh(8J\beta))}\frac{1}{J}
\end{aligned}$$

c. Derivation of χ lattice 2×2

$$\begin{aligned}
\chi_{abs} &= \frac{1}{L}\frac{< M^2 > - < M >^2}{T}\frac{1}{J} \\
&= \frac{32e^{8J\beta}+32}{12+2e^{-8J\beta}+2e^{8J\beta}}\frac{1}{LT}\frac{1}{J} = \\
&= \frac{4}{T}\frac{e^{8J\beta}+1}{6+2\cosh(8J\beta)}\frac{1}{J}
\end{aligned}$$

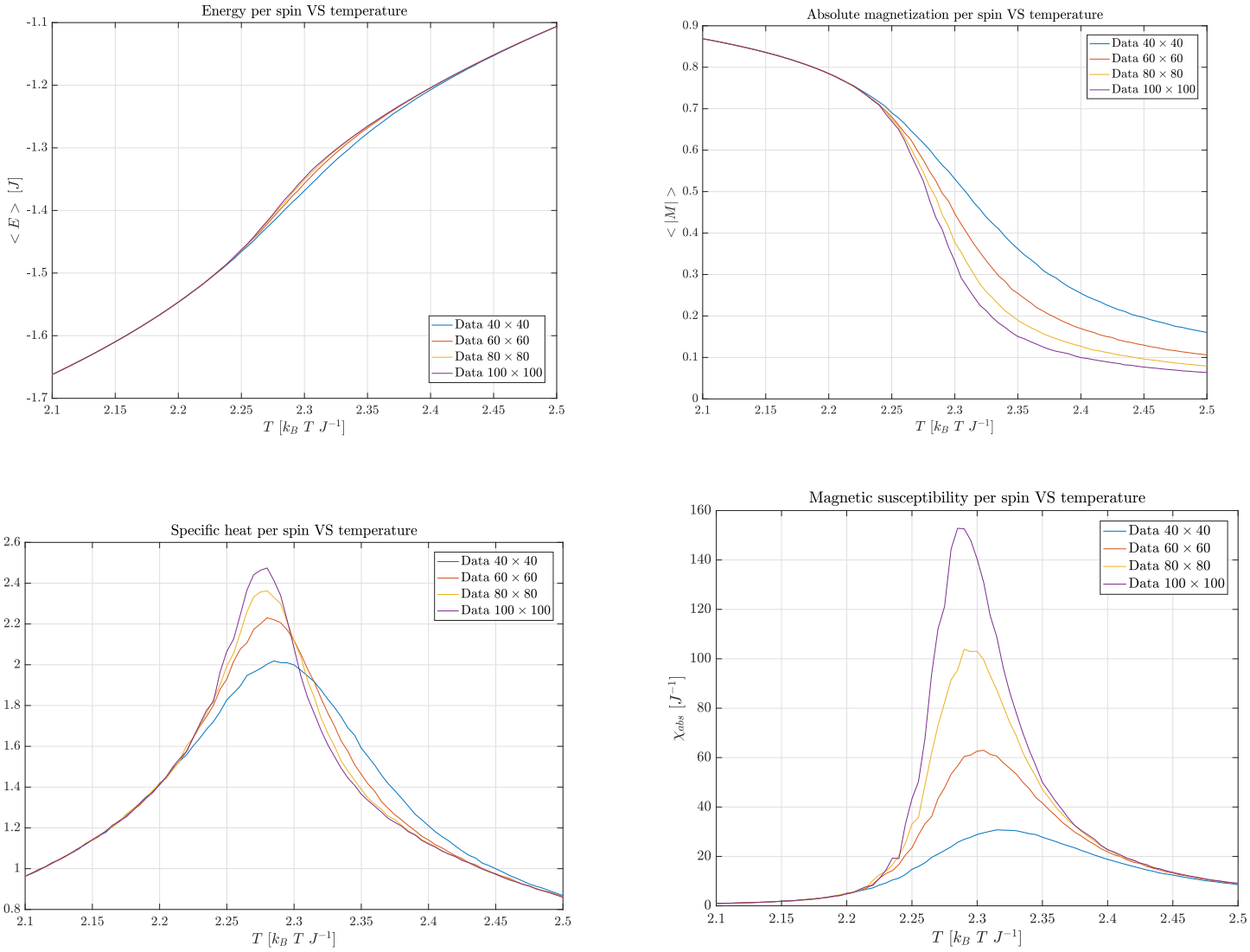


Figure 6: In these figures we show the behaviour the mean energy, mean absolute magnetization, specific heat and susceptibility as function of temperature for $L = 40 \times 40, 60 \times 60, 80 \times 80, 100 \times 100$. The results are obtained running the code in parallel with 8 processors and 10^6 MC cycles. The