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Modelling the Time Development of a 2D Ising Model by Means of a MCMC Algorithm

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Abstract

The source codes for this paper can be found at https://github.com/hakontan/FYS4150-Project-4

1. INTRODUCTION

An ever occuring problem in many fields of science is a binary system of interacting elements taking two possible values. Binary problems can be found in everything from political science, where one could model outcomes of a vote in a two party system, to modeling phase transitions in solid states physics. In this paper we will focus on the latter, where we will model a time evolving two-dimensional Ising model of interacting spins by means of a Markov Chain Monte Carlo (MCMC) algorithm in addition to a Metropolis algorithm as described by Ch. 3. and 4. by Newman & Barkema (1999). We will explore how different grid sizes and temperatures make the lattice behave, and how the systems energy and magnetisation developes in time, the final aim being to estimate the critical temperature of the phase transition when the lattice looses its magnetisation, as presented in Ch. 5. and 6. in Plischke & Bergersen (2006). This is then compared to the analytical value found by Onsager (1944).

This paper will present needed theory and implementation of the theory in the Method section 2, the results will be presented in the Results section 3 and be discussed in the Discussion section 4.

2. METHOD

2.1. *The Ising Model and Important Quantities from Statistical Menchanics*

The physical system considered by this paper will be a two-dimensional Ising model, consisting of a grid of $N \times N$ magnetic spins. Each spin can have the value $s = +1$ or $s = -1$, and they interact only with their nearest neighbours. The energy of the lattice is defined by the interaction of each neighbouring spin pair as

$$E = -J \sum_{l} \sum_{\langle kl \rangle} s_k s_l, \tag{1}$$

where $\langle kl \rangle$ denotes the sum over the nearest neighbours and J has units energy. When counting the energies we choose to use periodic boundaries, meaning that the nearest neighbour of a spin $s_{i,N-1}$ at the edge of the lattice is the spin $s_{i,0}$ at the opposite edge of the lattice. This is done so as to simulate a lattice that extends infinitly in space. The magnetisation is defined similarly as

$$M = \sum_i s_i, \tag{2}$$

simply being the sum of the systems spins. The probability density function (PDF) of the system having a cetain energy state is given by the Boltzmann distribution

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

where $\beta = \frac{1}{k_B T}$ for the Boltzmann constant k_B and the temperature T. The partition function of the system describing all statistical properties of the system in equilibrium is given as

$$Z = \sum_i e^{-\beta E_i}, \tag{4}$$

over all possible microstates (2^{N^2} in total for a 2×2 grid) of the system. The mean energy and absolute magnetisation of the system is then given as

$$\langle E \rangle = \sum_i E_i P(E_i) = \sum_i \frac{E_i}{Z} e^{-\beta E_i} = \frac{\partial \ln Z}{\partial \beta} \tag{5}$$

$$\langle |M| \rangle = \sum_i |M_i| P(E_i) = \sum_i \frac{|M_i|}{Z} e^{-\beta E_i} \tag{6}$$

and represent the most likely state of the system. Another important quantity from thermodynamics is the heat capacity measuring the change heat for a given temperature change. The heat capacity at constant volume is given as

$$C_V = \frac{\mathrm{d}\langle E \rangle}{\mathrm{d}T} = \frac{1}{k_B T^2} \left(\frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i} - \langle E \rangle^2 \right) \tag{7}$$

$$= \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{\sigma_E^2}{k_B T^2}, \tag{8}$$

Table 1. Table showing the possible energies E_i and magnetisations M_i of the 2×2 lattice and their corresponding number of spins up $N_\uparrow$ and their degenrecies d_i.

$N_\uparrow$	d_i	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
1	1	-8	-4

thus being analogous to the variance in energy states. Finally, the magnetic susceptibility measuring how the systems magnetisation responds to a temperature change, is defined as

$$\chi = \beta \left(\sum_i \frac{M_i^2}{Z} e^{-\beta E_i} - \langle |M_i| \rangle^2 \right) \tag{9}$$

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

These thermodynamical quantities will later be usefull when estimating the critical temperature of the phase transition when the system looses its net magnetisation. When later implementing these thermodynamical quantities numerically we will use natural units where $k_B = 1$ and the energy is in units J, the temperature will be unitless $k_B T/J$. Also the magnetisation is in this case a unitless quantity, and due to the energy and temperature scaling the heat capacity and susceptibility have units k_B and J^2 respectively.

2.2. *Analytical Solutions to the* 2×2 *Lattice*

Before discribing the algorithm modeling the time development of the lattice, we show the analytical solutions to the mean energy and absolute magnetisation as well as the heat capacity and the susceptibility as shown in 2.1, so as to later enable a comperison of the numerical results to known analytically quantities. When counting the energy and magnetisation of the 2×2 lattice as discribed in the previous subsection we get the possible states of the system shown in Table 1. This lattice has in all $2^{N^2} = 2^4 = 16$ possible microstates.

