Modelling Magnetic Phase Transitions with the Ising Model & Metropolis Algorithm

Benedicte Nyheim, Peder Hauge & William Eivik Olsen*
University of Oslo - Department of Physics

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The Ising model for simulating phase transitions have been studied for a two dimensional lattice by implementing the Metropolis algorithm and using periodic boundary conditions. Calculations of thermodynamical quantities for a 2×2 lattice were compared with analytical values to test the algorithm's reliability. The resulting accuracy was high, with relative error of order 10^{-5} for mean energy and magnetization after 10^6 Monte Carlo cycles. By increasing the size of the lattice and calculating the mean energy and absolute magnetization for varied numbers of Monte Carlo cycles we were able to establish a burn-in time of 10% of the Monte Carlo cycles independent of initial spin configuration and temperature. The peaks of heat capacity as a function of temperature for different lattice sizes were used to find the critical temperature for phase transformations. We estimated the critical temperature to be $T_C = (2.27 \pm 0.01)\ J/k$, which is in agreement of the analytical value $T_C \approx 2.269\ J/k$.

I. INTRODUCTION

The majority of everyday magnetic phenomena are known through ferromagnetic materials; materials that can maintain a net magnetic field without the influence of an external magnetic field. This is referred to as a spontaneous magnetization, caused by a macroscopic ordering of electron spins in the material. Such an ordering occurs when it is energetically favorable for the electron spins to be aligned.

In order to stay aligned it is necessary for the electron interactions to outweigh the thermal agitation which tends to randomize any atomic-level order. When a ferromagnetic material reaches a certain temperature known as the Curie temperature, a phase transition occurs in which the macroscopic ordering and the spontaneous magnetization disappears.

Phase transitions in magnetic systems are popularly simulated using the Ising model, where the total energy of the system is dependent on each electron spin and the relative spin of their neighbouring electrons. Despite the simplicity of the Ising model, numerical simulations of phase transitions quickly become demanding as a result of the probability of each microstate having a dependency on the partition function of the system. This requires a summation over the Boltzmann factors of every possible microstate, the number of them being 2^N for N particles.

In this paper we will study phase transitions in a two-dimensional spin lattice using the Ising model. To improve the efficiency of the calculations we will use the Metropolis algorithm, a Monte Carlo based algorithm for equation of state calculations, with periodic boundary conditions. This algorithm simplifies the calculations by only considering ratios of probabilities for the microstates, making the partition function unnecessary.

In the theory section we present analytical solutions for a 2×2 lattice with temperature $T = 1\ k/J$ and the Curie temperature for an infinitely large lattice. The former will serve as benchmark calculations for the algorithm while the latter will serve as a final test for the validity of our results.

II. THEORY

A. Ising Model

We will apply the Ising model to study phase transitions at finite temperature for magnetic systems. If there is no external magnetic fields interacting with the magnetic moments of the spins, the Ising model in its simplest form can be expressed with the energy

$$E = -J \sum_{\langle ij \rangle}^{N} s_i s_j, \tag{1}$$

where $s_i = \pm 1$, N is the total number of spins and J is a coupling constant determining the strength of the interaction between neighboring spins.

It is worth noting that for $J > 0$ it is energetically favorable for neighboring spins to be aligned. This means that at temperatures low enough, a spontaneous magnetization can occur. That is, a given magnetic moment can influence spins that are separated from it by a macroscopic distance. This leads to long range correlations between spins, causing a net magnetization of the system when there is no external magnetic field. The magnetization is defined as:

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

where we sum over all spins for a given configuration i.

* Code repository: https://github.com/williameivikolsen/FYS4150

B. Statistical mechanics

The partition function Z of a canonical ensemble of n microstates at a temperature T is given by

$$Z = \sum_{i=1}^{n} e^{-\beta E_i}, \tag{3}$$

where E_i is the energy of microstate i and $\beta = \frac{1}{kT}$, with k as Boltzmann's constant.

