Studies of phase transitions in magnetic systems based on the Ising model

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ABSTRACT

In the following project we study the two-dimensional Ising model (considering only square lattices, with the same number of spins in each direction). The numerical solution is based on Metropolis algorithm. First, the comparison between the analytical expressions for the 2×2 lattice and numerical results is being made. The analytically calculated quantities (per spin) are $< E >= -1.996$, $< |M| >= 0.9987$, $C_V = 0.0321$ and $\chi = 3.993$ (for $1.0\, k_B T/J$), which is in very good agreement with the numerical values produced with use of 10^6 Monte Carlo cycles ($< E >= -1.996$, $< |M| >= 0.9986$, $C_V = 0.0331$ and $\chi = 3.991$). Thereafter, we estimate the exact time (in number of MC cycles) needed in order to reach equilibrium for the system of 20×20 spins in temperatures $1.0\, k_B T/J$ and $2.4\, k_B T/J$, with both an ordered and a random initial spin configuration. The equilibration time (roughly $10^4 - 10^5$ MC cycles) is longer for temperatures closer to the critical temperature and, in general, for systems starting with disordered spin orientations. We also count the number of configurations accepted in the Metropolis algorithm (after a singular spin flip) and it is much larger for the higher temperature ($\approx 10^8$ after 10^6 MC cycles) than for the lower one ($\approx 3 \cdot 10^5$ after 10^6 MC cycles). We also make histograms of energy probability, $P(E)$, with energies of the system recorded after the steady state has been reached. The histogram corresponding to the higher $k_B T/J$ is much wider and associated with much larger σ_E^2 (≈ 3246.3 for system with 400 spins) than the histogram with lower $k_B T/J$ (≈ 9.3). Finally, we plot $< E >$, $< |M| >$, C_V and χ as a function of temperature in range $k_B T/J \in [2.1, 2.4]$ and for various lattice sizes (with $L = 40$, $L = 60$, $L = 80$ and $L = 100$ spins in each direction). Using the critical temperature read of the χ-curves and the finite size scaling relation, we estimate the critical temperature in the thermodynamical limit to be $k_B T_C(L = \infty)/J \approx 2.257$ (whereas the analytical result is ≈ 2.269).

1 Introduction

The Ising model is one of the most studied systems in statistical physics with respect to simulations of phase transitions. Based on the Ising model, we can analyze how a magnetic material responds to thermal energy and an external magnetic field. In two dimensions the model can be portrayed as a square lattice, where each site has its corresponding spin of north (with value +1) or south (with value -1). The directions of the spins have an impact on the total energy of the system in a given configuration i,

$$E_i = -J \sum_{<kl>}^{N} s_k s_l - B \sum_{<k>}^{N} s_k, \tag{1}$$

where $s_k \pm 1$, N is the total number of spins, J is a coupling constant expressing the strength of the interaction between neighboring spins and B is an external magnetic field interacting with the magnetic moment set up by the spins. The index $< kl >$ indicates summation over only nearest lattice sites. Here, we will consider the case without an external magnetic field applied, i.e. $B = 0$. The other quantity describing the system is magnetization,

$$M_i = \sum_{j=1}^{N} s_j, \tag{2}$$

being the sum over all spins for a given configuration.

In the thermodynamic limit, where $N \to \infty$, results do not depend on the way we treat the boundaries of the lattice. However, for smaller systems, the choice of boundary conditions is crucial. Throughout this project we will consider the model with periodic boundary conditions.

The analysis of the Ising model in this project is based on several quantities that will be evaluated for different lattice sizes and temperatures. These are introduced in the first subsection of Methods (Expectation values and related thermodynamical quantities). Next, we describe the Metropolis algorithm, which allows computing the various thermodynamical quantities numerically. Thereafter, we proceed to derive the analytical expressions for a small 2×2 square lattice (in order to test the program). Then, we introduce the properties of the system that will be analyzed. The Methods section is concluded with a closer description of how the results for different parts of the analysis can be produced. Next, in the Results and discussion section, we present and analyze the results produced by the programs.

