Ising Model

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(Dated: August 1, 2023)

The two-dimensional Ising model is used to study the phase transition of ferromagnets. To simulate the model, we use a parallelized version of the Metropolis-Hastings algorithm. First, we calculate the analytical solution of a model with a square 2×2 lattice and use the analytical results to verify our implementation of the model. We found that for a 20×20 lattice, the model needs approximately 10^5 Monte Carlo cycles to reach equilibrium. We estimate the probability distribution of the expected energy per spin and found that the variance for the temperature $T = 1\, J/k_B$ was of order 10^3 smaller than for the temperature $T = 2.4 J/k_B$. When using OpenMP to parallelize our code we made it run approximately 4 times faster using 8 threads. Lastly, we simulate the model for four different lattice sizes to study the phase transition. We use these simulated values to find an estimate of the critical temperature for an infinite Ising model. We find this to be ≈ 2.269282 J/k_B, which is close to the analytical result of $\frac{1}{\ln(1+\sqrt{2})} \approx 2.269185\ J/k_B$.

I. INTRODUCTION

The Ising model uses simple rules to demonstrate complex behaviour. It utilizes a square lattice with quantized spins to model change in ferromagnetic materials for different temperatures. We will use the Ising model to study the *phase transition* of a two-dimensional system. This is a transition where the ferromagnet changes between a magnetized phase and a phase with no net magnetization. In particular, we are interested in numerically approximating the *critical temperature* where the phase transition occurs.

The model was invented and suggested by *Wilhelm Lenz* in 1920 and later named after his student *Ernst Ising*. [1] It took 24 years before someone would solve the infinite two-dimensional Ising model analytically. That someone was Nobel laureate *Lars Onsager*. He found the analytical solution and could in 1944 represent the critical temperature for the infinite Ising model. [2] We will use Onsager's analytical results to analyze the accuracy of our estimate of the critical temperature.

The number of possible states of the Ising model grows exponentially as we increase the lattice size. Thus, it quickly becomes impractical or even impossible to calculate the probability distribution directly. To solve this problem we will use *Markov chain Monte Carlo* methods. We specifically use the *Metropolis-Hasting* algorithm to sample from the probability distribution. Despite the computationally effective model, it can be challenging to run the algorithm in an acceptable amount of time. For that reason, we utilize parallelization as a technique to efficiently run our simulations. In that fashion, we can study the phase transition and estimate the critical temperature in a reasonable amount of time.

In section II we present the theory necessary to understand the model, and the methods used to simulate it. In section III the relevant figures are presented. Then we move on to discussing the results in section IV. Finally, we summarize our findings in section V.

II. THEORY AND METHODS

A. the Ising Model

The Ising model uses a square lattice of lenght L to describe the state of ferromagnets. Each element in the lattice represents a spin s_i which can exist in two possible states: $s_i = 1$ and $s_i = -1$. In total the lattice will contain $N = L^2$ such spins. The *spin configuration* is the spin state of the entire system and is written as

$$\mathbf{s} = (s_1, s_2, \ldots, s_N). \tag{1}$$

For the Ising model to be able to study phenomena such as phase transitions we need to calculate the energy of the model. The total energy is given by the *Hamiltonian*

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l. \tag{2}$$

Here, $\langle kl \rangle$ means that the sum goes over all neighbouring pairs of spins, without double counting and J is the coupling constant. We see that the total energy is determined exclusively by the interaction between neighbouring spin pairs. In our model we will use *periodic boundary conditions*, i.e. every spin will interact with exactly four neighbouring spins. J is a constant that sets the energy associated with the interaction between the spins.

The total magnetization of the system is given by how many of the spins align in the same direction. It is found by summing over all the spins in the system:

$$M(\mathbf{s}) = \sum_{i}^{N} s_i. \tag{3}$$

To make it easier to compare results for different lattice sizes, we will mostly use the *energy per spin* (ϵ) and *magnetization per spin* (m) which are defined as:

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N}, \quad \text{and} \quad m(\mathbf{s}) = \frac{M(\mathbf{s})}{N}.$$

B. Statistical Mechanics

The probability of a spin configuration s for a temperature T is given by the *Boltzmann distribution*

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})}, \tag{4}$$

where $\beta = 1/(k_B T)$ is the "inverse temperature". k_B is the *Boltzmann contant*. The dimensionless normalization constant Z is the *partition function*, it is given by

$$Z = \sum_{\text{all } possible \ \mathbf{s}} e^{-\beta E(\mathbf{s})}. \tag{5}$$

When studying the Ising model for larger lattice sizes, the amount of unique spin configurations quickly become too large to practically handle. Therefore we avoid calculating the Boltzmann distribution directly, and rather use statistical methods to sample from the distribution.

The most fundamental properties of the model is the total energy and magnetization. Using the Boltzmann distribution we can calculate the expected values $\langle E \rangle$ and $\langle |M| \rangle$ as

$$\langle E \rangle = \sum_{\text{all } \mathbf{s}} E(\mathbf{s}) p(\mathbf{s}; T),$$
$$\langle |M| \rangle = \sum_{\text{all } \mathbf{s}} |M(\mathbf{s})| p(\mathbf{s}; T).$$

In a similar fashion we can define the expectance values $\langle E^2 \rangle$ and $\langle M^2 \rangle$.

Using these four values we can study two other main properties of the Ising model, namely the *specific heat capacity* C_V and the *magnetic susceptibility* χ. The specific heat capacity is defined as

$$C_V = \frac{1}{N} \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{6}$$

It tells us how much heat we have to introduce to the system to change its temperature. The magnetic susceptibility χ, expresses the degree of magnetization when introducing a material to a magnetic field. It is given by

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

The two properties C_V and χ will be used to study the phase transitions.

C. Markov Chain Monte Carlo Methods and the Metropolis-Hasting algorithm

We will use Markov chain Monte Carlo (MCMC) methods to sample from the Boltzmann distribution. A *Markov chain* describes a random sequence where the probability of the next state only depends on the previous state. The MCMC method produces a Markov Chain of sample steps whose stationary distribution is a given probability distribution. In our case we will generate a set of samples $\mathbf{s}_i$ from the Boltzmann distribution.