From the partition function we can calculate other thermodynamic quantities. The Boltzmann distribution is given by

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}. \tag{4}$$

We can also calculate the expectation value of an arbitrary thermodynamic quantity A through

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{n} A_i e^{-\beta E_i}. \tag{5}$$

The specific heat C_V and the magnetic susceptibility χ can be expressed as

$$C_V = \frac{1}{kT^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right), \tag{6}$$

$$\chi = \frac{1}{kT} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right). \tag{7}$$

where E is the energy and M is the magnetization.

C. Analytical solutions for 2×2 lattice

The energy and magnetization of each possible microstate in a 2×2 lattice can be calculated analytically using Eqs. (1) and (2). These quantities are presented in Table I. The energy of each configuration is presented in units of J, that is, $J = 1$.

Table I. Energy E and magnetization M of each possible microstate in 2×2 calculated analytically using Eqs. (1) and (2). $N_\uparrow$ is the number of spins up and d is the degeneracy.

$N_\uparrow$	d	M	E $[J]$
4	1	4	-8
3	4	2	0
2	4	0	0
2	2	0	8
1	4	-2	0
0	1	-4	-8

Using the energies calculated in Table I, the partition function Z can be found to be

$$Z = 4\cosh(8\beta) + 12.$$

The expressions for expectation values of the energy E, the absolute value of the magnetic moment $|M|$, in addition to E^2 and M^2 can then easily be obtained from Eq. (5):

$$\langle E \rangle = -32 \frac{\sinh(8\beta)}{Z},$$
$$\langle |M| \rangle = 8 \frac{e^{8\beta} + 2}{Z},$$
$$\langle E^2 \rangle = 256 \frac{\cosh(8\beta)}{Z},$$
$$\langle M^2 \rangle = 32 \frac{e^{8\beta} + 1}{Z}.$$

From this the specific heat and magnetic susceptibility could be calculated through Eqs. (6) and (7). For a temperature $T = 1\ k/J$ this gives the analytical values presented in Table II.

Table II. Analytical results for expectation value of energy E absolute magnetization $|M|$, heat capacity C_V and magnetic susceptibility χ per spin in the lattice with temperature $T = 1\ k/J$.

$\langle E \rangle / N$ $[J]$	$\langle |M| \rangle / N$	C_V/N $[J^2 \mathrm{k}^{-1}]$	χ/N $[k^{-1}]$
-1.99598	0.99866	0.03208	0.00401

D. Phase transitions

As the system reaches a temperature higher than the Curie temperature T_C, the magnetization of the system is expected to disappear.

Near the Curie temperature T_C we can characterize the thermodynamical quantities by a power law behavior. For our purposes we are interested in the heat capacity C_V and the susceptibility χ, which can be shown [1] to go as

$$C_V(T) \sim |T_C - T|^{\alpha}, \tag{8}$$

and

$$\chi(T) \sim |T_C - T|^{-\gamma}, \tag{9}$$

where $\alpha = 0$ and $\gamma = 7/4$ for the Ising model. The heat capacity and the susceptibility is therefore expected to have a peak around $T = T_C$.

Furthermore, it can be shown [1] that the critical temperature scales as

$$T_C(L) = \frac{a}{L} + T_C(L = \infty) \tag{10}$$

for the Ising model, where a is a constant. The critical temperature for an infinitely large lattice has been found analytically by Onsager [2] to be

$$T_C = \frac{2}{\ln\left(1 + \sqrt{2}\right)} \approx 2.269. \tag{11}$$

III. METHOD

A. Metropolis algorithm

The Monte Carlo based Metropolis algorithm simplifies calculations of thermodynamical quantities by only considering fractions of probabilities of microstates, making it unnecessary to calculate the partition function explicitly. The algorithm initializes a spin configuration of choice and suggests spin flips at random positions in the lattice. If the change in energy is negative the spin flip is accepted, moving the system towards an energy minimum. If not, there is still a probability for such a process to happen through thermal agitation. This is modelled by comparing the probability fraction $e^{\beta\Delta E}$ with a random number from a uniform distribution $[0, 1]$. If the Boltzmann factor is larger than the random number, the spin flip is accepted. If not, it is declined. The algorithm keeps suggesting spin flips at random positions for a chosen number of times. Then the thermodynamical quantities are added to a total expectation value. The entire process from the first spin flip suggestion to the update of the thermodynamical quantities is referred to as a Monte Carlo cycle (MC cycle). This process is then repeated for a chosen number of MC cycles before returning the expectation values. The full algorithm is described in a flow chart in Appendix A.

