

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

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Abstract

We model the time development of a 2D ferromagnetic Ising model using a Markov Chain Monte Carlo and the Metropolis algorithm for a lattice of $N \times N$ interacting spins with periodic boundaries. Our model behaves in good agreement with the known analytical results for a 2×2 lattice using more than 10^4 Monte Carlo cycles. When studying a $N = 20$ lattice we find that it stabilizes around an equilibrium after about 5000 Monte Carlo cycles for temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$ for an ordered and disordered initial spin configuration. Our results show that the lattice with the lower temperature stabilizes faster than for the higher temperature, effectively freezing at equilibrium. This is also reflected by the energy distributions around the equilibrium where the higher temperature lattice follows a Gaussian distribution while the lower temperature has a narrow distribution with a small number of likely energy states. For the critical temperature where the system loses its magnetization, we find it to be $k_B T_C/J \approx 2.284$, which corresponds to a relative error $\epsilon \approx 0.675\%$ compared to the analytical solution by [Onsager \(1944\)](#).

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

1. INTRODUCTION

An ever occurring 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 system's energy and magnetization develop with time. The final aim being to estimate the critical temperature of the phase transition when the lattice loses its magnetization, 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 Mechanics

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 neighbors. The energy of the lattice is defined by the interaction of each neighboring spin pair as

$$E = -J \sum_l \sum_{\langle kl \rangle} s_k s_l, \quad (1)$$

where $\langle kl \rangle$ denotes the sum over the nearest neighbors and J has units energy. When counting the energies we choose to use periodic boundaries, meaning that the nearest neighbor 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 infinitely in space. The magnetization is defined similarly as

$$M = \sum_i s_i, \quad (2)$$

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

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

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

$$Z = \sum_i e^{-\beta E_i}, \quad (4)$$

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

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

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

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

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

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

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

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

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

These thermodynamical quantities will later be useful when estimating the critical temperature of the phase transition when the system loses its net magnetization. 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 magnetization 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 describing the algorithm modeling the time development of the lattice, we show the analytical solutions to the mean energy and absolute magnetization as well as the heat capacity and the susceptibility as shown in 2.1, so as to later enable a comparison of the numerical results to known analytical quantities. When

Table 1. Table showing the possible energies E_i and magnetizations M_i of the 2×2 lattice and their corresponding number of spins up N_\uparrow and degrees of degeneracy 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 |

counting the energy and magnetization of the 2×2 lattice as described 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

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

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

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

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

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

Next this leads to the heat capacity being

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

and the susceptibility (when using the absolute magnetization) is

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

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

These analytical quantities can be compared 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 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

$$w_j = W(i \rightarrow j)w_i, \quad (17)$$

where $W(i \rightarrow j)$ is the transition matrix quantifying the probability of 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 $W(i \rightarrow j)$ having the largest eigenvalue. Since $W(i \rightarrow j)$ 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 losing the time dependence since the change from each iteration to the next becomes negligible. This means that effectively

$$w(t_i) - w(t_i + \epsilon) = 0, \quad (18)$$

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

$$\sum_i W(i \rightarrow j)w_i - W(j \rightarrow i)w_j = 0, \quad (19)$$

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

$$W(j \rightarrow i)w_j - W(i \rightarrow j)w_i = 0. \quad (20)$$

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

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

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 $W(j \rightarrow i)$ is larger than the backwards transition probability $W(i \rightarrow j)$. 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

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

where $r \in [0, 1]$ is a number drawn from a uniform distribution, effectively modeling all transition possibilities 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 magnetization. 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 neighbors contributing 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 magnetization ΔM from a spin flip have analytical expression;

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

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

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

$$\Delta M = 2s_l^2, \quad (25)$$

since the difference in magnetization at a spin flip is 2. This way of suggesting a new state is more efficient

than to compute the energy difference using a whole new lattice configuration, as it requires a lot less FLOPs.

The difference in energy is then used to determine whether the suggested spin flip is accepted or not through the described Metropolis algorithm.

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

2.4. The Analysis

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

The next step is 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 magnetization as

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

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

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 determined by a by-eye estimate. This is used as a starting time for the later sampling of energies and magnetization for the thermodynamical quantities 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 state at any given time step.