The main program (project4_main.cpp) is written in C++ and together with some selected results and the Python code (project4_read_plot.py), used to read the output files produced by the main program, process and plot the data, available in the following Github repository: github.com/jowborowska/CompPhysics

2 Methods

2.1 Expectation values and related thermodynamical quantities

Our model consists of a collection of microphysical systems from which we can derive expectation values and thermodynamical properties of the whole system. First of all, we need a

Boltzmann probability distribution,

$$P_i(\beta) = \frac{1}{Z} e^{-\beta E_i}, \tag{3}$$

where $\beta = \frac{1}{k_B T}$ and k_B is the Boltzmann constant, T is temperature, E_i is the energy of a microstate i, while Z is the partition function, given by

$$Z = \sum_{i=1}^{\Omega} e^{-\beta E_i} \tag{4}$$

for all microstates Ω. Using the probability distribution, we can find the expectation value for the energy (the mean energy) as

$$< E >= \sum_{i=1}^{\Omega} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{\Omega} E_i e^{-\beta E_i}. \tag{5}$$

The corresponding variance is defined as

$$\sigma_E^2 =< E^2 > - < E >^2 = \frac{1}{Z} \sum_{i=1}^{\Omega} E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{\Omega} E_i e^{-\beta E_i} \right)^2. \tag{6}$$

Having computed the variance, we can also find the specific heat at constant volume,

$$C_V = \frac{\sigma_E^2}{k_B T^2}. \tag{7}$$

Following a similar approach, we can evaluate the mean magnetization as

$$< M >= \sum_{i=1}^{\Omega} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{\Omega} M_i e^{-\beta E_i}, \tag{8}$$

as well as the mean absolute value of magnetization,

$$< |M| >= \sum_{i=1}^{\Omega} |M_i| P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{\Omega} |M_i| e^{-\beta E_i}, \tag{9}$$

and the variance

$$\sigma_M^2 =< M^2 > - < M >^2 = \frac{1}{Z} \sum_{i=1}^{\Omega} M_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{\Omega} M_i e^{-\beta E_i} \right)^2, \tag{10}$$

(which for $|M|$ is analogous). This can be used to define the magnetic susceptibility,

$$\chi = \frac{\sigma_M^2}{k_B T} \tag{11}$$

(here also $\sigma_{|M|}^2$ can be used, as we will see later).

2.2 Metropolis algorithm

We will employ the Metropolis algorithm, combining the Monte Carlo approach with Markov chains, in order to numerically estimate the quantities related to the Ising model for different lattice sizes and temperatures. The following part is meant to explain the usage of the algorithm specifically for the two-dimensional Isisng model, as implemented into the program. More general mathematical description of the self algorithm can be found in Hjorth-Jensen (2015), section 12.5.

For each Monte Carlo cycle, the following algorithm is performed, looping over all spins in the lattice. First of all, we establish the energy of the initial state, E_{start}. We choose a random position in the lattice and flip the spin located there, getting the corresponding energy of this trial state, E_{trial}. We calculate then the energy difference,

$$\Delta E = E_{trial} - E_{start} = J \sum_{<kl>}^{N} s_k^{start} s_l^{start} - J \sum_{<kl>}^{N} s_k^{trial} s_l^{trial} = -J \sum_{<kl>}^{N} s_k^{trial} \left(s_l^{trial} - s_l^{start} \right).$$

The flipped spin can take only two values, meaning that if $s_l^{start} = 1$ then $s_l^{trial} = -1$ and if $s_l^{start} = -1$ then $s_l^{trial} = 1$. Other spins keep their values, so that $s_k^{start} = s_k^{trial}$. Therefore, the energy difference can be computed more efficiently as

$$\Delta E = 2J s_l^{start} \sum_{<k>}^{N} s_k,$$

where the sum runs over the nearest neighbors k of spin l. The change in magnetization can be computed similarly. Since only spin l is flipped, we have

$$\Delta M = M_{trial} - M_{start} = s_l^{trial} - s_l^{start} = 2 s_l^{trial},$$

so that it can only take values 2 or -2.

Back to the Metropolis algorithm. Having computed ΔE, we can calculate the corresponding $w = e^{-\beta \Delta E}$. There are only five possible ΔE values for the Ising model in two dimensions (8J, 4J, 0, -4J and -8J). This means, that the array of $e^{-\beta \Delta E}$ can be created before the start of the Monte Carlo sweeps, in order to increase the computational efficiency of the algorithm, and we just need to access the correct element in the array of w values. Next, we compare w to a random number, r, drawn from the uniform distribution. If $r \leq w$, we accept the new spin configuration (and update magnetization and energy of the system with consecutively ΔM and ΔE), else we keep the old configuration. After a loop through the whole lattice, we add values of E_i, E_i^2, M_i, M_i^2 and $|M_i|$ to the corresponding sums. The whole process above constitutes one Monte Carlo cycle and is repeated many times. Afterwards, the sums are divided by the total number of Monte Carlo cycles to give the corresponding expectation values. In some parts of the project we also choose to divide the results with the total number of spins, $N = L^2$ (as we consider square $L \times L$ matrices only).