One crucial step in this algorithm is the calculations of the change of energy and magnetization, which should be done as efficient as possible as they have to be calculated many times. As only one spin is flipped at a time, the change of energy from one spin configuration to another is limited; only 5 values are possible for the Ising model in two dimensions. To explain this we illustrate one spin which we are going to flip, and its neighbours:

$$E = -4\ J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Longrightarrow \quad E = 4\ J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{array}.$$

Initially, the spins are aligned and the configuration has the lowest possible energy: $E = -4\ J$. After flipping the middle spin, the resulting energy is $E = 4\ J$ and the energy difference $\Delta E = 8\ J$. The result would be the same if all the spins were initially pointing down, and therefore we have 4 other possibilities:

$$E = -2\ J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Longrightarrow \quad E = 2\ J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$$

$$E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \downarrow & \end{array}$$

$$E = 2\ J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = -2\ J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \uparrow \\ & \downarrow & \end{array}$$

$$E = 4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = -4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{array}$$

with energy differences $\Delta E = 4\ J$, $\Delta E = 0$, $\Delta E = -4\ J$ and $\Delta E = -8\ J$, respectively. As a consequence we can calculate the different Boltzmann factors $e^{\beta\Delta E}$ in advance of applying the algorithm, and easily check the energy difference after a spin flip for which Boltzmann factor to use.

B. Calculations

We applied the Metropolis algorithm described to calculate the expectation value of the energy E, the absolute magnetization $|M|$, specific heat C_V and magnetic susceptibility χ using periodic boundary conditions. In addition, the acceptance rate of the proposed spin flips was found. The loop of spin flip suggestions was repeated N times for each Monte Carlo cycle where N is the total number of spins in the lattice.

The burn-in time for the Metropolis algorithm was estimated by simulating a 20×20 lattice for different numbers of Monte Carlo cycles. We discarded the equilibration time in all further calculations of the expectation values.

In all calculations we have scaled the thermodynamical quantities using natural units of the coupling constant, $J = 1$, and Boltzmann's constant, $k = 1$. For example the energy E will then have unit $[J]$ and the temperature $[J/k]$. All quantities are also scaled by the total number of spins to simplify comparison of different lattice sizes.

IV. RESULTS

The expectation value of energy E, absolute magnetization $|M|$, and the heat capacity C_v and magnetic susceptibility χ were calculated using the metropolis algorithm for the $L = 2$ lattice for different numbers of Monte Carlo cycles. The deviations from the analytical values in Table II are presented in Table III.

Table III. Relative error for calculated thermodynamics values when simulating for a $L = 2$ sized lattice with the Metropolis algorithm. The deviations were calculated for different numbers of Monte Carlo cycles c.

$\log_{10}(c)$	$\Delta \langle E \rangle$	$\Delta \langle \lvert M \rvert \rangle$	ΔC_v	$\Delta\chi$
4	1.2×10^{-3}	8.3×10^{-4}	6.0×10^{-1}	6.3×10^{-1}
6	1.2×10^{-5}	1.4×10^{-5}	5.9×10^{-3}	1.6×10^{-2}
8	2.1×10^{-6}	9.3×10^{-8}	1.1×10^{-3}	1.1×10^{-3}

The final spin configuration for a $L = 80$ lattice is shown in Figure 1 for temperatures both below ($T = 1.0\ J/k$) and above ($T = 2.4\ J/k$) the critical temperature,

and for different numbers of Monte Carlo cycles. The initial configuration for both temperatures are chosen to be random.