After generating a candidate $\mathbf{s}_i$ we need to implement an acceptance rule that decides if the candidate should be accepted or rejected. For the acceptance rule to distribute the samples according to the analytical Boltzmann distribution, the acceptance rule has to have two important properties: *ergodicity* and *detailed balance*. Ergodicity means that it is possible to reach all states from an arbitrary starting point with finitely many steps. Detailed balance implies that every step is reversible with equal probability, i.e. moving from state $\mathbf{s}_i$ to $\mathbf{s}'$ should have the same probability as moving from state $\mathbf{s}'$ to $\mathbf{s}_i$.

Using the MCMC method called the Metropolis-Hasting algorithm, we are secured both ergodicity and detailed balance. The algorithm calculates the acceptance probability as

$$\begin{aligned} A(\mathbf{s}_i \to \mathbf{s}') &= \min \left\{ 1, \frac{p(\mathbf{s}')}{p(\mathbf{s}_i)} \right\} \\ &= \min \left\{ 1, e^{-\beta(E(\mathbf{s}') - E(\mathbf{s}_i))} \right\}. \end{aligned}$$

We have not included the probabilities $T(\mathbf{s}' \to \mathbf{s}_i)$ and $T(\mathbf{s}_i \to \mathbf{s}')$. Since they are equal in the Ising model, they would cancel each other. Therefore, we are really using a special case of the Metropolis-Hasting algorithm simply called the *Metropolis* algorithm. Notice that we also do not have to calculate the partition function as it cancels out as well. We end up with an acceptance rule that always accepts a state that have a higher probability and rarely accepts states with a lower probability.

D. The Phase Transition

The phase transition phenomena occurs when there is a change from an amount of magnetization to zero magnetization and vice versa. For the two-dimensional Ising model this transition happens when we reach a critical temperature T_c. For T in a close proximity to T_c, the mean magnetization, specific heat capacity and susceptibility will behave as

$$\langle |m| \rangle \propto [T - T_c(L = \infty)]^{\beta}, \tag{8}$$
$$C_V \propto [T - T_c(L = \infty)]^{-\alpha}, \tag{9}$$
$$\chi \propto [T - T_c(L = \infty)]^{-\gamma}, \tag{10}$$

with critical exponents $\alpha = 0$, $\beta = 1/8$ and $\gamma = 7/4$. We observe from equations 9 and 10 that when $T \to T_C$, both C_V and χ diverge. Likewise, the *correlation length* ξ will also diverge as $T \to T_c$. It will behave as

$$\xi \propto [T - T_c(L = \infty)]^{-\nu},$$

with critical exponent $\nu = 1$. We will try to approximate the critical temperature with finite lattices. Looking at the correlation length for $\xi = L$ we get the equation

$$T_c(L = \infty) = T_c(L) - aL^{-1}, \tag{11}$$

where a is a constant. We will use this scaling relation to calculate an estimate to the critical temperature of an infinite, two-dimensional Ising model. $T_c(L = \infty)$ was, as mentioned, found analytically by Lars Onsager. He derived the following equation in 1944:

$$T_c(L = \infty) = \frac{2}{\ln\left(1 + \sqrt{2}\right)} J/k_B \approx 2.269 J/k_B. \tag{12}$$

E. Implementation

The implementation, which can be found here, is coded in C++. Here is a short summary of how the code works:

i) The Ising model is implemented through the use of classes and class methods.

ii) The class can either be initialised with a customized two-dimensional matrix or a random matrix. Our matrix represents the lattice. Here we also set the temperature.

iii) The approximation works by looping over the metropolis algorithm a given number of times. It finds a random index number in our matrix $\mathbf{s}$, and calculates the ΔE that would occur if we were to flip the spin on that index.

iv) We then sample a random number $x \sim U(0, 1)$, and if $x \leq e^{-\Delta E/T}$, we accept the new state, flip the spin and calculate our new energy and magnetism using $E_{new} = E_{old} + \Delta E$ and $M_{new} = M_{old} + 2s_{ij}$. If the new state is not accepted, we move on with our current state.

v) For every loop of the metropolis algorithm, we update the expected values by adding the current values of E and M, and at the very end, we divide by the number of cycles used.

The reason we implement ΔE is because we notice that the energy function is being called upon for every newly accepted state in the metropolis method. For our two dimensional problem, we can use the result of *flipping a single spin*:

$$\Delta E = E_{\text{after}} - E_{\text{before}}. \tag{13}$$

If we look closer at the possible values ΔE can take, we notice that it can only have 5 different states. This is because there are 5 different scenarios of values that the neighbouring spins can have, which are:

4 with opposite spins.
4 with identical spins.
3 with opposite spins and 1 with identical spin.
3 with identical spins and 1 with opposite spin.
2 with opposite spins and 2 with identical spin.

Below is an illustration of these scenarios:

$$\Delta E_1 : \begin{matrix} & \uparrow & \\ \uparrow & \uparrow & \uparrow, \\ & \uparrow & \end{matrix} \longrightarrow , \begin{matrix} & \uparrow & \\ \uparrow & \downarrow & \uparrow, \\ & \uparrow & \end{matrix} \quad \Delta E = 8J, \tag{14}$$

$$\Delta E_2 : \begin{matrix} & \uparrow & \\ \uparrow & \uparrow & \downarrow, \\ & \uparrow & \end{matrix} \longrightarrow , \begin{matrix} & \uparrow & \\ \uparrow & \downarrow & \downarrow, \\ & \uparrow & \end{matrix} \quad \Delta E = 4J, \tag{15}$$

$$\Delta E_3 : \downarrow \begin{matrix} & \uparrow & \\ \uparrow & \downarrow, \\ & \uparrow & \end{matrix} \longrightarrow , \downarrow \begin{matrix} & \uparrow & \\ \downarrow & \downarrow, \\ & \uparrow & \end{matrix} \quad \Delta E = 0J, \tag{16}$$

$$\Delta E_4 : \uparrow \begin{matrix} & \downarrow & \\ \downarrow & \downarrow, \\ & \uparrow & \end{matrix} \longrightarrow , \uparrow \begin{matrix} & \uparrow & \\ \uparrow & \downarrow, \\ & \uparrow & \end{matrix} \quad \Delta E = -4J, \tag{17}$$

$$\Delta E_5 : \uparrow \begin{matrix} & \downarrow & \\ \downarrow & \uparrow, \\ & \uparrow & \end{matrix} \longrightarrow , \uparrow \begin{matrix} & \uparrow & \\ \uparrow & \uparrow, \\ & \uparrow & \end{matrix} \quad \Delta E = -8J, \tag{18}$$

These different states will represent all the different types of states and their corresponding magnetization. Thus, we can replace calculating the energy using the Hamiltonian from equation 2 with the relation:

$$E_{\text{after}} = \Delta E + E_{\text{before}}. \tag{19}$$

We should also mention the periodic boundary conditions and the custom implementation. With such conditions, each state can at all times have four neighbouring states. The way we tackle this when calculating the total energy in our code is by first considering all the inner states. Then, by indexing, we consider the boundaries and their neighbours and periodic neighbours.