2.3 Analytical expressions for 2x2 lattice

For a square lattice model with $N = L \times L$ spins, we have $2^{L \cdot L}$ number of possible configurations (microstates). Assuming only two spins in each direction, i.e. $L = 2$, we have then 16 microstates, which allows finding the exact expressions related to the expectation values and

thermodynamical quantities (introduced in section 2.1). All these analytical values will be subsequently compared to the ones produced numerically, in order to test the implementation of the algorithm (we will compare the quantities per spin, so divided by the number of spins, $N = 4$).

We base the following derivations on the table in Hjorth-Jensen (2015), page 424, giving the possible spin-configurations with corresponding energy and magnetization for 2×2 lattice and periodic boundary conditions. First of all, we find the partition function according to Eq. 4,

$$Z = 1 \cdot e^{-\beta \cdot (-8J)} + 12 \cdot e^{-\beta \cdot 0} + 2 \cdot e^{-\beta \cdot 8J} + 1 \cdot e^{-\beta \cdot (-8J)} = 2e^{-8J\beta} + 2e^{8J\beta} + 12,$$

which follows from the fact that we have 12 possible configurations with energy equal zero, two configurations with energy equal -8J (all spins up or all spins down) and two configurations giving $E_i = 8$J. This partition function will be used in almost all expressions below.
Next, using formula 5, we can evaluate the expectation value of the energy,

$$< E >= \frac{1}{Z}\left(2 \cdot (-8J) \cdot e^{-\beta \cdot (-8J)} + 2 \cdot 8J \cdot e^{-\beta \cdot 8J}\right) = \frac{16J}{Z}\left(e^{-8J\beta} - e^{8J\beta}\right),$$

and similarly, expectation value of the energy squared,

$$< E^2 >= \frac{1}{Z}\left(2 \cdot (-8J)^2 \cdot e^{-\beta \cdot (-8J)} + 2 \cdot (8J)^2 \cdot e^{-\beta \cdot 8J}\right) = \frac{128J^2}{Z}\left(e^{-8J\beta} + e^{8J\beta}\right),$$

used in computation of the variance, as given by equation 6. The specific heat is then simply found according to formula 7. Using a similar approach, we can compute the mean magnetization (Eq. 8) and the mean magnetization squared. We have

$$< M >= \frac{1}{Z}\left(1 \cdot 4 \cdot e^{-\beta \cdot (-8J)} + 4 \cdot 2 \cdot e^{-\beta \cdot 0} + 4 \cdot (-2) \cdot e^{-\beta \cdot 0} + 1 \cdot (-4) \cdot e^{-\beta \cdot (-8J)}\right) = 0,$$

which comes from the fact that there is one possible configuration with magnetization 4 and energy -8J (all spins up), one configuration with magnetization -4 and energy -8J (all spins down), four configurations with magnetization 2 and energy 0 and four configurations with magnetization -2 and energy 0, as well as six configurations resulting in magnetization equal zero. Furthermore,

$$< M^2 >= \frac{1}{Z}\left(4^2 \cdot e^{-\beta \cdot (-8J)} + 4 \cdot 2^2 \cdot e^{-\beta \cdot 0} + 4 \cdot (-2)^2 \cdot e^{-\beta \cdot 0} + (-4)^2 \cdot e^{-\beta \cdot (-8J)}\right) = \frac{32}{Z}\left(e^{8\beta J} + 1\right),$$

which together with the previous expression allows finding the corresponding variance, σ_M^2, (Eq. 10), as well as the magnetic susceptibility (Eq. 11). Finally, the mean absolute value of magnetization, according to Eq. 9, is

$$< |M| >= \frac{1}{Z}\left(4 \cdot e^{-\beta \cdot (-8J)} + 4 \cdot 2 \cdot e^{-\beta \cdot 0} + 4 \cdot |-2| \cdot e^{-\beta \cdot 0} + 1 \cdot |-4| \cdot e^{-\beta \cdot (-8J)}\right) = \frac{8}{Z}\left(e^{8\beta J} + 2\right).$$

2.4 Analyzed properties of the model

2.4.1 Time of reaching the equilibrium

We want to perform the study of a time corresponding to the number of Monte Carlo sweeps of the lattice, needed in order to reach an equilibrium situation (thermalization time). When

this happens, the expectation values oscillate around the mean, not changing drastically. The contributions to the expectation values prior to the steady state situation can then be discarded, in order to achieve a better accuracy of measurments. For this part we will use a square lattice with $L = 20$ spins in each direction.