Using the possible energy states in Table 1 we can write the partition function of the system as

$$Z = \sum_{i=1}^{2^{N^2}} e^{\beta E_i} = 4\cosh(8J\beta) + 12. \tag{11}$$

Using this we get the expectation value for the energy to be

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{2^{N^2}} E_i e^{-E_i \beta} = -\frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3}. \tag{12}$$

Similarly we find that the expectation value of the absolute magnetisation is given by

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{2^{N^2}} |M_i| e^{-E_i \beta} = \frac{2e^{8J\beta} + 4}{\cosh(8J\beta) + 3}. \tag{13}$$

Next this leads to the heat capacity being

$$C_V = \frac{\mathrm{d}\langle E \rangle}{\mathrm{d}T} = -\frac{1}{k_B T^2} \frac{\mathrm{d}\langle E \rangle}{\mathrm{d}\beta} = \frac{192(\cosh(8J\beta) + 1)}{k_B T^2 (\cosh(8J\beta) + 3)^2}, \tag{14}$$

and the susceptibility (when using the absolute magnetisation) is

$$\chi_{|M|} = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right) \tag{15}$$

$$= \frac{1}{k_B T} \left(\frac{8e^{8J\beta} + 8}{\cosh(8J\beta) + 3} - \frac{(2e^{8J\beta} + 4)}{(\cosh(8J\beta) + 3)^2} \right). \tag{16}$$

These analytical quantities can be compares to the numerical results.

2.3. *The MCMC and Metropolis Algorithms*

Now that we have looked at how the lattice of $N \times N$ interacting spins is set up, we can begin describing the algorithm used to simulate the evolution of the lattice in time. The algorithm used to simulate the time evolution of the lattice is a Markov Chain Monte Carlo (MCMC) algorithm. We will, however, only outline the algorithm used here, which is derived in detail in Ch. 3. and 4. of Newman & Barkema (1999). The main idea behind a Markov Chain is that we want to let the system, in our case being the lattice of spins, transition from one state w_i to the next state w_j in time. This can be written as

$$w_j = W(i \to j) w_i, \tag{17}$$

where $W(i \to j)$ is the transition matrix quantifying the probability transitioning to w_j. If we iterate over many such changes-of-states the system will converge to

the state corresponding to the eigenvector of the transition probability matrix $W(i \to j)$ having the largest eigenvalue. Since $W(i \to j)$ is a stochastic matrix, the largest eigenvalue is one. Applying the matrix to an initial state w_i many times the system thus converges towards equilibrium, effectively loosing the time dependence since the change from each iteration to the next becomes negligable. This means that effectively

$$w(t_i) - w(t_i + \epsilon) = 0, \tag{18}$$

for a small change ϵ, near the equilibrium position. This can be rewritten as

$$\sum_i W(i \to j)w_i - W(j \to i)w_j = 0, \tag{19}$$

simply multiplying out the matrix product of the forward and backward transitions. There are multiple ways (19) can be fulfilled, but we impose detailed balance (Newman & Barkema 1999, Ch. 3. and 4.) so that each element of the sum fulfills the equation, making

$$W(j \to i)w_j - W(i \to j)w_i = 0. \tag{20}$$

Now, because we do not know the transition probabilities W because they are unknown or too complicated to model, we can use the above relation to model the transition probability using the Metropolis algorithm (Newman & Barkema 1999, Ch. 3. and 4.). From the detailed balance we get that

$$\frac{w_j}{w_i} = \frac{W(j \to i)}{W(i \to j)} \equiv r. \tag{21}$$

Since the w's are probabilities, the l.h.s. quantifies whether the next state is more probable than the previous state. Thus if the ratio $\frac{w_j}{w_i} \geq 1$ we let the system transition to the next state as the forward transition probability $W(j \to i)$ is larger than the backwards transition probability $W(i \to j)$. However if the l.h.s. of (21) is less than one there is a finite probability that the system may transition forwards or backwards. This must be included in the acceptance rule so as to not include a bias freezing the system at the state of highest probability, as we want the system to transition to as many, if not all possible states.

In our case we can rewrite (21) as

$$r \leq \frac{P(E_2)}{P(E_1)} = \frac{\frac{1}{Z}e^{-\beta E_2}}{\frac{1}{Z}e^{-\beta E_1}} = e^{-\beta \Delta E}, \tag{22}$$

where $r \in [0, 1]$ is a number drawn from a uniform distribution, effectively modeling all transition posibilities and at the same time eliminate the unknown partition function Z.

When implementing the Markov Chain in practice we first must initialize the system by computing the $N \times N$ lattice energy and magnetisation. This is simply done by using (1) and (2) as described previously.

We simulate the time evolution by looping through a number of m Monte Carlo cycles. Then at each Monte Carlo cycle we sweep through the lattice $N \times N$ times to roughly cover the whole grid, by picking a random grid point i, j drawn from a uniform distribution $i, j \in [0, N-1]$ using a Mersenne-Twister pseudo-random number generator, at each sweep. At each sweep we suggest a spin flip and compute the energy of the lattice after the flip. Since each spin only has four different nearest neighbours contributiong to the energy we find that the change in energy for any suggested flip is among five possible values $\Delta E \in -8J, -4J, 0, 4J, 8J$. Both the change in energy ΔE and the change in magnetisation ΔM from a spin flip have analytical expression;

$$\Delta E = E_2 - E_1 = -J \sum_{\langle kl \rangle} s_k^2 s_l^2 + J \sum_{\langle kl \rangle} s_k^1 s_l^1 \tag{23}$$

$$= -J \sum_{\langle kl \rangle} s_k^2 (s_l^2 - s_l^1) = 2 s_l \sum_{\langle k \rangle} s_k, \tag{24}$$

since the surrounding spins $s_k = s_k^1 = s_k^2$ are unchanged and the fliped spin $s_l^2 = -s_l^1$. The magnetisation change is

$$\Delta M = 2 s_l^2, \tag{25}$$

since the difference in magnetisation at a spin flip is 2. This way of suggesting a new state is more efficient than to compute the energy diffence using a whole new lattice configuration, as it requires a lot less FLOPs.