F. Burn-in time

When using the Metropolis-Hastings algorithm, we should be wary of the so called *burn-in time* (or the *equilibrium time*). The reason why we consider the burn-in time is because the samples in MCMC methods are *correlated*, i.e. the samples are not independent:

$$p(x_{i+1}|x_i) \neq p(x_{i+1}). \tag{20}$$

To avoid inaccurate draws, we find where the relative error stabilizes at a small value. Here the system reaches an *equilibrium*. The equilibrium is important because when it is reached, the data points from then on are more accurate. We refer to the period between the first MC cycle and the equilibrium as the burn-in time.

We will estimate the burn-in time for different initial states and temperatures. We want to show that for various configurations both ϵ and $\langle|m|\rangle$ reach an equilibrium after a certain number of cycles. We want to be conservative since the burn-in time for different configurations are unknown. For instance, the size of the lattice might change the burn in time. When the burn-in time is found we get rid of the data gathered up until the equilibrium point is reached. This will make the results more accurate in case the start is at an improbable state.

G. Analyzing the 2×2 Case

Now that the theory is in place, it is time to study an example. We will consider an Ising Model with a 2×2 lattice and periodic boundary conditions. A 2×2 lattice will have a total of $2^4 = 16$ possible states. Two examples of possible states are:

$$\mathbf{s}_1 = \begin{matrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{matrix}, \quad \mathbf{s}_2 = \begin{matrix}\uparrow & \downarrow \\ \downarrow & \downarrow\end{matrix}. \tag{21}$$

We are interested in calculating four key properties of the lattices: the number of spins in the $+1$ state (represented by $(\uparrow)$), the total energy, magnetization and the degeneracy of the system. In equation 21 we see that $\mathbf{s}_1$ have four spins in the $+1$ state, with a total energy of $-8J$ and a total magnetization of 4. $\mathbf{s}_2$ have three spins in the $+1$ state, with a total energy of $0J$ and a total magnetization of 2. in table I there is an overview of all the possible configurations of the 2×2 Ising Model.

Spins Up	Energy	Magnetization	Degeneracy
4	-8J	4	1
3	0	2	4
2	0	0	4
2	8J	0	2
1	0	-2	4
0	-8J	-4	1

TABLE I. The total energy, total magnetization and degeneracy of all the possible number of spins in the $+1$ position for a 2×2 lattice.

Using the equations from the previous sections we can derive the following equations which are given in appendix A

$$Z = 12 + 4\cosh(8\beta J), \tag{22}$$

$$\langle E \rangle = -8J\frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3}, \tag{23}$$

$$\langle E^2 \rangle = 64J^2\frac{\cosh(8\beta J)}{\cosh(8\beta J) + 3}, \tag{24}$$

$$\langle |M| \rangle = \frac{2e^{8\beta J} + 4}{\cosh(8\beta J) + 3}, \tag{25}$$

$$\langle M^2 \rangle = 8\frac{e^{8\beta J} + 1}{\cosh(8\beta J) + 3}, \tag{26}$$

$$C_V = \frac{1}{N}\frac{1}{k_B T^2}\frac{64J^2}{\cosh(8\beta J) + 3} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3}\right), \tag{27}$$

$$\chi = \frac{1}{N}\frac{1}{k_B T}\frac{4}{\cosh(8\beta J) + 3} \left(2e^{8\beta J} + 2 - \frac{e^{16\beta J} + 4e^{8\beta J} + 4}{\cosh(8\beta J) + 3}\right). \tag{28}$$

These analytical results will serve as a test for our numerical results.

H. Parallelization and RNG

Drawing several samples and calculating the Metropolis-algorithm with only a single thread for all the operations is not efficient. Therefore we chose to parallelize our code with *OpenMP*, by dividing the simulation of multiple Ising models between the different threads. Using this method, we got around half the best possible speedup using OpenMP, which is $\frac{\text{total runtime}}{\text{number of threads}}$. For us to be able to use OpenMP smoothly in our code, we also had to make sure it was thread safe.

Random numbers serve as the backbone of the MC-simulations. It is, however, not possible for computers to generate true random numbers. Therefore we generate *pseudorandom* numbers that mimics the properties of true random numbers.

In our code we implemented our own method for extracting random numbers. The rand() function in C++ has a reputation of giving low quality random sequences. In addition, it is difficult to use for parallel programs, since it is not thread safe. Our own methods give us a thread safe and reliable way to generate different types of random numbers. In our implementation we use the *Mersenne Twister* (MT19937) to extract our random sequences. To make the RNG implementation thread safe and replicable, we give each thread running in our program a unique seed.

III. FIGURES

Table II shows the numerical values we get when simulating the 2×2 case for different amount of cycles, compared to the analytical results. Figure 1 shows how the expected energy and magnetization values change over temperature and shows that we get accurate results over the whole temperature spectrum. Figure 2 shows how a 20×20 system reaches equilibrium for two different temperatures. Next, figure 3 shows the probability of different energies per spin for the same two different temperatures. The figures 4 and 5 compares estimated values for four different lattice sizes over a range of temperature $T \in [2.1, 2.4]$. Finally, figure 6 shows a linear regression of the maximum values of C_V and χ from the figure 5. As a bonus we have included figure 7, which visualizes the spin configuration of two systems as they undergo a phase transition.

Cycles	$\langle$E$\rangle$ [J]	$\langle$M$\rangle$	χ [1/J]	C_V [k$_B$]
10^2	-8	4	0	0
10^3	-7.9760	3.9880	0.005984	0.047856
10^4	-7.9832	-1.1894	0.005090	0.033529
10^5	-7.9840	-0.0843	0.003843	0.031776
10^6	-7.9838	0.0297	0.004021	0.032334
Analytical	-7.9839	0	0.004010	0.032146

TABLE II. Simulated values of expected energy, expected magnetization, magnetic susceptibility and specific heat capacity.