The recorded and plotted quantities are the mean energy, $< E >$, and the mean absolute value of magnetization, $< |M| >$, as functions of number of Monte Carlo cycles (representing time) for two different values of temperature ($T = 1.0$ and $T = 2.4$ in units of k_BT/J) and for both an ordered - ground state (all spins aligned upwards) and a random initial spin orientation as a starting configuration. We will also count the total number of accepted configurations (after an individual spin flip) in the Metropolis algorithm as a function of the total number of Monte Carlo cycles for the two mentioned temperature values.

2.4.2 Probability distribution, P(E)

Thereafter, we will count the number of times a given energy appears in the computations, starting after the equilibrium state has been reached. This gives the probability, $P(E)$, which will be subsequently plotted in the form of histogram and compared with the variance in energy, σ_E^2. Here, the system with $L = 20$ spins in each direction and temperatures $T = 1.0$ and $T = 2.4$ in units of k_BT/J are used again.

2.4.3 Phase transitions and critical temperature

A phase transition is associated with some abrupt macroscopic changes during the course of changing an external parameter, such as temperature. This happens as we pass through the critical point (with the corresponding critical temperature, T_C). An important quantity in studies of phase transitions is the correlation length, ξ. The Ising model in two dimensions with $B = 0$ undergoes a phase transition of second order, where the correlation length diverges at the critical point,

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

and in our case (with finite lattice sizes) is proportional to the size of the lattice, $\xi(T) \propto L$.

The analysis of phase transitions will be performed for two thermodynamical functions - the heat capacity (Eq. 7) and the magnetic susceptibility (Eq. 11). At the crititcal point these quantities are discontinuous or diverge in the thermodynamic limit ($N \to \infty$). However, our lattices will always have finite sizes (with N spins total, $N = L \times L$), so that $C_V(T)$ and $\chi(T)$ will not diverge, but instead exhibit a peak near T_C, which sharpness is dependent on the lattice size, L. We will analyze this dependence and estimate T_C by plotting $C_V(T)$ and $\chi(T)$ (as well as expectation values $< E > (T)$, $< |M| > (T)$) for square lattices with four different sizes (with $L = 40$, $L = 60$, $L = 80$ and $L = 100$ spins in each direction) in the temperature range $k_BT/J \in [2.1, 2.4]$ and $k_B\Delta T/J = 0.02$. The choice of temperature step is not accidental here (more about it in the Results and Discussion section). Having the estimates of the critical temperature as a function of lattice size, $T_C(L)$, we can also estimate the critical temperature in the thermodynamical limit, following the finite size scaling relation,

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{12}$$

where a is a constant and ν is defined by the correlation length relation above. We will use the exact result, $\nu = 1$, which gives

$$T_C(L = \infty) = T_C(L) - \frac{a}{L}. \tag{13}$$

Both a and $T_C(L=\infty)$ can be estimated based on the results of simulations. Thereafter, we can compare our estimate to the exact analytical result, $kT_C(L=\infty)/J = 2/ln(1+\sqrt{2}) \approx 2.269$ (after Lars Onsager).

2.5 Numerical implementation

The main program is written in C++ and consists of several functions. Naturally, different parts of the analysis require production of different results. First of all, a test of the code implementation is performed on the 2×2 lattice, by comparing the results of analytical expressions (shown in the terminal and produced by the function Analytical_2times2) with the numerical ones. The values of L, temperature (in units k_BT/J) and the number of MC cycles can easily be adjusted in the main function. The numerical results are then written to an output file. The same concerns the part where we study phase transitions and loop over a range of temperatures (the only difference is that we use the absolute value of magnetization in the χ computations instead).

In the analysis of the equilibration time a different set of values is needed (we want to see the temporary results after each Monte Carlo sweep of the entire lattice). Therefore, we alter the functions performing Metropolis algorithm and writing data to a file, in order to produce the set of values of interest. This alternative of the program can be chosen in the main function with a simple likely_state_computations == true statement.

All of the produced output files with data are subsequently read and processed by the program written in Python. Here, we interpolate the data sets for temperature plots (using scipy.interpolate.spline) and create all of the ramaining figures shown in this report.

Since some of the computations, especially for larger lattices and more Monte Carlo cycles, are computationally heavy, the attempt of temperature-loop parallelization with OpenMP has been made. Unfortunately, despite a thorough investigation and many implemented changes, all of the attempts ended with "Segmentation fault (core dumped)" error, aborting the program. Nevertheless, with added optimization flags to the compiler (-O3 -o) and the choice of 10^5 Monte Carlo cyclces and temperatures spanning over the range $T \in [2.1, 2.4]$ with $\Delta T = 0.02$ or even $\Delta T = 0.01$, the computations took not so long, so the results could be produced without a problem.