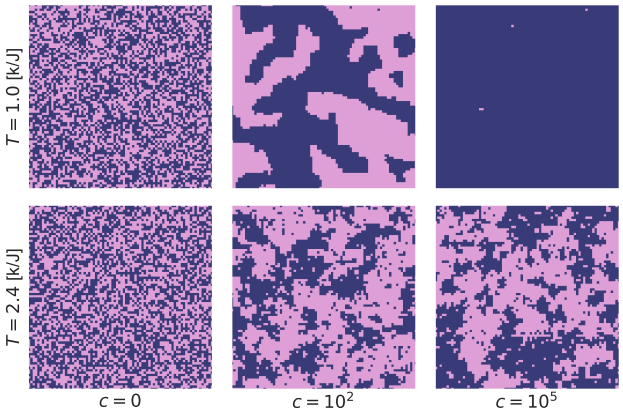

Figure 1. Illustration of the spin configurations in the $L = 80$ lattice. The light shade of purple illustrates spin up and the dark spin down. The top row shows the configurations for temperature $T = 1.0\ J/k$, and the bottom row for $T = 2.4\ J/k$. Both configurations are shown for different number of Monte Carlo cycles, from the left: $[0, 10^2, 10^5]$.

We have studied how many Monte Carl cycles are needed before the most likely state of the system is reached (burn-in time), using a lattice with size $L = 20$. In particular, this has been investigated for different initial temperatures and spin configuration.

In Figure 2 the mean energy per spin is plotted for a varying number of Monte Carlo cycles $\in [10^3, 10^6]$, both for random and fully aligned initial states and for temperatures $T = 1.0\ J/k$ and $T = 2.4\ J/k$. A similar figure for the mean absolute magnetization per spin is presented in Figure 3.

Using the same temperatures and initialization states as above, we have also seen how the rate of accepted spin flip proposals changes as a function of the number of MC cycles. This is shown in Figure 4.

We can find the the probability $P(E)$ of measuring the system's energy at a given value. A system with size $L = 20$ ran for 10^5 Monte Carlo cycles, of which 10% were discarded before collection of system energies started. We calculated the system's energy after going through each of the remaining cycles. This was done for $T = 1.0\ J/k$ and $T = 2.4\ J/k$. The number of different energy occurrences was counted and then scaled in order to produce the discrete probability distribution shown in Figure 5.

The expectation values of the energy E, absolute magnetization $|M|$, heat capacity C_V and magnetic susceptibility χ was calculated for square lattices of length $L = 40$, $L = 60$, $L = 80$ and $L = 100$ for temperatures in the range $T \in [2.0, 2.6]$. The temperatures were linearly spaced with steps $\Delta T = 0.004\ J/k$ between 2.2 J/k and 2.4 J/k, and with steps $\Delta T = 0.02\ J/k$ otherwise. Every calculation was run with 2×10^6 MC cycles. The results are shown in Figures 6, 7, 8 and 9.

The critical temperature was found as the maxima of the heat capacities displayed in Figure 8 and are plotted as a function of $1/L$ in Figure 10 with a linear regression

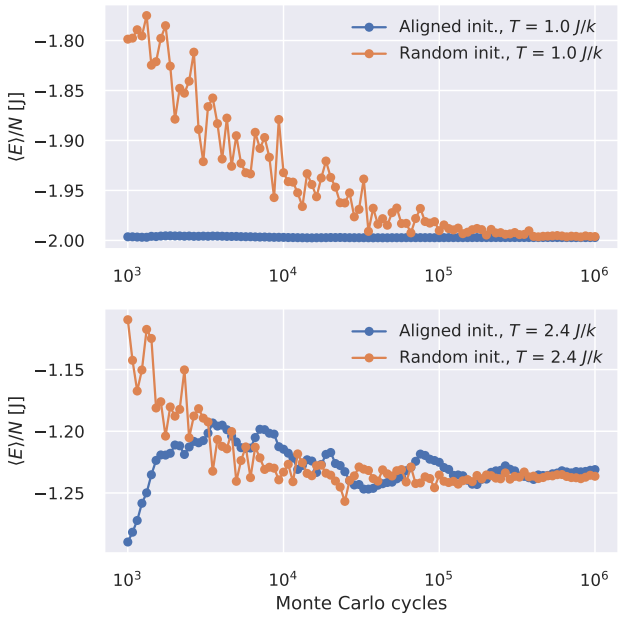

Figure 2. Mean energy per spin for a 20×20 system, run for 100 logarithmically spaced MC cycles in the interval $[10^3, 10^5]$.