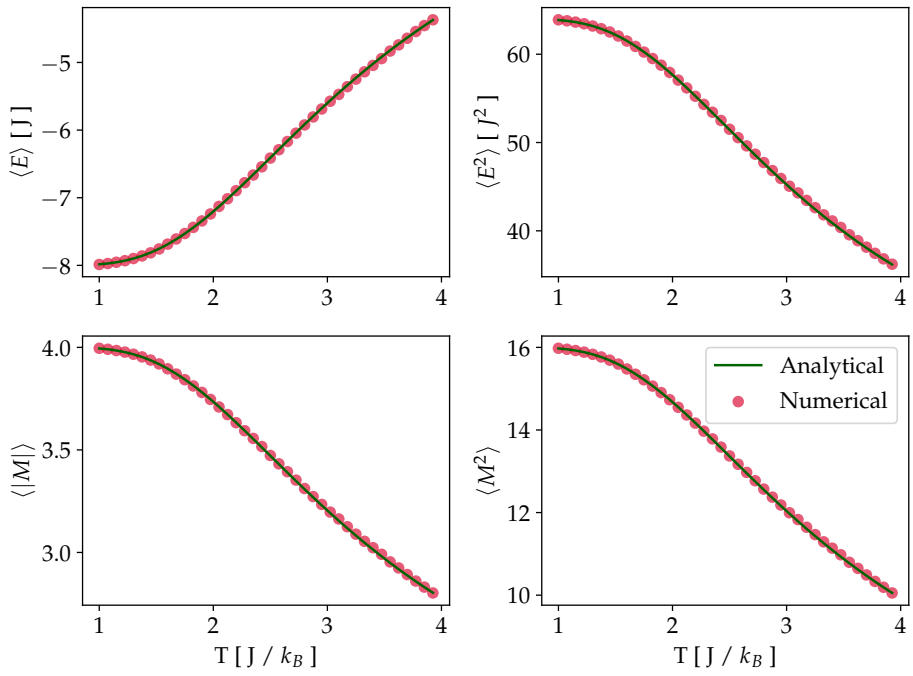

FIG. 1. A comparison between the numerical value (shown as red dots) and the analytical value of $\langle E \rangle$, $\langle E^2 \rangle$, $\langle |M| \rangle$ and $\langle M^2 \rangle$. The answers correlate to the 2×2 case studied in section II G. The analytical answers are calculated using equations 23 - 26. The numerical solutions are calculated using 100 000 MC cycles and a change in temperature of 0.075 J/k_B between each simulation. All plots share the same x-axis of Temperature between 1 and 4 J/k_B.

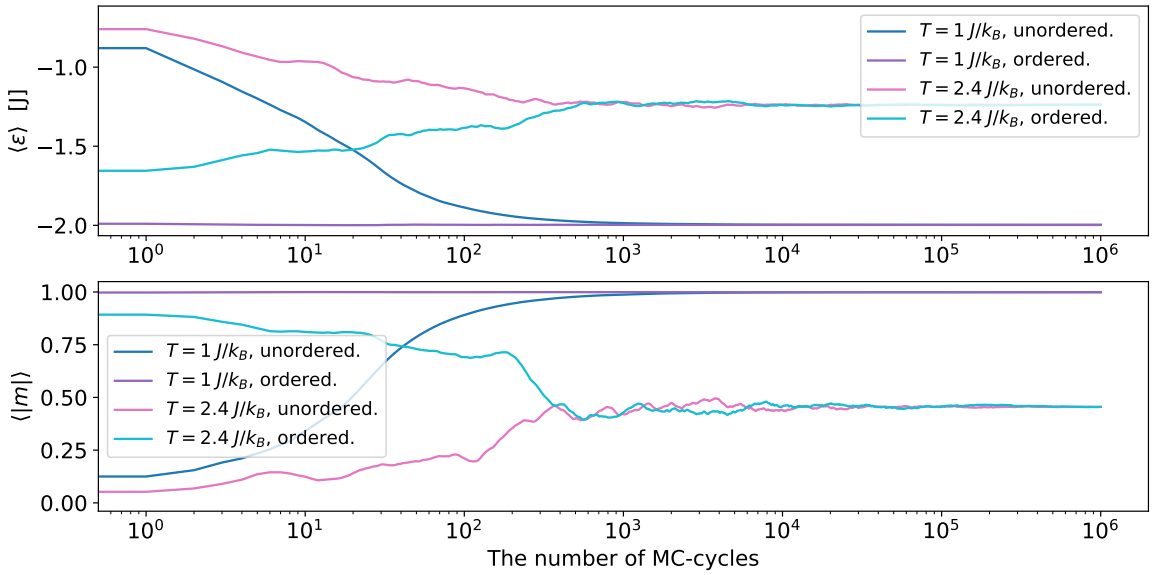

FIG. 2. The expectation values of energy per spin $\langle \epsilon \rangle$ and magnetization per spin $\langle |m| \rangle$ for an Ising model with a 20×20 lattice. The calculations are done for two different temperatures $T = 1\, J/k_B$ and $T = 2.4\, J/k_B$ as well as in both an ordered and unordered state. The orderer state represents an antiferromagnetic ordering (like a checkerboard) while the unordered state means that every spin in the initial lattice were chosen as (+1) or (-1) with equal probability. The simulation was done using 10^6 MC cycles. The x-axis of both plots are logarithmic.