To further see if the lattice behaves as expected we can approximate the Boltzmann distribution $P(E)$ for a given temperature $k_B T/J$ by making a histogram of the energy states of the system. We would expect that for a low temperature like $k_B T/J = 1.0$ 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 $k_B T/J$ the PDF will look more like a Gaussian distribution as the system has many more possible (symmetric) energy states around the equilibrium that it can oscillate around.

The distributions are then compared to the sample variance given by the central limit theorem (Jensen

2015, p. 357) defined as

$$\sigma^2 = \frac{\sigma_E^2}{m}, \quad (28)$$

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 deviation σ_E .

Next, we want to study the phase transition where the lattice loses its net magnetization. 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 magnetization is given by

$$\langle M(T) \rangle \sim (T - T_C)^\beta, \quad (29)$$

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

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

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

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 temperature T approaches 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

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

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

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

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

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

the heat capacity becomes

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

and the susceptibility is

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

where we have set $T_C(N) = T$ and $T_C(N \rightarrow \infty) = T_C$. Thus if we plot the mean energy and magnetization as well as the heat capacity and susceptibility as a function of temperatures we can estimate the critical temperature for an infinite grid $N \rightarrow \infty$. 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 magnetization suddenly bend at $T = T_C(N)$, and that the heat capacity and susceptibility peak at $T = T_C(N)$. When $N \rightarrow \infty$ this peak will diverge. Using (33) for two grid sizes N_1 and N_2 we can estimate the constant a to be

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

since we know that $T_C(N \rightarrow \infty)$ is the same for all grids. Knowing a we can use (33) to compute an estimate for $T_C(N \rightarrow \infty)$. 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 decently large number of Monte Carlo cycles is very time consuming, we parallelized the temperature loops using MPI and different compiler flags. To check the speed-up factor we timed code using different degrees of parallelization and compiler flags.

3. RESULTS

The following results were produced running on an Intel Core i7-6700HQ CPU with a clock speed of 2.60 GHz and 8Gb RAM. The computations were made using C++ using the mpic++ compiler in Ubuntu 16.04.

To determine how many Monte Carlo cycles that were required for the solutions to stabilize 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 highest precision found in Table 2 obtained with 10^6 Monte Carlo cycles, we computed the mean energy and absolute value of the magnetization 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 quantities were computed for the $k_B T/J = 1.0$ case. This is tabulated in Table 3.

In order to find how long it takes for the model to reach equilibrium we calculate the energy E , absolute

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 |

magnetization $|M|$ and heat capacity C_V all as functions of the temperature T for lattices 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 PDF $P(E)$ was plotted as a histogram 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 are shown in Table 5.

To study the behavior of the 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 $\langle |M(T)| \rangle$ were calculated in the interval $k_B T/J \in [2.0, 2.5]$. These thermodynamical quantities were plotted per particle in the given temperature interval using 50 points. 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 calculations were also timed using a varying amount of threads for parallelization and compiler flags for a lattice with dimensions $N = 10$

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

| $k_B T/J$ | $\langle E \rangle [J]$ | $\langle M \rangle$ | $C_V [k_B]$ | $\chi_{ M } [J^{-1}]$ |
|---------------------------------------|-------------------------|-----------------------|-------------|-----------------------|
| 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 $\frac{k_B T}{J} = 1.0$ | $4.967 \cdot 10^{-6}$ | $2.780 \cdot 10^{-5}$ | 0.003 | 0.0391 |