The differnece in energy is than used to deterain whether the suggested spin flip is accepted or not through the described Metropolis algorithm.

For each accepted spin flip the energy and magnetisation sample means and variances are updated. After many cycles the system will than converge to the most like state $\langle E \rangle$, and oscillate around it.

2.4. *The Analysis*

Now that we have an algorithm computing the discribed thermodynamic quantites, we can compare the output to the known analytical values for a 2×2 grid for say a temperature $k_B T/J = 1.0$.

The next step would be to choose a larger lattice, for instance $N = 20$, both with an ordered and disordered initial spin configuration. Then we let the system run through a large number of Monte Carlo cycles, representing a long time, and computing the sample mean of

energy and absolute magnetisation as

$$\langle E\rangle = \frac{1}{m}\sum_{i=1}^{m} E_i \tag{26}$$

$$\langle |M|\rangle = \frac{1}{m}\sum_{i=1}^{m} |M_i|, \tag{27}$$

at each Monte Carlo cycle m. This cumulative mean we can use to find how much time, i.e. how many Monte Carlo cycles, the system needs to reach a state close to the most likely state where $\langle E\rangle$ and $\langle |M|\rangle$ start flattening out. This is deterained by a by-eye estimate. This is used as a starting time for the later sampling of energies and magnetisation for the thermodynamical quantites C_V and χ when looking at the phase transitions. Also we plot the number of accepted flips as a function of the Monte Carlo cycles to see how much the system changes states at any given time.

To further see if the lattice behaves as expected we can approximate the Boltzmann distribution $P(E)$ for a given temperature k_BT/J by making a histogram of the energy states of the system. We would expect that for a low temperatue like $k_BT/J = 1.0$ that $P(E)$ approaches a δ-function at small energies as β becomes large, and the exponential function $P(E)$ quickly dies out when energies become larger. The lattice effectively freezes at the lowest possible energy state. Therewhile for higher temperatures like k_BT/J the PDF will look more like a Gaussian distribution as the system has meany more possible (symmetric) energy states around the equilibrium that it can oscillate around.

The distributions are than compared to the sample variance given by the central limit theorem (Jensen 2015, p. 357) defined as

$$\sigma^2 = \frac{\sigma_E^2}{m}, \tag{28}$$

for the number of experiments (Monte Carlo cycles) m and the energy variance $\sigma_E^2 = \langle E^2\rangle - \langle E\rangle^2$. This will be an error estimate of the statistical experiment as it measures the deviation between the true mean and the sample mean. Also the spread in the histogram is compared to the standard diviation σ_E.

Next, we want to study the phase transition where the lattice looses its net magnetisation. In the theory presented in Ch. 5. and 6. Plischke & Bergersen (2006) we see that many physical properties of the system near the critical temperature can be described by a power law. Near the critical temperature T_C for when the lattice undergoes the phase transition, the mean magnetisation is given by

$$\langle M(T)\rangle \sim (T - T_C)^{\beta}, \tag{29}$$

where $\beta = 1/8$ is the so-called critical exponent. The heat capacity and the susceptibility follow analogous relations as

$$C_V(T) \sim |T_C - T|^{-\alpha} \tag{30}$$

$$\chi(T) \sim |T_C - T|^{-\gamma}, \tag{31}$$

where $\alpha = 0$ and $\gamma = 7.4$. When the lattice is heated to $T \gg T_C$ the correlation length ξ of the lattice becomes of the order of the lattice size. The correlation length is a measure of how far two correlated spins are separated. As the temperatue T appreaches the critical temperature T_C, the correlation length increases as more and more of the lattice spins are correlated, exerting a divergent behaviour close to T_C as

$$\xi(T) = |T_C - T|^{-\nu}, \tag{32}$$

where we let $\nu = 1$. Since we study a second order phase transition the correlation length will eventually span the whole system, in our case being limited to a finite grid this corresponds to the lattice size N. Therefore since $\xi \propto N$ we get that

$$T_C(N) - T_C(N \to \infty) = aN^{-1/\nu}, \tag{33}$$

where a and ν are constants. Then the mean magnetisation becomes

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \to N^{-\beta/\nu}, \tag{34}$$

the heat capacity becomes

$$C_V(T) \sim |T_C - T|^{-\alpha} \to N^{\alpha/\nu} \tag{35}$$

and the susceptibility is

$$\chi(T) \sim |T_C - T|^{-\gamma} \to N^{\gamma/\nu}, \tag{36}$$

where we have set $T_C(N) = T$ and $T_C(N \to \infty) = T_C$. Thus if we plot the mean energy and magnetisation as well as the heat capacity and susceptibility as a function of temperatres we can estimate the critical temperature for an infinite grid $N \to \infty$. For this we use $N = 40, 60, 80$ and 100, and a temperature range of $T \in [2.0, 2.5]$ with 50 temperature steps. We expect that the mean energy and absolute magnetisation suddenly bend at $T = T_C(N)$, and that the heat capacity and susceptibility peak at $T = T_C(N)$. When $N \to \infty$ this peak will diverge. Using (33) for two grid sizes N_1 and N_2 we can estimate the constant a to be

$$a = \frac{T_C(N_1) - T_C(N_2)}{N_1^{-1/\nu} - N_2^{-1/\nu}}, \tag{37}$$

Table 2. Table showing the mean value for the energy and the absolute magnetization for a 2×2 lattice. The absolute error computed by comparing the calculated values with the analytical values given by (12) and (13) is also tabulated to illustrate the discrepancy.