maxima of C_V and χ_{abs} are signals of phase transition and they are located in correspondence of the value of T_C.

[1] M. H. Jensen, *Computational physics - Lecture notes Fall 2015*, University of Oslo - Department of Physics, 2015.

[2] `https://arxiv.org/pdf/0906.0653v2.pdf`

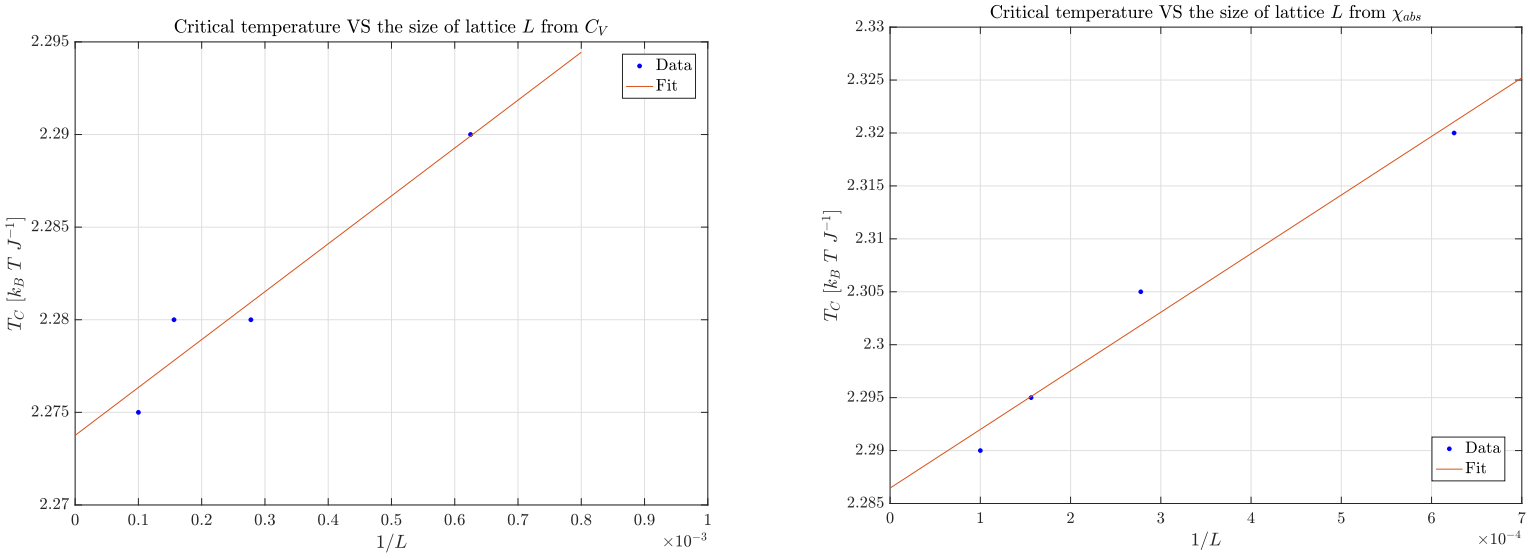


Figure 7: In these figures, we show the fit of the critical temperatures as functions of the inverse of the lattice dimensions. The prolongation of the fit line gives us $T_C(L = \infty)$. As we can see the two values are particularly different, this could be caused by the fact that the maxima of χ_{abs} are less determined with respect to the maxima of C_V.