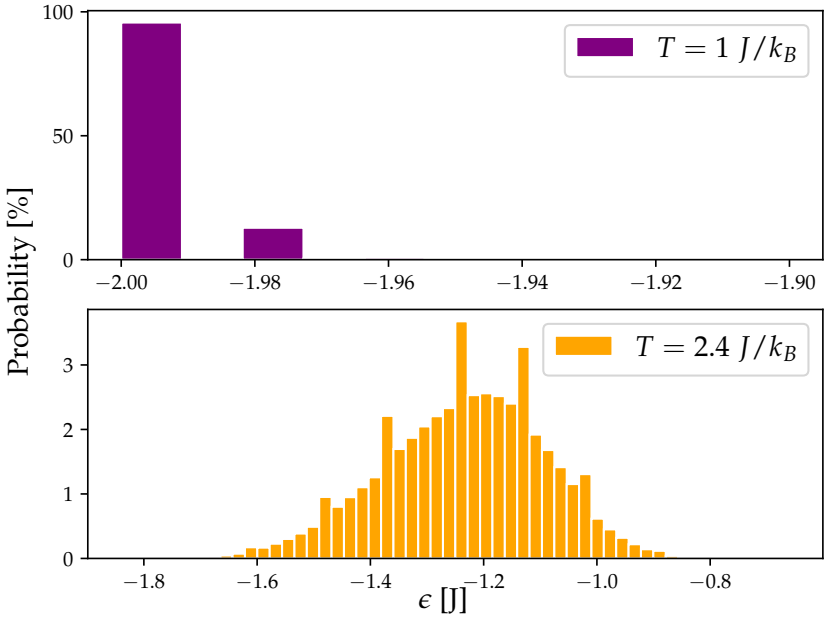

FIG. 3. A histogram of different energies per spin ϵ for two different temperatures T = 1 J/k_B and $T = 2.4 J/k_B$. The size of the lattice is 20 and the results are generated using 10^6 MC cycles with a burn-in time of 10^5. There are 11 bins used in the histogram for $T = 1\ J/k_B$ and 54 bins used for the other histogram. Every spin in the initial lattice was chosen at random.

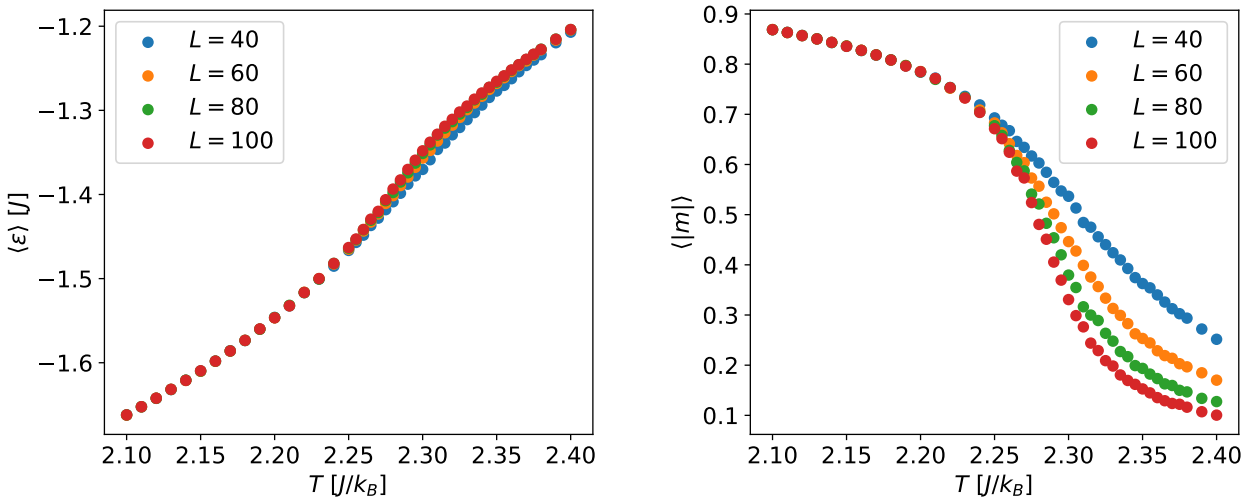

FIG. 4. The expected energy and magnetization per spin plotted against the temperature $T \in [2.1, 2.4]\ J/k_B$, for four different lattice sizes $L = 40$, 60, 80 and 100. We have used 10^6 MC cycles with a burn-in time of 10^5 to generate the results. The step size used for the temperature is 0.01 J/k_B for $T \in [2.1, 2.25] \bigcup [2.39, 2.4]\ J/k_B$ and 0.005 J/k_B for $T \in [2.255, 2.38]\ J/k_B$.

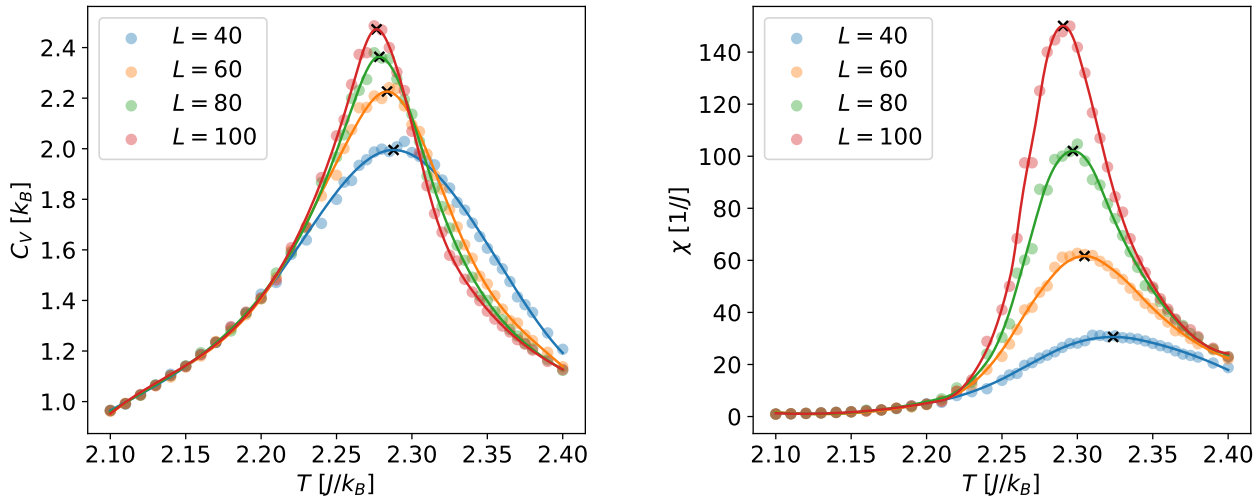

FIG. 5. The specific heat capacity C_V and susceptibility χ plotted against the temperature $T \in [2.1, 2.4]\ J/k_B$, for four different lattice sizes $L = 40$, 60, 80 and 100. We have used 10^6 MC cycles with a burn-in time of 10^5 to generate the results. The step size used for the temperature is 0.01 J/k_B for $T \in [2.1, 2.25] \bigcup [2.39, 2.4]\ J/k_B$ and 0.005 J/k_B for $T \in [2.255, 2.38]\ J/k_B$. The values are normalized to the number of spins in the lattice.