MC cycles	$\langle E \rangle$ $[J]$	$\langle M \rangle$	E_{error}	M_{error}
10	-4.8	2.8	3.183	1.194
10^2	-8.0	4.0	0.016	0.005
10^3	-7.968	3.990	0.015	0.004
10^4	-7.988	3.996	0.004	0.001
10^5	-7.982	3.994	0.0019	0.0006
10^6	-7.9833	3.9944	0.0005	0.0002

since we know that $T_C(N \to \infty)$ is the same for all grids. Knowing a we can use (33) to compute an estimate for $T_C(N \to \infty)$. This estimate can be compared to the analytical value found by Onsager (1944); $k_B T/J = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$, for $\nu = 1$. As looping over several temperatures using a desently large number of Monte Carlo cycles is very time consuming, we parallelized the temperature loops using MPI and used compiler flags. To check the speed-up we timed code using diffent degrees of parallisation and compiler flags.

3. RESULTS

To determine how many Monte Carlo cycles that were required for the solutions to stabilize using a 2×2 lattice, the model was compared to the analytical values for the energy and the absolute magnetization given by (12) and (13) respectively for a 2×2 lattice. This shows that the error became sufficiently small after approximately 10^4 Monte Carlo cycles.

Using the higherst precision found in Table 2 obtaines with 10^6 Monte Carlo cycles, we computed the mean energy and absolute value of the magnetisation as well as the heat capacity and susceptibility for different temperatures $k_B T/J \in [1.0, 2.12]$. The relative errors to the analytical solutions described in Section 2.2 of the computed quanteties were computed for the $k_B T/J = 1.0$ case. This is tabulated in Table 3.

In order to find how long it would take for the model to reach equilibrium we calculate the energy E, absolute magnetisation $|M|$ and heat capacity C_v all as functions of the temperatue T for lattice with size $N = 20$. The values were divided by the lattice area N^2 in order to illustrate these quantities per spin particle. The number of accepted flips was also counted for these calculations. These results are shown in Figures 1, 2 and 3 respectively. Here we calculated for two separate temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$ with two initial spin configurations. One ordered configuration where all initial spins point in the same direction and a disordered configuration where all initial spins are randomly chosen.

The probability $P(E)$ was plotted for the two temperatures. This is shown in Figure 4. Here we started counting after 5000 Monte Carlo cycles to allow the solution to stabilize first. The variance σ_E^2 of the Boltzmann distribution and total variance according to the central limit theorem σ^2 for this result is shown in Table 5.

To study the behaviour of Ising model close to the critical temperature, the mean energy $\langle E(T) \rangle$, heat capacity $C_v(T)$, magnetic susceptibility $\chi(T)$ and the mean of the absolute value of the magnetization $\langle |M(T)| \rangle$ was calculated in the interval $T \in [2.0, 2.5]$. These thermodynamical quantities were plotted per particle in the given interval with a timestep of $\Delta T = 0.01$. This is shown in Figure 5. For this calculation 10^6 Monte Carlo cycles were used for each temperature in the interval. The calculations were done on four different lattice dimensions $N = 40$, $N = 60$, $N = 80$ and $N = 100$ to study how this affects the solution.
The same calculation was also timed using a varying amount of threads for parallisation and compiler flags for a lattice with dimensions $N = 10$. This is tabulated in Table 4.

Finally we used the peaks of the heat capacity C_v of the $N = 80$ and $N = 100$ lattices seen in Figure 5, to estimate the critical temperature $T_C(N \to \infty)$ of an infinite grid according to the method described in section 2.4. We found that the critical temperature $k_B T_C/J \approx 2.284$ with a relative error to the analytical value (by Onsager (1944)) of $\epsilon \approx 0.675\%$.

4. DISCUSSION

When studying the mean energy and absolute mangetization for the ordered and disordered configurations for $N = 20$, our results show significant differences for the four combinations of temperature and initial spin configuration. When studying the mean energy, illustrated in Figure 1, one can see that the ordered configuration for $k_B T/J = 1$ starts very close to its most likely state. The disordered configuration with $k_B T/J = 1$ has an initial value that is more off than the ordered configuration, but it quickly reaches an equilibrium. The same behaviour can be seen for the same combinations for temperature and initial configuration for the absolute mangetization as seen in Figure 2. The fluctuations around the most likely state is also relatively small for

Table 3. Table showing the mean energy and mean absolute magnetization as well as the heat capacity and susceptibility for different temperatures. The values where computed with a number of Monte Carlo cycles of 10^6.

k_BT/J	$\langle E \rangle$ $[J]$	$\langle M \rangle$	C_V $[k_B]$	$\chi_{\lvert M \rvert}$ $[J^{-1}]$
1	-7.9841	3.9947	0.1263	0.0158
1.28	-7.9086	3.9697	0.4415	0.0698
1.56	-7.7279	3.9096	0.8654	0.1683
1.84	-7.4251	3.8092	1.2673	0.2907
2.12	-7.0192	3.6734	1.5442	0.4131
Rel. Error at $\frac{k_BT}{J} = 1.0$	$4.967 \cdot 10^{-6}$	$2.780 \cdot 10^{-5}$	0.003	0.0391