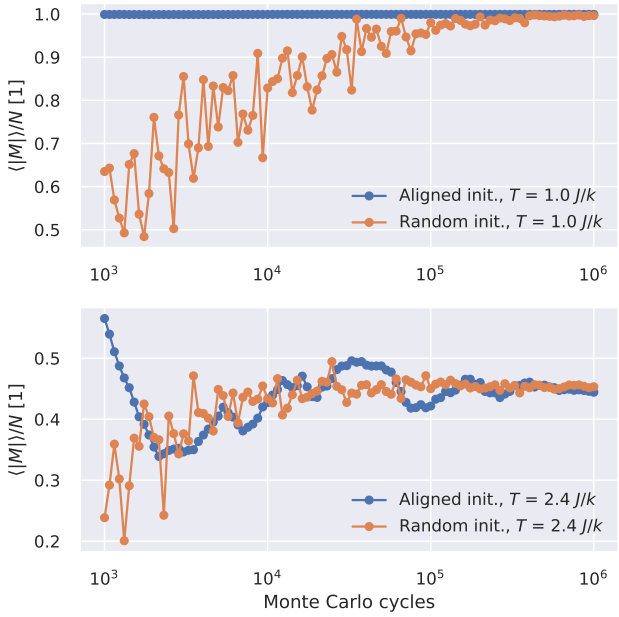

Figure 3. Mean abs. magnetization per spin for a 20×20 system, run for 100 logarithmically spaced MC cycles in the interval $[10^3, 10^5]$.

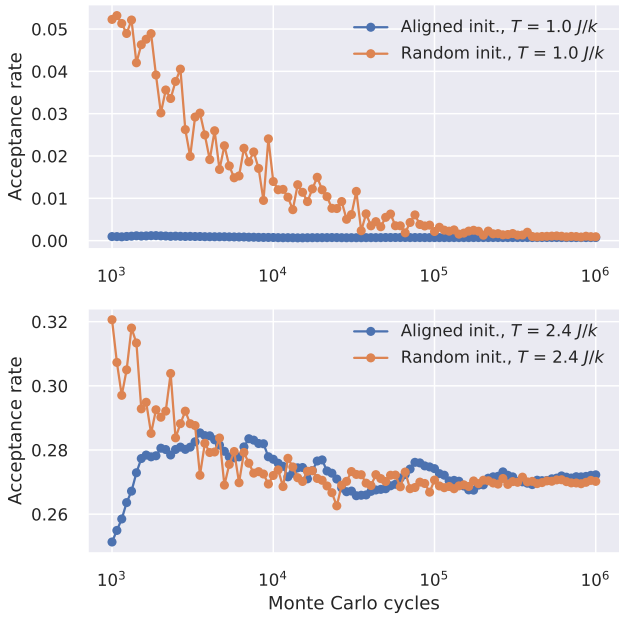

Figure 4. Acceptance rate for proposed spin flips for a 20×20 system, run for 100 logarithmically spaced MC cycles in the interval $[10^3, 10^5]$.

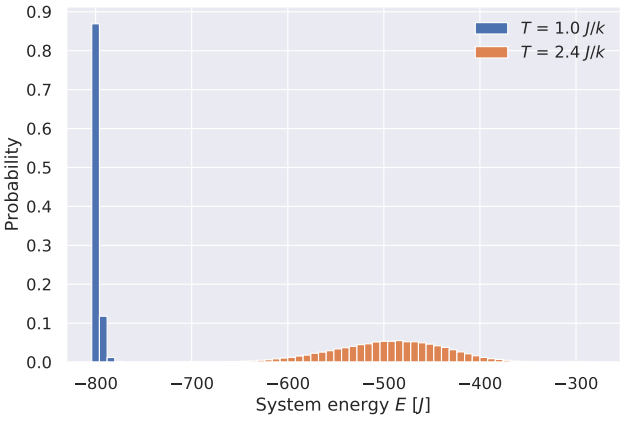

Figure 5. Histogram showing the probability of calculating possible system energies with $T = 1.0J/k$ and $T = 2.4J/k$. The height of bars sum up to 1 for both colors.