3 Results and discussion

3.1 Analytical vs numerical results for 2×2 lattice

First of all, the test of implementation of the code has been performed on the example of 2×2 lattice and temperature $T = 1.0$ (in units k_BT/J). The analytical values, computed according to the expressions described in section 2.3, are: the mean energy per spin, $< E >= -1.99598$, the mean absolute value of magnetization per spin, $< |M| >= 0.998661$, the specific heat per spin, $C_V = 0.0320823$, and the magnetic susceptibility per spin, $\chi = 3.9933$. The numerical values have been produced for various numbers of Monte Carlo cycles (see Table 1). As expected, the more MC cycles, the better agreement with the exact solution. The best accuracy corresponds to 10^6 MC sweeps of the whole lattice, with the results shown in the table.

	Expectation values and variances per spin			
no. of MC cycles	$< E >$	$< \|M\| >$	C_V	χ
10^3	-1.998	0.999	0.015984	0.003996
10^4	-1.9964	0.9988	0.02874816	2.4963136
10^5	-1.99578	0.998625	0.033688766	3.936524
10^6	-1.995848	0.9986215	0.033147044	3.9905608

Table 1: The numerical results produced by the code for 2 $\times$ 2 lattice, $T = 1.0$ (in units k_BT/J) and different numbers of Monte Carlo cycles. The analytical values are: $< E >= -1.99598$, $< |M| >= 0.998661$, $C_V = 0.0320823$ and $\chi = 3.9933$. We can see a very good agreement with the numerical results for 10^6 MC cycles.

3.2 Thermalization time

As described in the Methods section (2.4.1), we want to find the time (represented by the number of Monte Carlo cycles) for which the system reaches equilibrium. Figure 1 shows the behavior of the mean energy of the whole system as a function of the number of performed Monte Carlo cycles. For the lower temperature, we see that the ordered system almost immediately reaches the steady state, whereas it takes approximately $5 \cdot 10^4$ MC cycles for the system starting from a random configuration to reach equilibrium. Nevertheless, for the higher temperature systems in both variants of initial configuration reach the equilibrium around the same time, $\approx 10^5$ MC cycles. The plots of the mean absolute value of magnetization (see Figure 2) show that $< |M| >$ exhibits a similar behavior. It turns out that the time needed to reach steady state is longer for temperatures close to the critical temperature than for the temperatures away from the critical one. In general, it is also better to start with an ordered spin configuration, since then the steady state is reached faster (especially for low temperatures).

We have also counted the total number of accepted lattice configurations (after individual spin flips in the Metropolis algorithm), which is plotted as a function of the total number of Monte Carlo cycles and shown on Figure 3. For the lower temperature, a system with initially random configuration takes slightly higher values than an initially ordered one, whereas for the temperature close to the critical temperature, the two curves are almost entirely aligned. It is also worth noticing that the number of accepted configurations is much higher for the higher temperature ($\approx 10^8$ after 10^6 MC cycles) than for the lower one ($\approx 3 \cdot 10^5$ after 10^6 MC cycles). This will be later explained in the discussion about phase transitions.

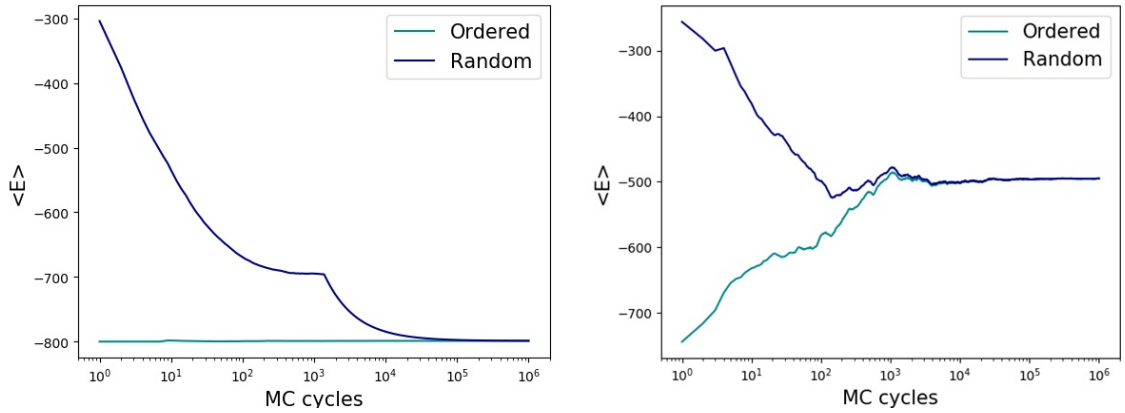

Figure 1: The mean value of energy of the whole system (lattice 20×20 spins) as a function of the number of Monte Carlo cycles for temperatures $1.0\, k_B T/J$ (left panel) and $2.4\, k_B T/J$ (right panel). Cases of both an ordered (cyan curve) and a random (navy blue curve) initial spin configurations are shown. Number of MC cycles is scaled logarithmically.