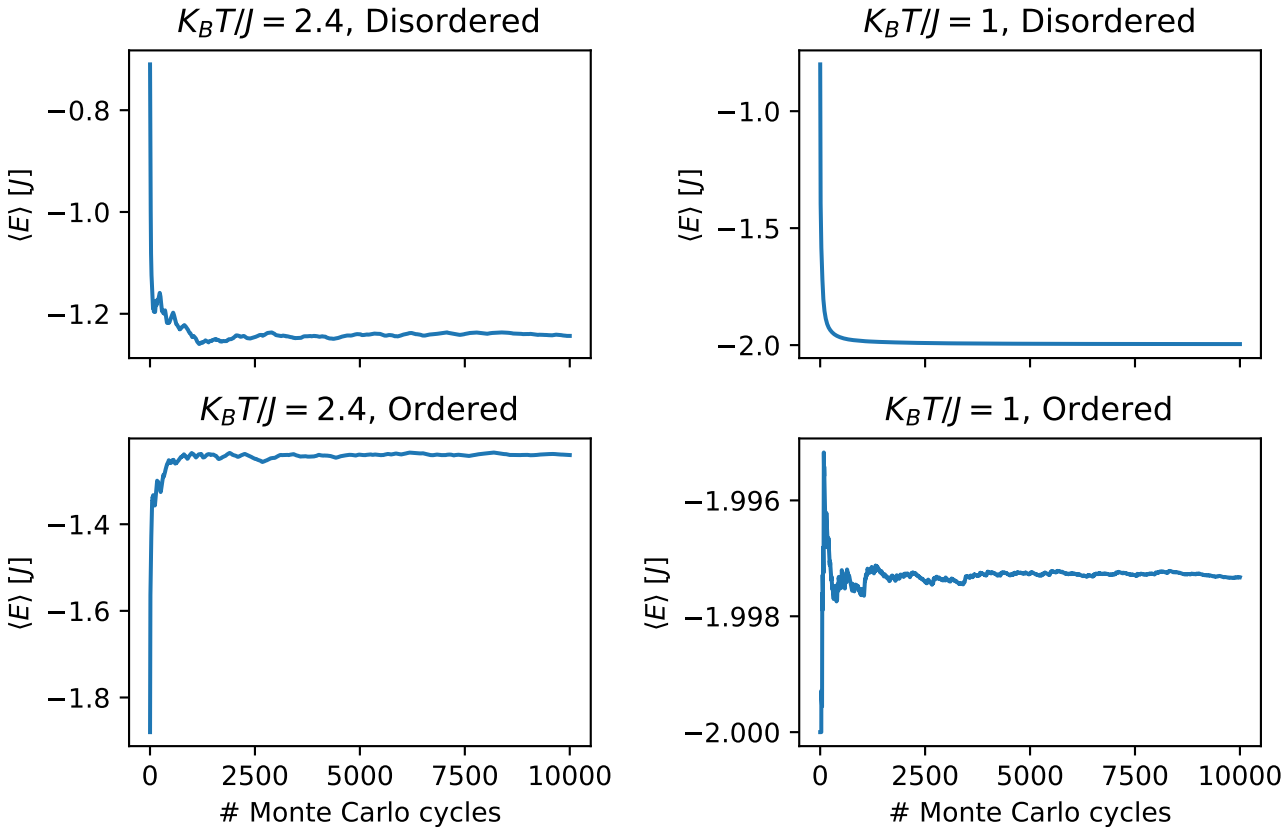

Figure 1. Figure showing the energy E as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_BT/J = 1$ and $k_BT/J = 2.4$ for and ordered lattice where all initial spins point in the same direction and an unordered lattice where all initial spins are chosen randomly.

this temperature. For the temperature $k_BT/J = 2.4$, one can see that for both initial spin configurations the discrepancy between the most likely state and the initial state is relatively large for both the mean energy and absolute magnetization. The solution stabilizes around the most likely state relatively fast, allthough not as fast as for the lower temperature previously discussed. One can also see that for the higher temperature, the fluctuations around the most likely state is a lot higher than for $k_BT/J = 1$. This can also be seen by studying the number of accepted flips per Monte Carlo cycle as shown in Figure 3. After the quantities have stabilized one can see that the number of flips for the higher temperature is a lot higher than for $k_BT/J = 1$. While the lower temperature ranges zero to four flips, the solution with $k_BT/J = 2.4$ ranges from approximately 50