$a/L + b$. The slope and intercept were found to be $a = 0.8 \pm 0.7$ and $b = 2.27 \pm 0.01$, respectively.

The linear regression in Figure 10 was repeated with critical temperatures from the maxima of the susceptibilities in Figure 9. The intercept was then found to be $b = 2.2 \pm 0.3$.

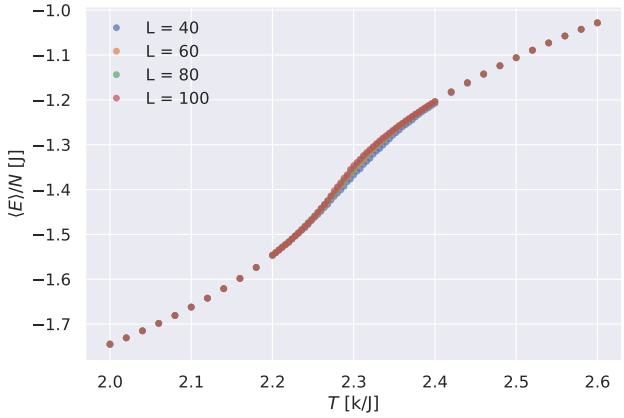

Figure 6. Expectation value of the energy E per spin in the system for lattices of length $L = 40$, $L = 60$, $L = 80$ and $L = 100$ as a function of temperature T.

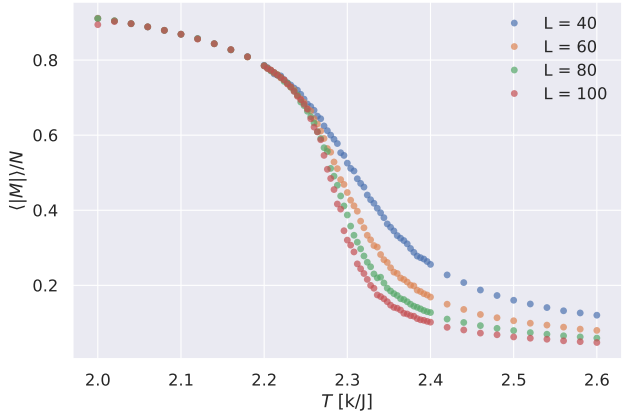

Figure 7. Expectation value of the absolute magnetization $|M|$ per spin in the system for lattices of length $L = 40$, $L = 60$, $L = 80$ and $L = 100$ as a function of temperature T.

V. DISCUSSION

To test the reliability of the algorithm we calculated the expectation values of the mean energy E, mean magnetization $|M|$, heat capacity C_v and magnetic susceptibility χ for a 2×2 lattice and compared these with the analytical values (Tables II and III). The relative errors of the heat capacity C_v and susceptibility χ are quite large, of order 10^{-1} for 10^3 Monte Carlo cycles. However for more than 10^6 MC cycles the algorithm reproduces the analytical values to a good accuracy, with for example the mean energy having a relative error of size order 10^{-5}.

We also made a visualization of the final spin configurations after applying varied numbers of MC cylces, for temperatures both below and above the critical temperature (Figure 1). We initialized the spin configuration to be random, and observed that the spin configurations

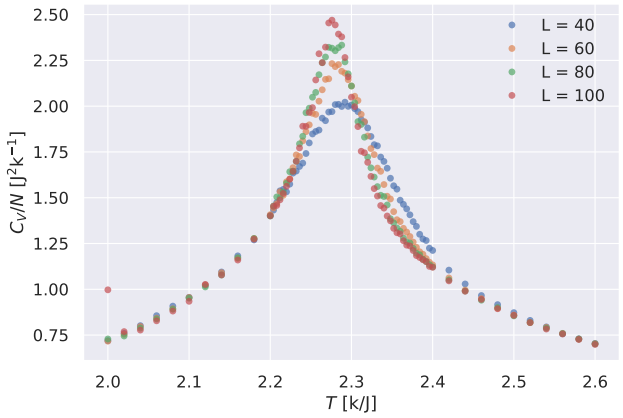

Figure 8. Heat capacity C_V per spin in the system for lattices of length $L = 40$, $L = 60$, $L = 80$ and $L = 100$ as a function of temperature T.