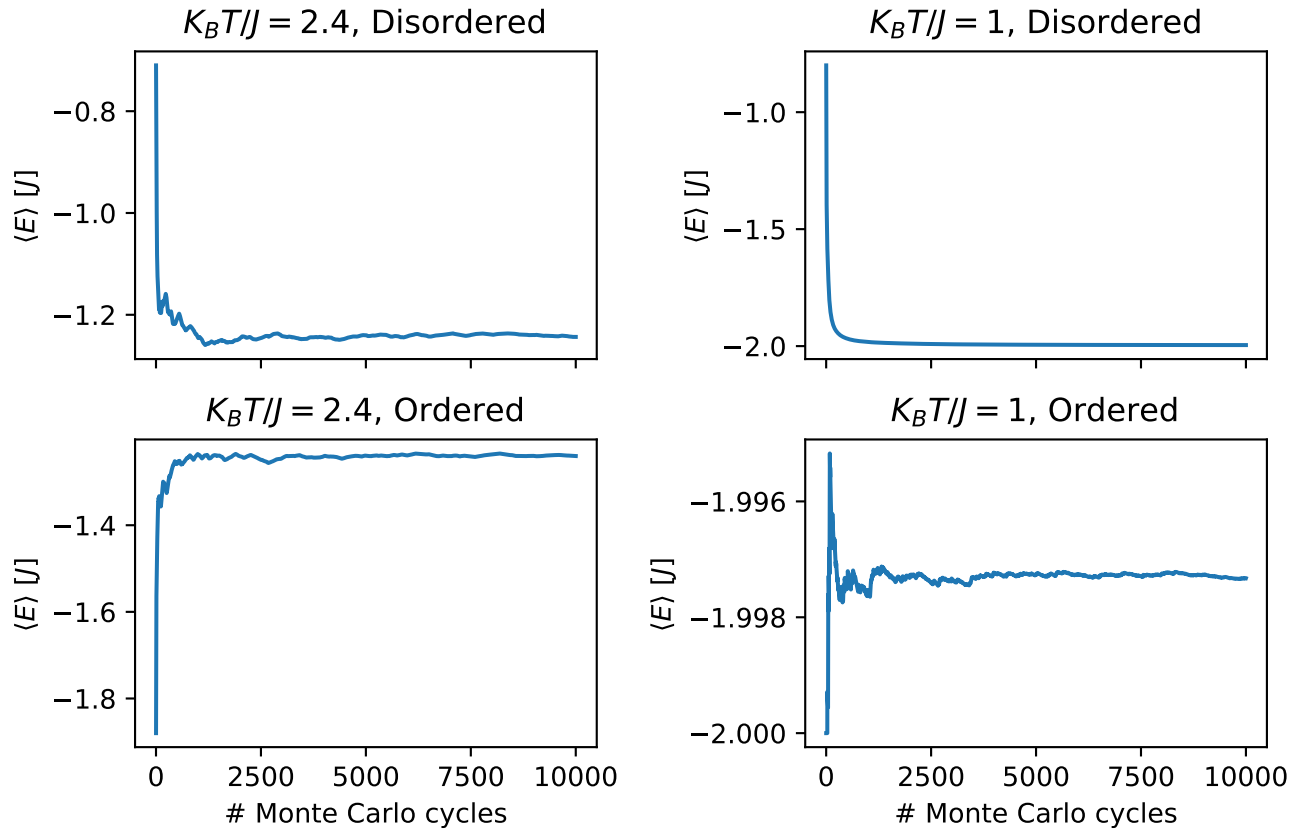


Figure 1. Figure showing the mean energy $\langle E \rangle$ as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$ for an ordered lattice where all initial spins point in the same direction and an unordered lattice where all initial spins are chosen randomly.

and 10^6 Monte Carlo cycles. 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 $T_C(N \rightarrow \infty)$ 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 of $\epsilon \approx 0.675\%$ relative to the analytical value by [Onsager \(1944\)](#).

4. DISCUSSION

The results in Table 2 and 3 indicate that the system approaches equilibrium close to the analytical value at 10^4 Monte Carlo cycles. At temperature $k_B T/J = 1.0$ and 10^6 Monte Carlo cycles, all thermodynamical quan-