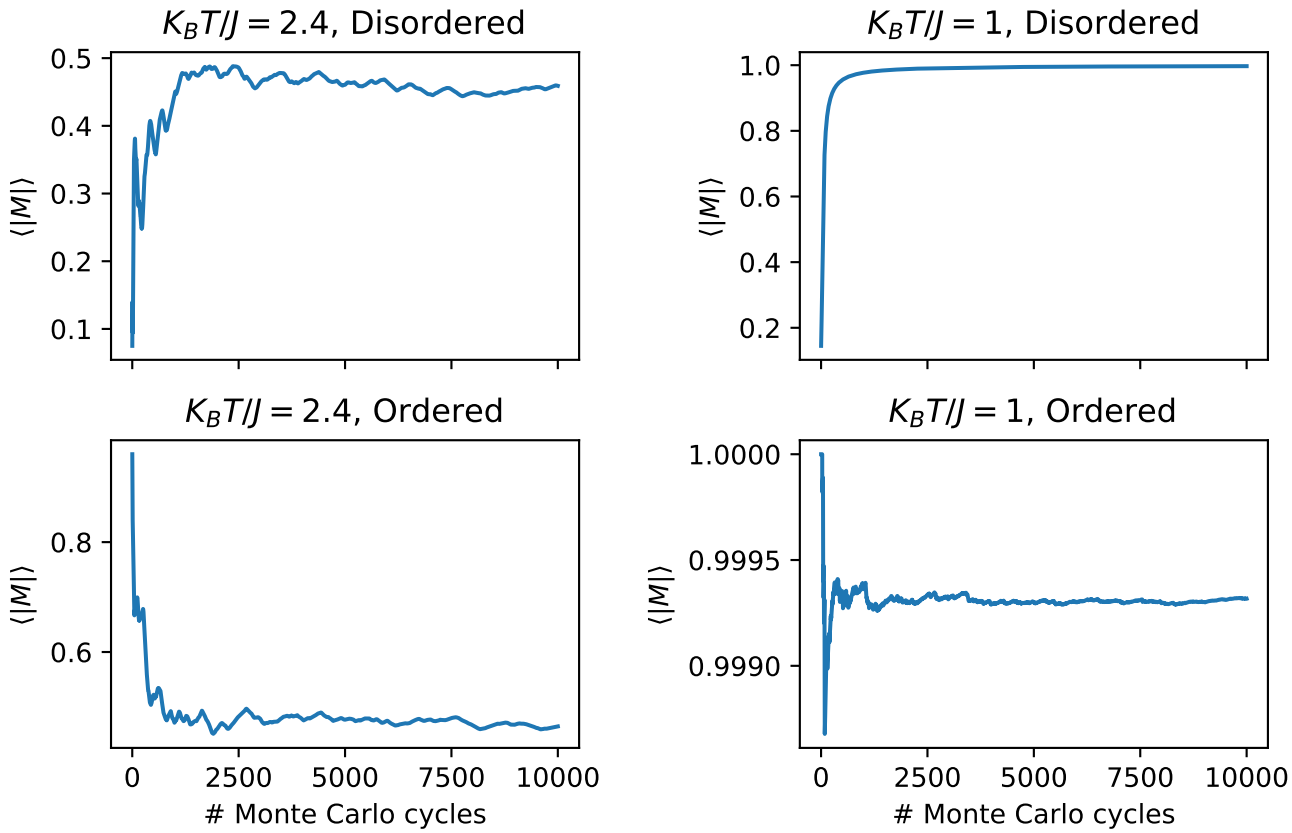

Figure 2. Figure showing the absolute value of the magnetization $|M|$ as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_BT/J = 1$ and $k_BT/J = 2.4$ for and ordered lattice where all initial spins point in the same direction and an unordered lattice where all initial spins are chosen randomly.

Table 4. Table showing the timing of a loop over 50 different temperatres using 10^6 Monte Carlo Cycles for each loop iteration. The grid size for the lattice used was $N = 10$.

Threads	Flag	Run time [s]
1	-O3	195.636
4	-O3	55.539
8	-O3	45.61
8	-O1	220.689

Table 5. Table showing the variance in the energy σ_E^2 and the total variance according to the central limit theorem σ^2 for to temperatures. The grid size used was $N = 20$ and 10^6 Monte Carlo cycles with a sample start at 5000 cycles.

k_BT/J	σ_E^2 $[J^2]$	σ^2 $[J^2]$
1.0	$5.848 \cdot 10^{-5}$	$5.848 \cdot 10^{-12}$
2.4	0.0203	$2.03 \cdot 10^{-9}$

to 100 flips per Monte Carlo cycle. By studying the histogram, as shown in Figure 4, one can see that for $k_BT/J = 2.4$ the variance in the energy is a lot higher than for $k_BT/J = 1$. This is also tabulated in Table 5. Here we can see that for a higher temperature the particles in the crystal will be more suscebtible to change due to the thermal energy causing the devations around the most likely state to be larger than for a lower temperature. Since the histogram for $k_BT/J = 2.4$ is relatively gaussian one can also compare the standard deviation, given as $\sqrt{\sigma_E^2}$, with the FWHM. Four our result this seems like a good match by an eye estimate. For the lower temperature, the shape appears too narrow with a small number of bins making it hard to conduct the same estimation. The variance of the sample mean σ^2 of the energy provides an error estimate for the mean of the energy distribution. To improve our method further, one could include a similar error estimate for the other