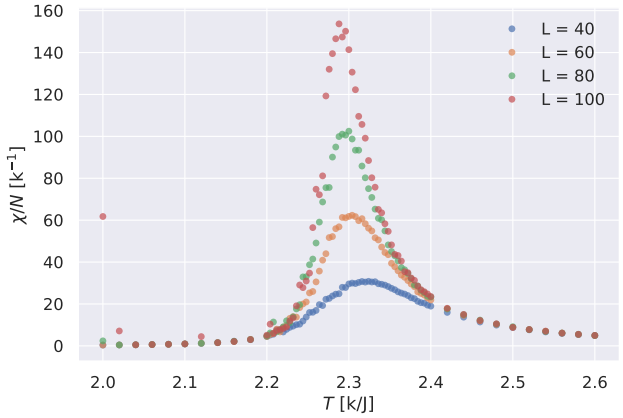

Figure 9. Magnetization χ per spin in the system for lattices of length $L = 40$, $L = 60$, $L = 80$ and $L = 100$ as a function of temperature T.

seem to evolve as expected after some MC cycles; below the critical temperature the spins aligns and there is a net magnetization, as expected for ferromagnetic materials. Above the critical temperature we observe that the spin configuration seems more random as the macroscopic ordering disappears. This is also as expected.

Figures 2 to 4 provide a good picture of how long it takes before a system reaches its most likely state. In all cases (mean energy/magnetization and acceptance rate) we see that regardless of how the initial spin state of the system, the random and aligned initializations both converge towards the same values.

For the low temperature cases ($T = 1.0\ J/k < T_C$), the burn-in time/equilibrium time is nearly non-existent when the system starts in an aligned state. This is due to the system being in a ferromagnetic phase with small thermal agitations, and thus the values of $\langle E \rangle$, $\langle |M| \rangle$ and the acceptance rate stay close to constant. The near-zero

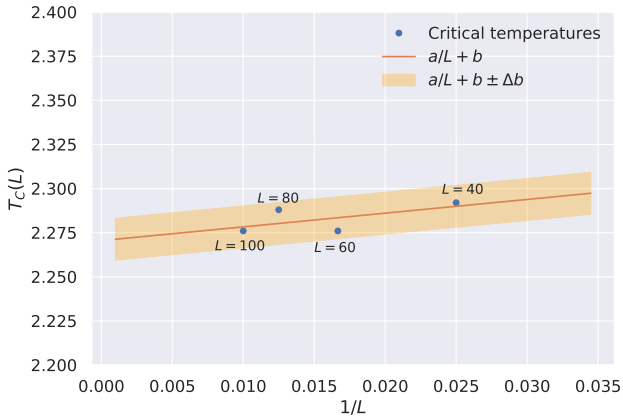

Figure 10. Critical temperatures as the maxima of the heat capacities in Figure 8 as a function of lattice size L with linear regression $a/L + b$. The slope and intercept were found to be $a = 0.8 \pm 0.7$ and $b = 2.27 \pm 0.01$, respectively.

acceptance rate means that it's very hard to unalign any of the spins.

Although the difference in expectation values calculated using random and aligned initializations decrease over time, the difference is considerable when calculating with few ($c = 100$) Monte Carlo cycles, with the deviation for all expectation values being above 10% . By inspection, we see that around 90% of this difference is gone when increasing the number of MC cycles to $c = 10^5$. If we plan to make a calculation with 10^6 MC cycles, the contributions to the expectation values before cycle number 10^5 are generally unreliable, and this motivates the inclusion of a cut-off fraction of 0.1. This means that we discard the first 10 % of MC cycles when calculating expectation values, no matter the total number of MC cycles chosen.

For higher temperatures ($T = 2.4\ J/k > T_C$), the differences between expectation values are less dramatic for the aligned and random initialization. The paramagnetic phase leads to the system accepting more thermal agitations, thus allowing for a greatly increased number of accessible energy states. There is then a reduced probability of the system being in the lowest energy state, so the advantages of choosing an aligned initial state diminishes.