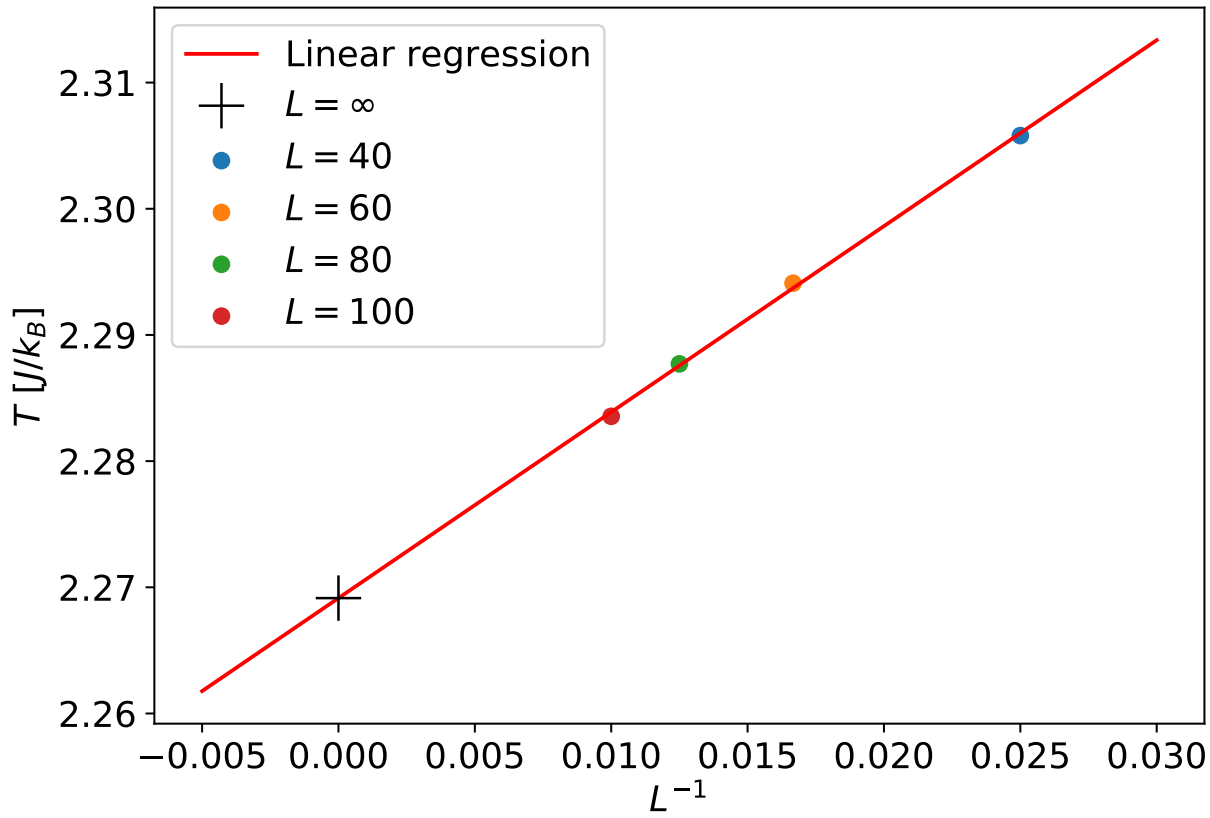

FIG. 6. The average temperature of the maximum specific heat capacity and susceptibility plotted against the inverse of the lattice size. The linear regression is done using the least squares method. The approximated value when $L = \infty$ is shown as a black cross.

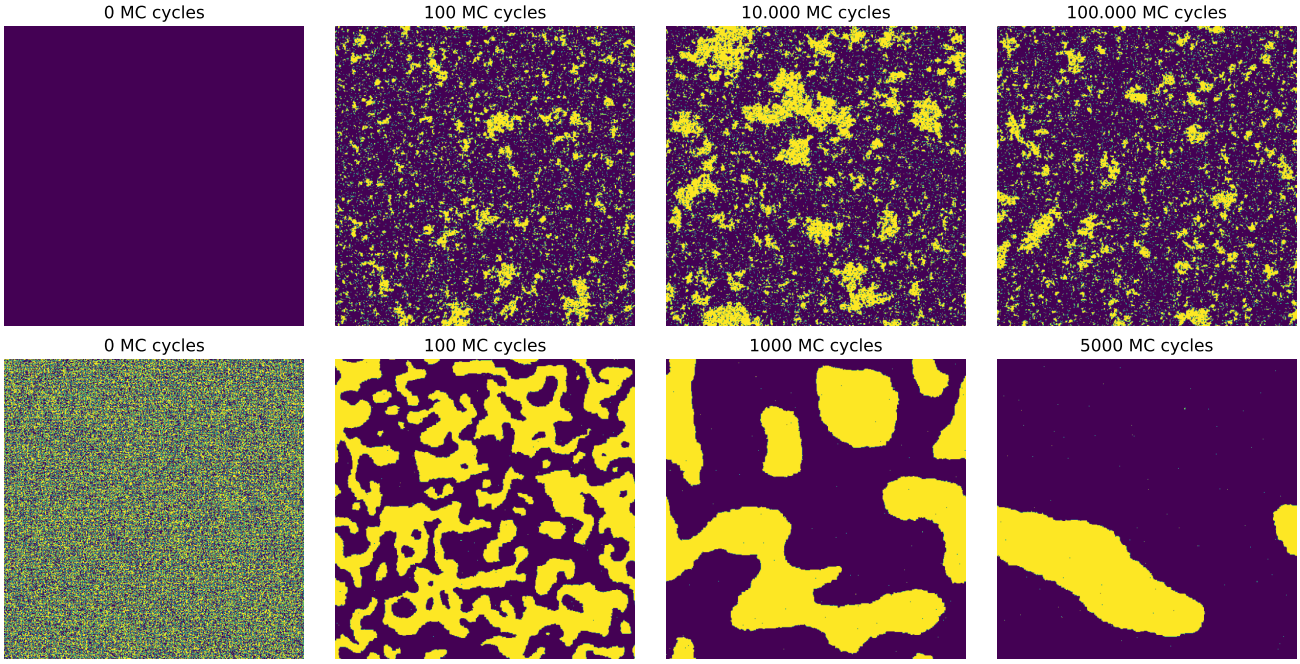

FIG. 7. A satisfying figure that shows how the spin configuration changes as a system undergoes a phase transition. The top row illustrates a ferromagnetic initial state with a temperature of 2.269 J/k_B (close to the critical temperature), while the bottom row shows a random initial state with a temperature of 1 J/k_B. The blue color represents a spin up (+1) while the yellow color represents a spin down (-1). The results are calculated using a 500×500 lattice.