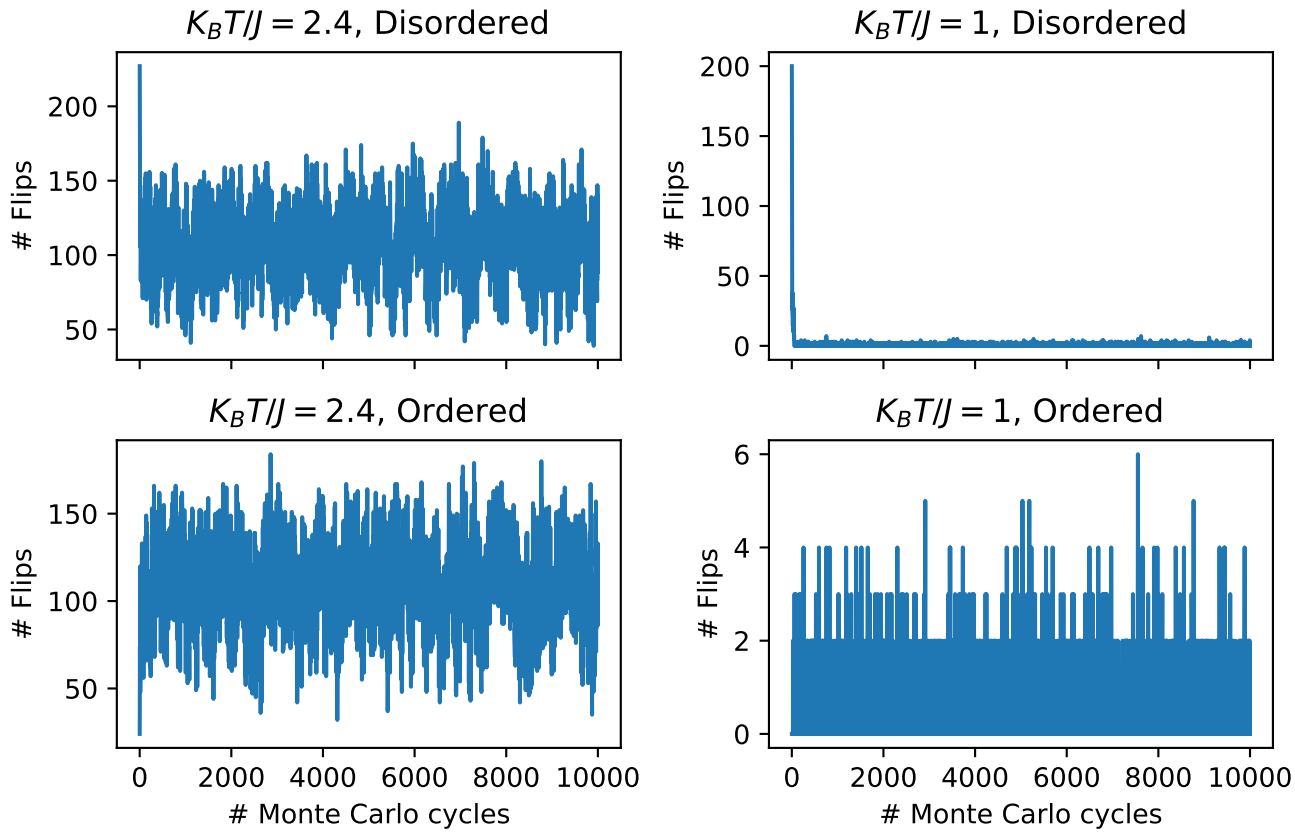

Figure 3. Figure showing the number of flips done to the spin values as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_BT/J = 1$ and $k_BT/J = 2.4$ for and ordered lattice where all initial spins point in the same direction and an unordered lattice where all initial spins are chosen randomly.

results as well.

The implementation of the model was also timed using parallelization and different compiler flags with $N = 10$. This is tabulated in Table 4. Here we can see that there is a significant increase in efficiency between one and four threads using the compiler flag -O3. However, the difference between eight and four threads compiled with the -O3 flag is not that significant. An interesting result is the difference between using eight threads using the -O1 compiler flag compared to using one thread with the -O3 compiler flag. We found that one thread with the -O3 compiler flag turned out to be the fastest. This result indicates that compiler flags have a larger impact on CPU time than parallelization. Our results however were only produced computing once for every combination of parallelization and compiler flag. To improve this result and draw a safer conclusion one should test a wider range of parallelization and compiler flag combinations and run the calculations more than once to provide a better statistical analysis.

When computing the thermodynamical quanitites $\langle E(T)\rangle$, $C_v(T)$, $\chi(T)$ and $\langle|M(T)|\rangle$, as shown in Figure 5, our results proved to be in good compliance with theory as described in section 2.4. By looking at the figure one can see that the heat capacity $C_v(T)$ peaks close to the critical temperature T_C with a higher peak as the lattice size increases. This is in compliance with what one would expect from (35). The same is the case for the behavior of the magnetic susceptibility given by (36). The plot for the energy shows that it is not very sensible to lattice dimensions N. It shows a slight bend when the temperature approaches the T_C. The absolute magnetization is, in contrast to the energy, a lot more sensitive to the lattice dimensions when the temperature approaches T_C. As expected it goes to zero when the temperature approaches. This indicates that the crystal approaches a disordered state where we have an equal amount of spins in both direction cancelling each other.

5. CONCLUSION

We have implemented the Ising model to simulate magnetic phase transitions in a lattice with periodic boundary conditions. Our simulations behave as ex-