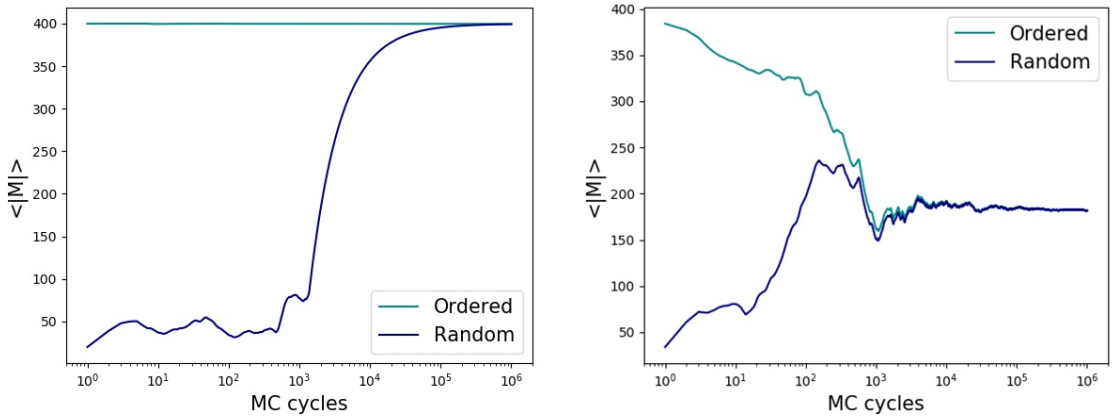

Figure 2: The mean absolute value of magnetization of the whole system (lattice 20×20 spins) as a function of the number of Monte Carlo cycles for temperatures $1.0\, k_B T/J$ (left panel) and $2.4\, k_B T/J$ (right panel). Cases of both an ordered (cyan curve) and a random (navy blue curve) initial spin configurations are shown. Number of MC cycles is scaled logarithmically.

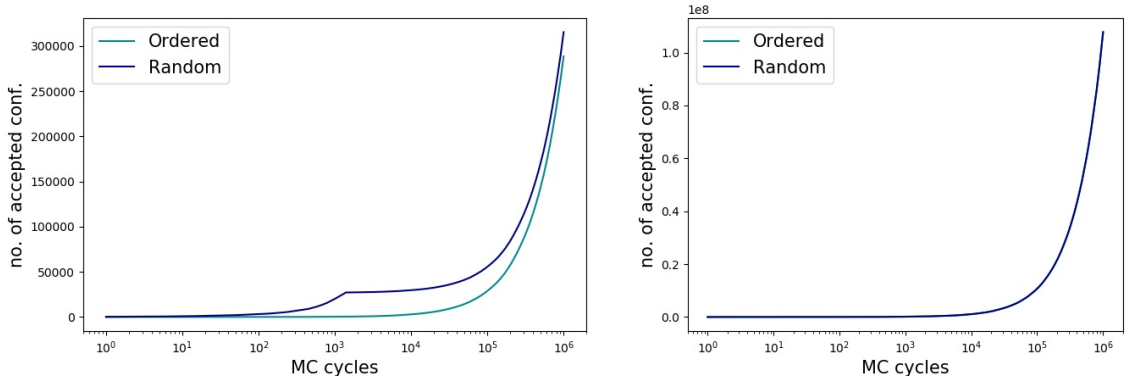

Figure 3: The number of accepted configurations (in the Metropolis test) of lattice with 20 × 20 spins as a function of the number of Monte Carlo cycles for temperatures 1.0 k_BT/J (left panel) and 2.4 k_BT/J (right panel). Cases of both an ordered (cyan curve) and a random (navy blue curve) initial spin configurations are shown. Number of MC cycles is scaled logarithmically.

3.3 Analysis of probability distribution, P(E)

We have estimated the time of reaching the steady state to be $\approx 10^4$ MC cycles. Now, we count the number of times a given energy of the system (20 × 20 lattice) appears in the computations, starting after 10^4 MC cycles and finishing with 10^6 MC cycles performed. The resulting probability distributions are shown in Figure 4. We can observe a narrow histogram for the lower temperature and a broad symmetric histogram for the temperature closer to the critical one. This is in agreement with the plots from Figure 1., where the mean energy goes towards minimum (-800J) for lower T, whereas it oscillates around ≈ -500J for higher T. The computed variances in energy (for the whole system of 400 spins) are $\sigma_E^2 \approx 9.3$ for the lower temperature and $\sigma_E^2 \approx 3246.3$ for the higher one. This is in agreement with the broadness of observed histograms.