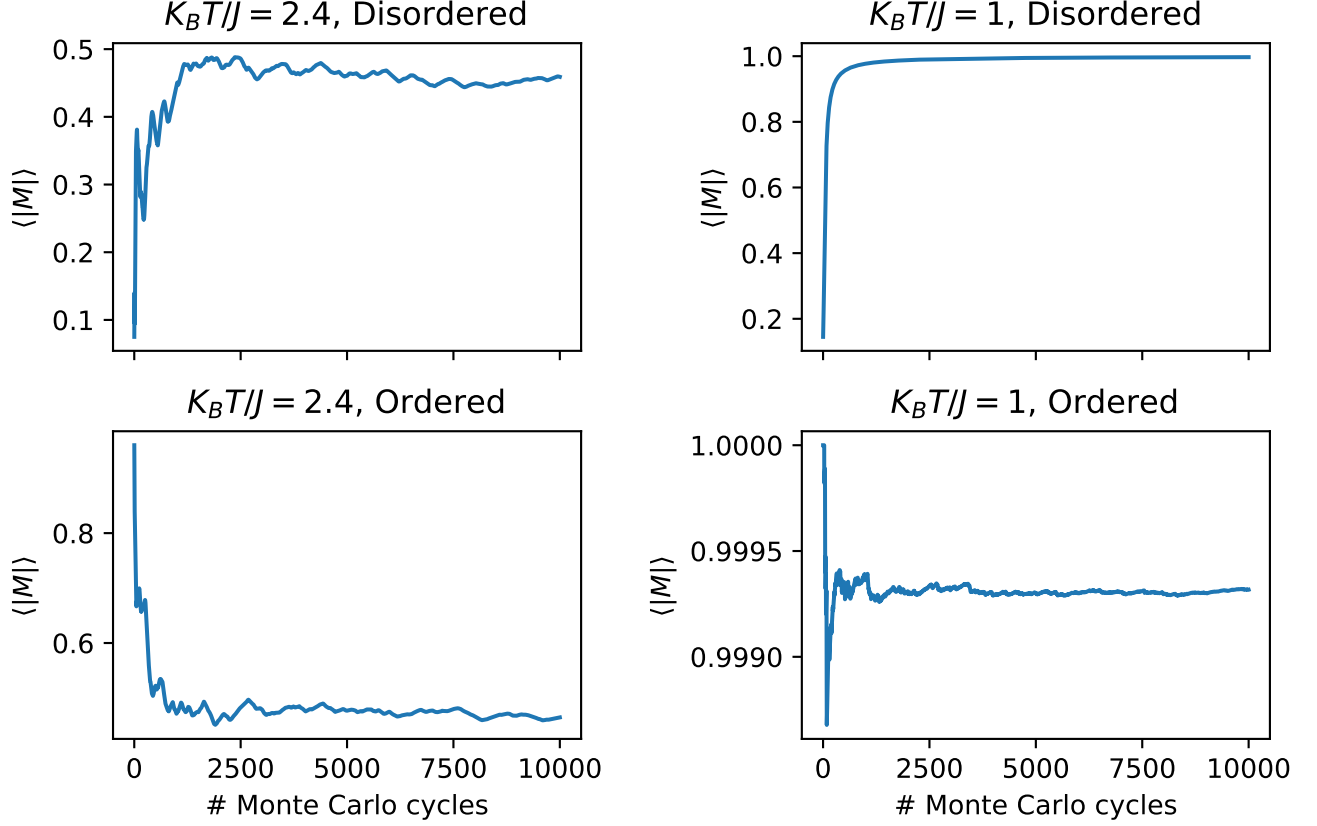


Figure 2. Figure showing the mean absolute value of the magnetization $\langle |M| \rangle$ as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$ for an ordered lattice where all initial 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 temperatures 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 distribution σ_E^2 and the total variance according to the central limit theorem σ^2 for the two temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$. The grid size used was $N = 20$ and 10^6 Monte Carlo cycles with a sample start at 5000 cycles.

| $k_B T/J$ | $\sigma_E^2 [J^2]$ | $\sigma^2 [J^2]$ |
|-----------|-----------------------|------------------------|
| 1.0 | $5.848 \cdot 10^{-5}$ | $5.848 \cdot 10^{-12}$ |
| 2.4 | 0.0203 | $2.03 \cdot 10^{-9}$ |

tities in Table 3 approach the analytical values within satisfactory relative errors. We see that the mean energy and absolute magnetization increase and decrease respectively with increasing temperatures. Both the heat capacity and the magnetic susceptibility increase within the chosen temperature interval, as they are expected to peak at the critical temperature and then fall off again.

When studying the mean energy and absolute magnetization 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 $k_B T/J = 1.0$ starts very close to its most likely state.