IV. RESULTS AND DISCUSSION

A. Error estimation and burn-in time:

Table II and figure 1 compares our numerical methods against the analytical results for the 2×2 lattice studied in section II G. This is done to validate our algorithm. Figure 1 shows the analytical and numerical values of expected energy and magnetization against temperatures between 1 J/k_B and 4 J/k_B. The results shows that our numerical results correspond well to the analytical values.

Table II shows the simulated values of $\langle E \rangle, \langle M \rangle, C_v, \chi$, against their respective analytical solutions for cycles ranging from $10^2 - 10^6$. We observe that the simulated values get very close to the analytical solution for 10^6 cycles.

In figure 2 we study the burn-in time for different initial states and temperatures. To make it more relevant for studying the phase transition, we use a 20×20 lattice and look at temperatures both above and below the critical temperature found by Lars Onsager. In figure 2 we show the numerical value of $\langle \epsilon \rangle$ and $\langle |m| \rangle$ plottet against the number of MC cycles. The temperatures used are 1 J/k_B and 4 J/k_B. For both temperatures we use an ordered and an unordered initial spin matrix. The ordered matrix represents an anti-ferromagnetic ordering where every neighbour of all the spins have the opposite state. The unordered matrix simply chooses spin with equal probability. Together, the two plots in figure 2 gives an estimation of the burn-in time. They show that for our configurations, both $\langle \epsilon \rangle$ and $\langle |m| \rangle$ reach an equilibrium somewhere between 10^4 and 10^5. Therefore it is natural to set the burn-in time to 10^5. This means that we will ignore the first 10^5 MC cycles in future simulations to make our estimations as accurate as possible. We are ideally running for a million MC cycles, possibly more, so ignoring the first 10^5 is not significant.

B. Probability Distribution of ϵ

In figure 3 we see the frequencies of different energy levels per spin ϵ for temperatures $T = 1\, J/k_B$ and $T = 2.4\, J/k_B$ for an unordered 20×20 lattice. The figure shows how ϵ is distributed for both temperatures. It gives us an estimate of the probability distribution of ϵ $p_\epsilon(\epsilon; T)$, which tells us the probability that ϵ is in a given range. In other words, it is a discretized approximation to the Boltzmann distribution. This is most obvious in the case where $T = 2.4\, J/k_B$, since it has a wider range of energy states. When $T = 1\, J/k_B$, we see that almost every energy calculated has the same value. This is because the ferromagnet will want to align all the spins to the (+1) state for lower energies. We can deduce from table I and the Hamiltonian given in equation 2 that an arbitrary lattice with only spins up will have a total energy per spin of -2 J. Furthermore, from table II E we see that flipping a single spin from a ferromagnetic arrangement leads to a large positive change in energy, therefore it is not probable. This is why we only see two bins clearly in the histogram, the energy will be stable at -2 J and only occasionally move to higher energy states with decreasing probability.

Calculating the variance from the two histograms yields:

$$\sigma_1^2 \approx 5.8 \cdot 10^{-5} \quad \text{and} \quad \sigma_2^2 \approx 2 \cdot 10^{-2}.$$

We see that the variance for the temperature $T = 1\, J/k_B$ is much lower than for $T = 2.4\, J/k_B$. This agrees with our understanding of the model and the figure. For higher temperatures there are far more probable energy states for the system, leading to a variance that is of order 10^3 larger for the higher temperature.

This is perhaps best illustrated in figure 2, where we see that for the ordered ferromagnetic state for $T = 1\, J/k_B$ looks like a constant function, while for $T = 2.4\, J/k_B$ there is much more fluctuation. (Keep in mind that we have used a burn-in time of 10^5 when generating the histogram.)

C. Estimating the Critical Temperature

In figure 4 we have plotted the expected energy and magnetization per spin against temperature $T \in [2.1, 2.4]\, J/k_B$. The expected energy increases for higher temperatures in a regular pattern. For the smallest lattice $L = 40$, the pattern appear almost linear, but we see that around the analytical critical temperature 2.269 J/k_B the larger lattices get steeper and steeper. We see a similar pattern in the plot of expected absolute magnetization. We expect $\langle |m| \rangle$ to approach zero at the critical temperature for an infinite lattice. This might be why the graph becomes steeper for larger L, such that for $L = \infty$ we get an infinitely steep curve at the critical temperature and zero after that.[3]

In figure 5 we have plotted the specific heat capacity and susceptibility for 4 different lattice sizes against temperature $T \in [2.1, 2.4]\, J/k_B$. We want to use these plots to find the temperature for each curve and their corresponding maximum value. To estimate the most accurate values, we do regression analysis on these plots using a univariate spline method. Then we find the critical temperature $T_c(L)$ by picking out the temperature corresponding to the maximum point for each of the graphs. Since we have a plot for C_v and χ, we get two critical temperature values for each lattice size. To achieve a higher accuracy, we use the mean value of the two critical temperatures.

To estimate $T_c(L = \infty)$, we plot $T_c(L)$ against L^{-1} for $L = 40$, 60, 80 and 100. We then do linear regression on these points using the least squares method. This gives an estimate of the function given in 11. When $L \to \infty$ we have $L^{-1} \to 0$. Therefore, if we find where the regression line crosses the y-axis, we get our estimate $T_c(L = \infty) \approx$

$2.269282\,J/k_B$. This is close to Lars Onsager's analytical solution of $\frac{2}{\ln(1+\sqrt{2})} \approx 2.269185\,J/k_B$. The results of this is in figure 6.