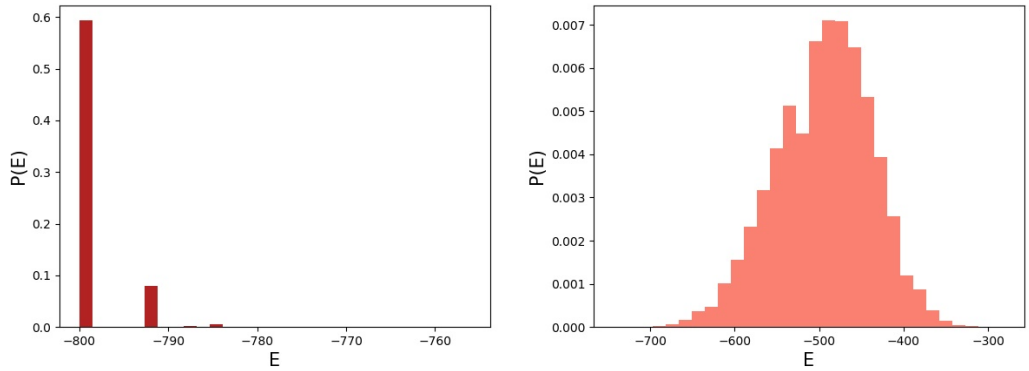

Figure 4: Histograms showing the normed probability, $P(E)$, of energies (in units J) of the whole system (lattice 20 × 20 spins with initially ordered configuration), recorded after the equilibrium state has been reached (around 10^4 MC cycles) for temperatures 1.0 k_BT/J (left panel) and 2.4 k_BT/J (right panel).

3.4 Phase tranistions and critical temperature

Finally, we study the behavior of the Ising model closer to the critical temperature as a function of the lattice size, $N = L \times L$, for square lattices. Figure 5. shows how the mean energy per spin, the mean absolute magnetization per spin, the specific heat, as well as the megnetic susceptibility vary with temperature for different lattice sizes. We have chosen $T \in [2.1, 2.4]$ (in units $k_B T/J$), making sure that the critical temperature, T_C, is enclosed in the studied range. As it has been mentioned, the computations are performed with $\Delta T = 0.02$ and post-interpolation. Higher ΔT gives less data points to interpolate between (and hence less accurate result), whereas lower ΔT gives even less smooth curves (they look "noisy", as if the values oscillated around the best-fit). For the data sets with discarded pre-equilibrium contributions to the expectation values (the ones from less than $\approx 10^4$ MC cycles) plots look almost identical.

In the phase transition, we move from a state where most of the spins are aligned at low temperatures (high degree of order, ferromagnetic phase) to a phase where both spin directions are equally probable (high degree of disorder - more accepted configurations in the Metropolis algorithm for higher temperature, paramagnetic phase). This results in net magnetization close to zero, as can be seen on the plot of the mean absolute value of magnetization per spin on Figure 5. Since we are plotting the absolute value, $< |M| >$, our mean magnetisation will always be above zero (we are taking the average of a number which is never negative).

The peaks of $C_V(T)$ and $\chi(T)$ curves have been marked as the moments of undergoing the phase transition. We see that both quantities, as the lattice size increases, develop a sharper and sharper peak centered around the critical temperature, $T_C(L)$. Since χ provides a more reliable, clear relation between L and the peak position, we will use the maxima of magnetic susceptibility for the estimation of the critical temperature. Then, $T_C(L = 40) \approx 2.32$, $T_C(L = 60) \approx 2.3$, $T_C(L = 80) \approx 2.3$ and $T_C(L = 100) \approx 2.28$. As described in the section 2.4.3, we can use these results to estimate the critical temperature in the thermodynamical limit. Following Eq. 13. we have,

$$T_C(L = \infty) = 2.32 - \frac{a}{40} = 2.3 - \frac{a}{60} = 2.3 - \frac{a}{80} = 2.28 - \frac{a}{100}$$

$$\Rightarrow 2.32 - \frac{a}{40} = 2.28 - \frac{a}{100} \Rightarrow a \approx 2.67.$$

Implementing the above value of constant a to Eq. 13 with different L and averaging the results gives a rough estimate of $T_C(L = \infty) \approx 2.257$, which is not that far from the analytical result, $T_C(L = \infty) \approx 2.269$ (units $k_B T/J$ again).