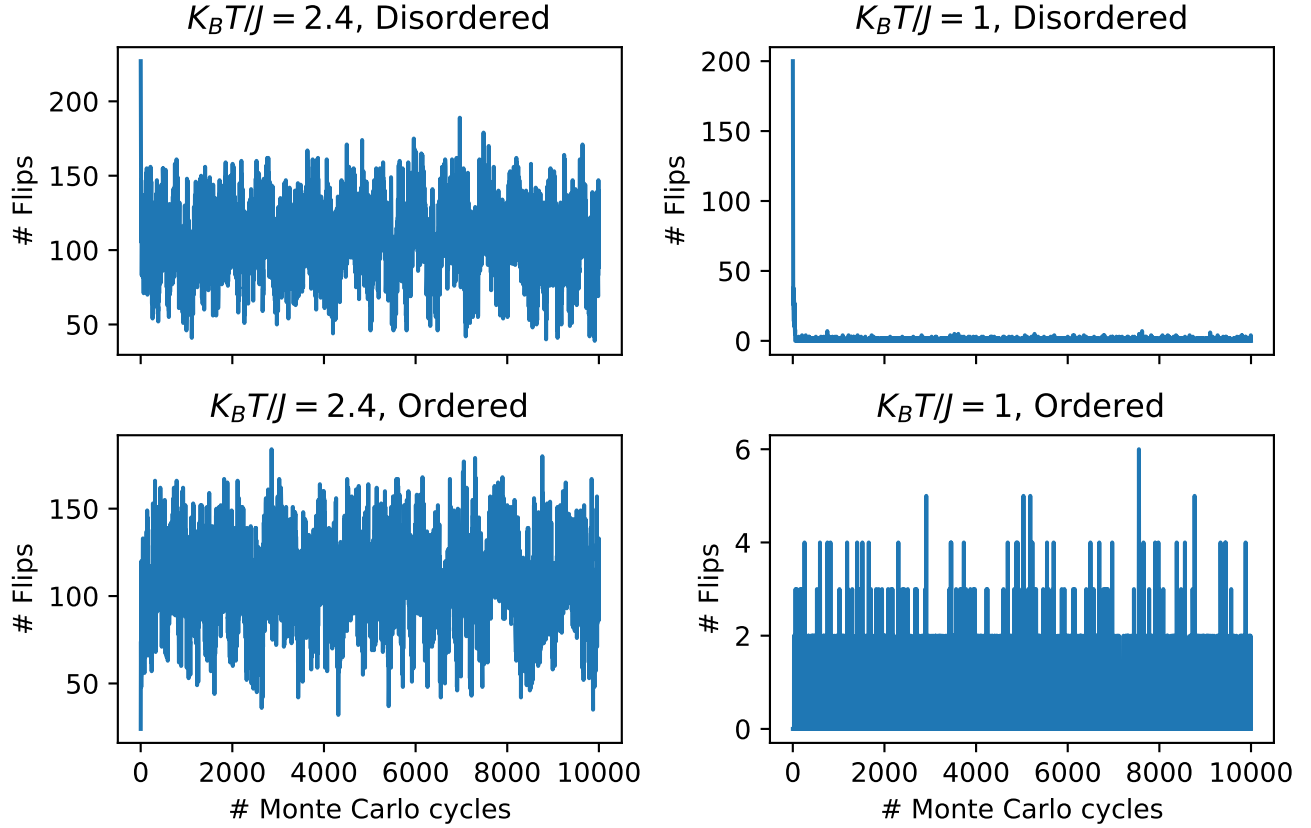


Figure 3. Figure showing the number of accepted flips performed to the spin values as a function of Monte Carlo cycles for a lattice with dimensions $N = 20$. The simulations were done with two different temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$ for an ordered lattice where all initial spins point in the same direction and an unordered lattice where all initial spins are chosen randomly.