D. Visualizing Phase Transitions

Our system starts with an initial spin configuration $\mathbf{s}_1$. For each MC cycle we run the Metropolis algorithm and update the spin configuration. After N such cycles, we end up with the following Markov chain of length N:

$$\mathbf{s}_1 \to \mathbf{s}_2 \to \cdots \to \mathbf{s}_N. \tag{29}$$

Another way to view these Markov chains is as spin configurations for different times $t_1, t_2, \ldots, t_N$. This means that we can rewrite the Markov chain from equation 29 as

$$\mathbf{s}(t_1) \to \mathbf{s}(t_2) \to \cdots \to \mathbf{s}(t_N).$$

This allows us to visualize how the spin configurations, and therefore the Ising model, change over time. We do this in figure 7 for two different temperatures and initial spin configurations. The top row shows how a ferromagnet with all spins in the (+1) state, changes to a state of no net magnetization at a temperature close to T_c. The bottom row shows how a random initial spin configuration goes from zero magnetization to a ferromagnetic arrangement at $T = 1\,J/k_B$.

V. CONCLUSION

We have used the two-dimensional Ising model to study the phase transition of ferromagnets. To simulate the model we used a Markov chain Monte Carlo based algorithm called the Metropolis-Hastings algorithm. First, we simulated an Ising model with a 2×2 lattice and found that the numerical values corresponded nicely to the analytical answers. Then we studied a model with a 20×20 lattice and found that a conservative estimate for the burn-in time is 10^5 MC cycles. Both $\langle\epsilon\rangle$ and $\langle|m|\rangle$ reached an equilibrium for temperatures above and below the critical temperature after 10^5 cycles. We then estimated the Boltzmann distribution by making a histogram of different energies per spin ϵ. This enabled us to estimate the distribution without actually calculating it. We found that the variance in the histogram for $T = 1\,J/k_B$ was of order 10^3 smaller than for the temperature $T = 2.4\,J/k_B$. We then calculated the mean energy per spin $\langle\epsilon\rangle$, the mean magnetization per spin $\langle|m|\rangle$, the specific heat capacity C_V and the magnetic susceptibility χ for models with $L = 40$, 60, 80 and 100. For efficiency we parallelized our code using OpenMP. We used the results to estimate the critical temperature of an infinite two-dimensional Ising model. The estimate we got of the critical temperature was $2.269282\ J/k_B$. This is close to Onsager's analytical result of $\approx 2.269185\ J/k_B$.

VI. CODE

The code used to simulate the Ising Model is available at this Github repository.

Appendix A: Analytical

$$\begin{aligned} Z &= \sum_{\text{all possible } \boldsymbol{s}} e^{-\beta E(\boldsymbol{s})} = 2e^{\beta 8J} + 12e^0 + 2e^{-\beta 8J} \\ &= \frac{4e^{\beta 8J} + 4e^{-\beta 8J}}{2} + 12 = 4\cosh(\beta 8J) + 12 \end{aligned} \tag{A1}$$

$$\begin{aligned} \langle E\rangle &= \sum_{\text{all } \boldsymbol{s}} E(\boldsymbol{s})p(\boldsymbol{s};T) = \frac{1}{Z}\sum_{\text{all } \boldsymbol{s}} E(\boldsymbol{s})e^{-\beta E(\boldsymbol{s})} \\ &= -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -8J\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3} \end{aligned} \tag{A2}$$

$$\begin{aligned} \langle E^2\rangle &= \sum_{\text{all } \boldsymbol{s}} (E(\boldsymbol{s}))^2 p(\boldsymbol{s};T) = \frac{1}{Z}\sum_{\text{all s}} (E(s))^2 e^{-\beta E(s)} \\ &= \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} = \frac{1}{Z}64J^2\cosh(8\beta J)\cdot 4 \\ &= 64J^2\frac{\cosh(8\beta J)}{\cosh(8\beta J)+3} \end{aligned} \tag{A3}$$

$$\begin{aligned} \langle M\rangle &= \sum_{\text{all } \boldsymbol{s}} M(\boldsymbol{s})p(\boldsymbol{s};T) = \frac{1}{Z}\sum_{\text{all } \boldsymbol{s}} M(\boldsymbol{s})e^{-\beta E(\boldsymbol{s})} \\ &= \frac{1}{Z}(-4e^{8\beta J} - 8e^0 + 8e^0 + 4e^{8\beta J}) = 0 \end{aligned} \tag{A4}$$

$$\begin{aligned} \langle |M|\rangle &= \sum_{\text{all } \boldsymbol{s}} |M(\boldsymbol{s})|p(\boldsymbol{s};T) = \frac{1}{Z}\sum_{\text{all } \boldsymbol{s}} |M(\boldsymbol{s})|e^{-\beta E(\boldsymbol{s})} \\ &= \frac{1}{Z}(4e^{8\beta J} + 16e^0 + 4e^{8\beta J}) = \frac{2e^{8\beta J}+4}{\cosh(8\beta J)+3} \end{aligned} \tag{A5}$$

$$\begin{aligned} \langle M^2\rangle &= \frac{1}{Z}(16e^{8\beta J} + 16e^0 + 16e^0 + 16e^{8\beta J}) \\ &= \frac{32e^{8\beta J}+32}{4\cosh(8\beta J)+12} = 8\frac{e^{8\beta J}+1}{\cosh(8\beta J)+3} \end{aligned} \tag{A6}$$

$$C_V = \frac{1}{N}\frac{1}{k_B T^2}(\langle E^2\rangle - \langle E\rangle^2)$$
$$= \frac{1}{N}\frac{1}{k_B T^2}\frac{64J^2}{\cosh(8\beta J)}(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J)+3}) \tag{A7}$$

$$\chi = \frac{1}{N}\frac{1}{k_B T}(\langle M^2\rangle - \langle|M|\rangle^2) = \frac{1}{N}\frac{1}{k_B T}$$
$$\frac{4}{\cosh(8\beta J)+3}(2e^{8\beta J} + 2 - \frac{e^{16\beta J} + 4e^{8\beta J} + 4}{\cosh(8\beta J)+3}) \tag{A8}$$

[1] R. Fitzpatrick, The ising model (2006), (accessed: 19.11.2021).

[2] L. Onsager, Phys. Rev. **65**, 117 (1944), (accessed: 16.11.2021).

[3] M. Hjorth-Jensen, *Computational Physics*, Vol. 13 (Department of Physics, University of Oslo, 2015) pp. 415–448, (accessed: 01.11.2021).