4 Conclusions

As we have seen, the two-dimensional Ising model exhibits some very interesting behavior that can be studied numerically. It is a good practice to verify the code by checking the agreement with analytical results (if there are any exact solutions, even for a simple case), which we have done. We have also seen that the accuracy of the results produced by Metropolis algorithm is strictly dependent on the number of Monte Carlo sweeps through the entire spin-lattice. Nevertheless, the more MC cycles, the longer computations, so we have to find a balance between the accuracy and computational efficiency. Establishing the thermalization time, when the system reaches equilibrium, and discarding the contributions to the expectation

values prior to equilibrium is a way of increasing the accuracy even more.

Another aspect, that we have studied, is that the initial configuration of spins' orientation matters, especially for lower temperatures. In addition, the distribution of energies of the system for lower temperatures is much sharper (system mostly stays around the ordered configuration energy) than for ones close to the critical temperature. Finally, even though we were limited to a finite lattice-sizes in our simulations, we were able to estimate the critical temperature in the thermodynamical limit. This shows that even if a given process is not possible to exactly model numerically, we can still make some estimations, employing mathematical relations.

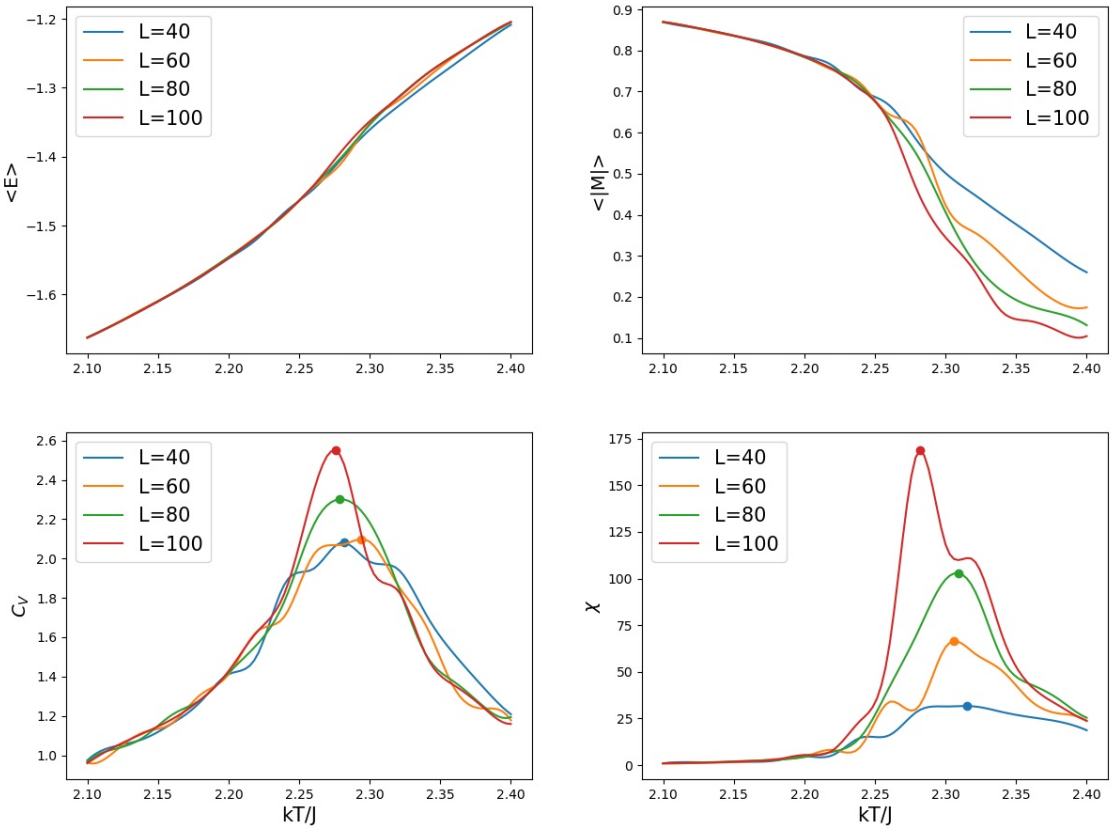

Figure 5: The behavior of the mean energy per spin, $< E > (T)$ (upper left panel), the mean absolute magnetization per spin, $< |M| > (T)$ (upper right panel), the specific heat per spin, $C_V(T)$ (lower left) and the magnetic susceptibility per spin, $\chi(T)$ (lower right), for the temperatures in range $[2.1, 2.4]\, k_B T/J$ and various square lattice sizes ($L = 40$ (blue), $L = 60$ (orange), $L = 80$ (green) and $L = 100$ (red) spins in each direction). The peaks of each C_V and χ curve, corresponding to the phase transition, are marked on the plots.

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