The disordered configuration with $k_B T/J = 1.0$ has an initial energy with a larger deviation from equilibrium than the ordered configuration, but it quickly reaches an equilibrium. The same behaviour can be seen for the same combinations of temperature and initial configuration for the absolute magnetization as seen in Figure 2. The fluctuations around the most likely state are also relatively small for this temperature. Therefore the plots of the mean energy and mean absolute magnetization with a disordered initial configuration seem very smooth. For the temperature $k_B T/J = 2.4$, 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, although 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 are a lot higher than for $k_B T/J = 1.0$. 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 $k_B T/J = 1.0$. While the lower temperature ranges from zero to four flips, the solution with $k_B T/J = 2.4$ ranges from approximately 50 to 100 flips per Monte Carlo cycle. By looking at the figures for the energy and absolute magnetisation, one can see that the solution stabilizes after approximately 5000 Monte Carlo cycles. Therefore this value is used as a cutoff when computing the thermodynamic quantities used for estimating the critical temperature, as we are interested in the oscillations around the equilibrium. By studying the histogram, as shown in Figure 4, one can see that for $k_B T/J = 2.4$ the variance in the energy is a lot higher than for $k_B T/J = 1.0$. This is also tabulated in Table 5. Here we can see that for a higher temperature the particles in the crystal has more permitted energy states around the equilibrium due to the thermal energy causing larger changes in the configuration of spins compared to crystal of lower temperature. Since the histogram for $k_B T/J = 2.4$ is relatively Gaussian, one can also com-

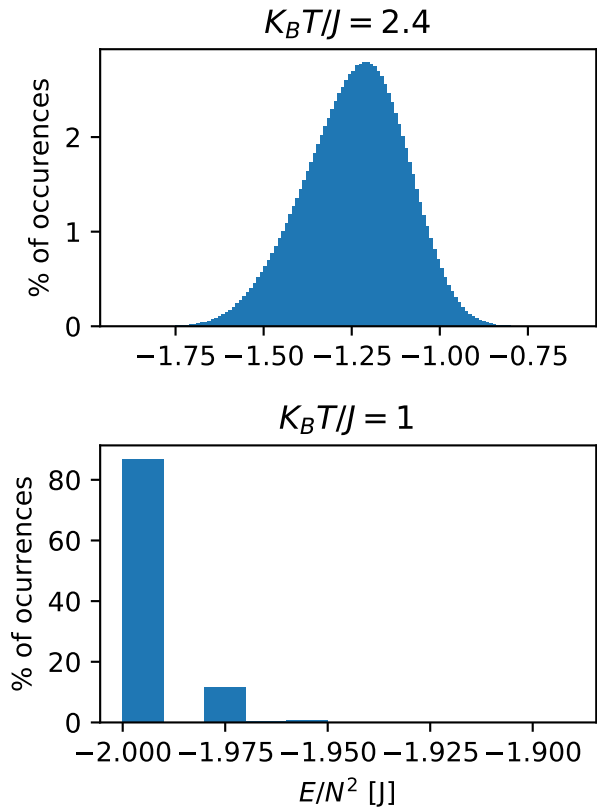


Figure 4. Figure showing the probability distribution function $P(E)$ of energies for a system with lattice size $N = 20$ for two different temperatures $k_B T/J = 1.0$ and $k_B T/J = 2.4$. The energies were counted continuously after 5000 Monte Carlo cycles to allow the solution to stabilize. The total amount of Monte Carlo cycles used were 10^7 .

pare the standard deviation, given as $\sqrt{\sigma_E^2}$, with the FWHM. For our result this seems like a good match using a by-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 shape of the distribution is consistent with expectation described in section 2. 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 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 faster than eight threads with the -O3 compiler flag. This result indicates that compiler flags have a larger impact on CPU time than parallelization. However parallelization also provides a significant increase in performance. 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 quantities $\langle E(T) \rangle$, $C_V(T)$, $\chi(T)$ 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 decreases rapidly after the temperature reaches the critical temperature. This indicates that the crystal approaches a disordered state where we have an equal amount of spins in both direction cancelling each other leading to a loss of magnetization. We found the critical temperature to in very good agreement with Onsager (1944).

5. CONCLUSION

We have implemented the Ising model to simulate magnetic phase transitions in a lattice with periodic boundary conditions. Our simulations behave as expected for the temperatures and initial lattice configurations tested, for $N = 20$ with a sample start after 5000 Monte Carlo cycles where we can safely assume the system to close to equilibrium. Our estimated critical temperature of the studied phase transition T_C aligns well with the results of Onsager (1944).