One shortcoming of Figure 3 is that it implies that the net magnetization per spin converges to a value $\langle |M| \rangle / N \approx 0.45$ for $T = 2.4\ J/k$. This temperature is above the critical temperature T_C, so we should in reality expect $\langle |M| \rangle / N \to 0$. The explanation is the finite (and small) size of L used to make this plot ($L = 20$). As Figure 2 shows, the magnetization falls towards zero as L grows for $T = 2.4\ J/k$.

Figure 5 shows how the number of accessible energy states explodes for higher temperatures. Computing the variance of the sampled energies gives $\sigma_E^2(T = 1.0\ J/k) = 9.324\ J^2$ and $\sigma_E^2(T = 1.0\ J/k) = 3295\ J^2$, which illus-

trates how much broader the energy probability $P(E)$ becomes for higher temperatures.

There is a point to be made about the necessity of considering burn-in time. This effect stems from the fact that we can't perform infinitely many MC cycles, and consequently that we can't perfectly reconstruct the probability density $P(E)$ (made possible due to the ergodicity of the system). With a limited number of MC cycles available, we can only approximate the true probability density $P(E)$ and hence the actual value of $\langle E \rangle$. In addition, our calculated distribution $P(E)$ will be susceptible to changes in initial spin configurations. However, this is still much preferable to calculating $\langle E \rangle$ analytically, as we have argued that this quickly becomes impossible for larger systems.

In Figure 7 we see that as the temperature of the system increases, the absolute magnetization drops towards zero, indicating an increasing randomness in the configuration. This causes a higher energy of the system as an increasing number of neighboring spins are oppositely aligned, as illustrated in Figure 6. This increase in energy originates from the thermal agitations increasing with the temperature.

In Figure 8 we see that the heat capacity has a peak between $T = 2.2$ and $T = 2.3$ for all the lattice sizes, indicating a phase transition. This can also be seen in the peak of the susceptibility in Figure 9. Note that the temperatures of the peaks in susceptibility are slightly different from those of heat capacity.

The linear regression displayed in Figure 10 shows that all the data points are within one standard deviation of the intercept b from the linear relation we expected from Eq. (10). The numerical approximation of the critical temperature of the infinitely large lattice is then

$$T_C(L = \infty) \approx b = (2.27 \pm 0.01)\ J/k,$$

which is in agreement with Onsager's analytical result $T_C \approx 2.269\ J/k$.

We see that the result obtained with the critical temperatures taken from the peaks in the susceptibility χ also agrees with Onsager's analytical result, but with a higher uncertainty. This might be caused by the discontinuity in the absolute magnetization $|M|$ which is used to calculate χ. The heat capacity is on the other hand dependent on the energy, which is continuous around the critical temperature as can be seen in Figure 6. This gives a smoother curve around the critical temperature for the heat capacity, which might be the cause of the better estimate of $T_C(L = \infty)$.

VI. CONCLUSION

We have studied the Ising model for simulating phase transitions using the Metropolis Monte Carlo algorithm with periodic boundary conditions. Thermodynamical quantities for the 2×2 system were calculated and compared to the analytical values, with mean energy and absolute magnetization having a relative error of the order 10^{-5} for 10^{-6}. For the algorithm to match the analytical values to a satisfying accuracy, about 10^6 Monte Carlo cycles were needed. The lattice were increased in size and the expectation values were studied for an increasing amount of MC cycles to find the equilibrium time for different temperatures and initial configurations, which were estimated to be around 10^5 cycles. By using the peak of the heat capacity against temperature for different lattice sizes we used linear regression to estimate the critical temperature for the infinitely large lattice to be $T_C = (2.27 \pm 0.01)\ J/k$, in accordance with Onsager's analytical value of $T_C \approx 2.269\ J/k$.

[1] Hjort-Jensen, M. *Computational Physics, Lecture notes.* 2015, pp. 430–432.
[2] Onsager, L. Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition. *Phys. Rev. 65* (Feb 1944), 117–149.

Appendix A: Metropolis algorithm