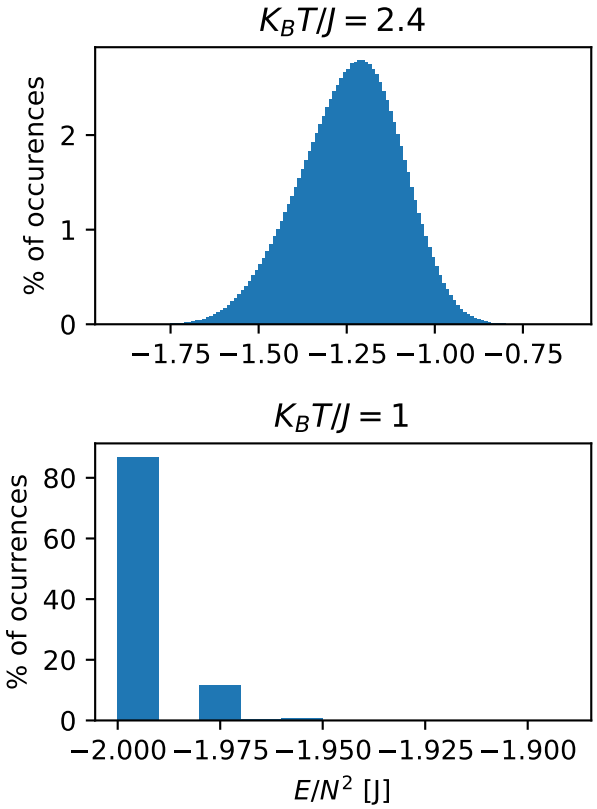

Figure 4. Figure showing the probability $P(E)$ for a system with lattice size $N = 20$ for two different temperatures $k_BT/J = 1.0$ and $k_BT/J = 2.4$. The energies were counted continously after 5000 Monte Carlo cycles to allow the solution to stabilize.

pected, reaching their equilibriums after $\sim 10^3$ Monte Carlo cycles and our estimated critical temperature of the studied phase transition T_c aligns well with the results of Onsager (1944).

For future research we should consider more than two temperatures to get better statistics, also running over a better grid resolution onmore powerful hardware. The analysis in this projects last error estimation of (?), which is important for robust results and should be looked into further. Purely in the interest of computational performance, the simulations should also be run and timed on different amounts of threads to get a better indication of how well the algorithm scales.

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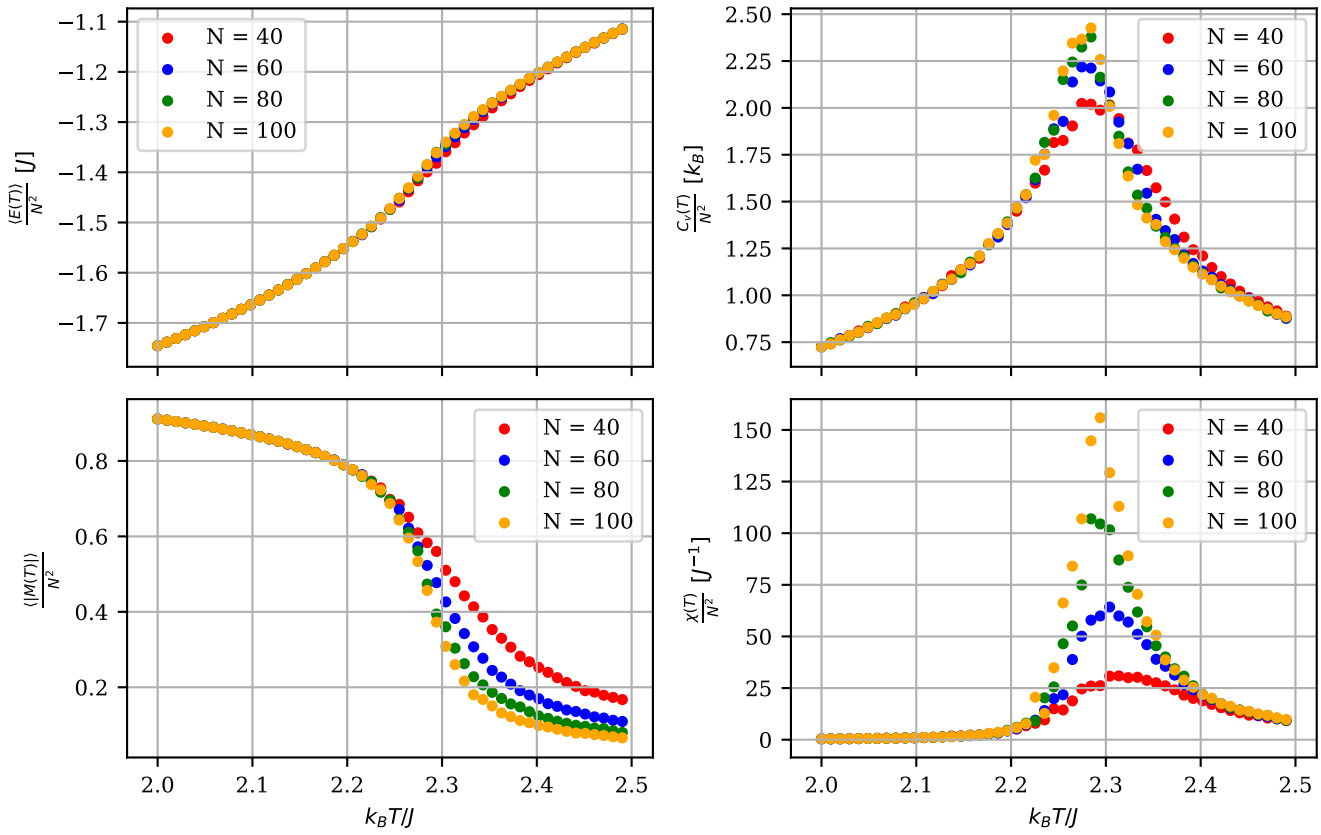

Figure 5. Figure showing thermodynamical quantitites per particle as a function of temperature for varying lattice dimensions N after 5000 Monte Carlo cycles when the system has stabilized. Starting clockwise from the upper left the figure illustrates the mean energy $\langle E(T)\rangle$, heat capacity $C_v(T)$, magnetic susceptibility $\chi(T)$ and the mean of the absolute value of the magnetization $\langle |M(T)|\rangle$. The plot was produced using 50 temperature poins in the range $k_BT/J \in [2.0, 2.5]$.