Further research into the problem would be to see how the system behaves for more than two temperatures. The problem could also be expanded to three dimensions in order to reflect a more realistic crystal. In general good statistical error estimates are missing from most of our results. Including this could enable a safer ground for conclusions. When performing the timing

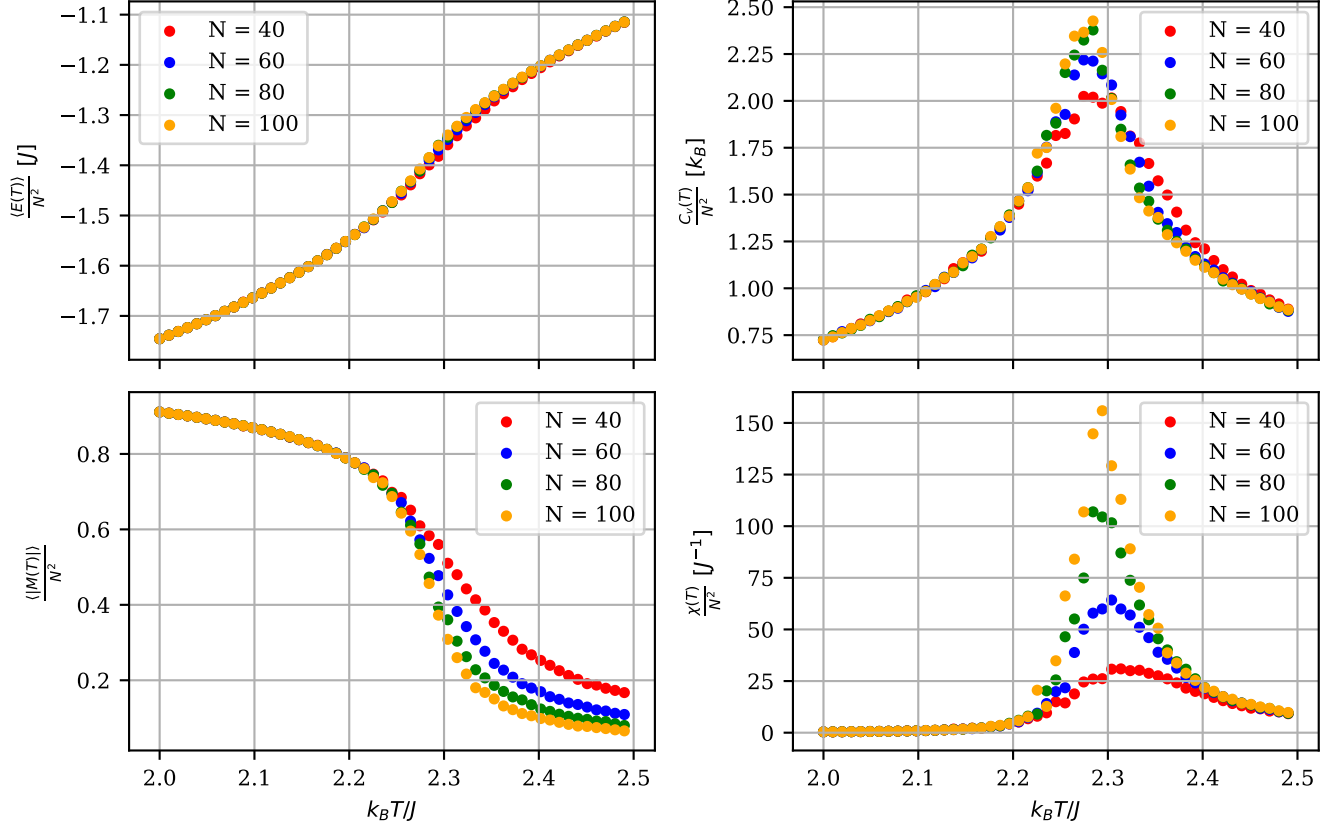


Figure 5. Figure showing thermodynamical quantities per particle as a function of temperature for varying lattice dimensions N after 5000 Monte Carlo cycles where the system has stabilized. Starting clockwise from the upper left the figure illustrates the mean energy $\langle E(T) \rangle$, heat capacity $C_V(T)$, 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 points in the range $k_B T/J \in [2.0, 2.5]$.

of the calculations one could include a larger amount combinations for compiler flags and degrees of paral-

lization as well as averaging over several runs giving a better foundation for conclusions.

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