

Simulation of the 2D Ising Model using Monte Carlo Methods and the Metropolis Algorithm

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Abstract

Monte Carlo methods implemented through the Metropolis algorithm were used to simulate the behaviour of the Ising model of ferromagnetism for finitely sized square lattices. The energy, absolute magnetisation, heat capacity, and entropy per lattice site were all found to approach Onsager's analytic results in the thermodynamic limit of an infinite lattice. The zero field magnetic susceptibility, as well as the hysteretic behaviour of the lattice in the presence of an external field, were also found to agree with the theoretical expectations for the model. The finite-size scaling of the model was investigated, and an estimate for the critical temperature of the continuous phase transition in the thermodynamic limit was found, having a value of $T_C = 2.259 \pm 0.057$, which is in agreement with Onsager's solution.

1 Introduction

Many important problems in statistical physics are difficult to handle analytically and hence computational methods must be employed to arrive at the relevant results. One very common and powerful such approach are Monte Carlo simulations, and the Ising model is one example to which they have been applied extensively. This model, introduced by Wilhelm Lenz in 1920^[1], and later solved in 1 dimension by his student Ernst Ising in 1925^[2], concerns ferromagnetism in materials. It treats the magnet as a lattice of spins $\{s_i\}$, each of which can be in one of two states – either $+1$ or -1 . Each spin can interact with its neighbours and an externally applied magnetic field. This results in the following Hamiltonian for the system:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - \mu H \sum_i s_i, \quad (1)$$

where J is the exchange interaction strength between spins, μ is the magnetic moment of a single spin, and H is the externally applied magnetic field strength. The first sum appearing in eq.(1), i.e., $\sum_{\langle ij \rangle}$, goes over all lattice sites i and j which are nearest neighbours.

This project is concerned with the Ising model in 2 dimensions. An analytic solution for this case has also been found, by Lars Onsager in 1944^[3]. It showed the existence of a continuous phase transition (for $H = 0$) in the thermodynamic limit of an infinite lattice at the critical temperature:

$$T_C = \frac{J}{k_B} \frac{2}{\ln(1 + \sqrt{2})}. \quad (2)$$

Here, however, the problem is approached in a numerical fashion, modelling the thermodynamic behaviour of 2-dimensional lattices of finite size using a Monte Carlo simulation implemented through the Metropolis algorithm. The goal is to compare the computational results with those predicted by Onsager, specifically investigating the existence

of the phase transition and determining the finite-size scaling of the model. This will exemplify the strengths of the Monte Carlo approach to statistical mechanics, and justify why it is so widely used.

The overall computational approach is summarised in the next section, with the actual implementation and its performance discussed after that. In section 4 the results of the project are presented and discussed, and section 5 provides the overall conclusions. An appendix is given at the end containing a listing of the numerical code.

2 Computational Analysis

The aim of this project is to investigate the equilibrium behaviour of finitely-sized 2-dimensional square lattices of spins at fixed temperature. In order to incorporate the translational symmetry of an infinite lattice, i.e., have every site equivalent to any other, periodic boundary conditions are applied. Effectively, the 2-dimensional lattice becomes topologically equivalent to a torus.

Two approaches exist for finding the equilibrium properties of the system. One can either numerically calculate the partition function using the following sum going over all possible arrangements of spins on the lattice:

$$Z = \sum_{\{s_i\}} e^{-\beta \mathcal{H}(\{s_i\})}, \quad (3)$$

where $\beta \equiv \frac{1}{k_B T}$. The relevant properties of the system, such as the mean magnetisation, energy, and heat capacity, can then be found from Z .^[4] However, for $H = 0$ the number of spin configurations scales as 2^{N^2} for $N \times N$ lattices, and is even larger in the $H \neq 0$ case. Thus, this approach becomes very computationally heavy for large N .

A more efficient approach, scaling quadratically as N^2 , involves evolving the lattice using Monte Carlo methods and sampling its relevant properties during this evolution. The simulation of the Ising model for a $N \times N$ lattice in this way proceeds as follows. A lattice with all spins aligned in the same direction is initialised. The system is then evolved using the Metropolis algorithm, where each time step consists of the following:

1. Choose a lattice site at random, with each site having equal probability $\frac{1}{N^2}$ of being selected.
2. Determine the energy change $\Delta \mathcal{H}$ of the system when the spin at the chosen site is flipped.
3. If $\Delta \mathcal{H} \leq 0$, i.e., the overall energy of the system does not increase, the spin flip is accepted.
4. If $\Delta \mathcal{H} > 0$, a random number $p \in [0, 1)$ is drawn uniformly. If $\exp(-\beta \Delta \mathcal{H}) > p$, the spin flip is accepted. Otherwise, the original spin is retained.

It is this specific choice of acceptance probabilities

$$A_{\mu \rightarrow \nu} = \begin{cases} 1, & \Delta \mathcal{H}_{\mu \rightarrow \nu} \leq 0 \\ \exp(-\beta \Delta \mathcal{H}_{\mu \rightarrow \nu}), & \Delta \mathcal{H}_{\mu \rightarrow \nu} > 0 \end{cases} \quad (4)$$

for the spin flip taking the lattice from state μ to ν that define the Metropolis algorithm. This is a valid choice of probabilities since they satisfy the principle of detailed balance.^[5] Moreover, the fact that only single-spin-flip dynamics are considered during each time step is justified by the assumption that the energy of a system in thermal equilibrium fluctuates within a narrow range and rarely changes dramatically. Single spin flips provide such small changes and so it is reasonable to use them as the main drive for transitions in the system.

The system is then evolved for multiple time steps using this algorithm, ensuring that it equilibrates. When equilibrium has been reached, the behaviour is simulated further, recording the absolute magnetisation and energy at each time step. This data is then used to find the average equilibrium properties of the system (per lattice site), namely:

$$\overline{|m|} = \frac{1}{N^2} \overline{|M|}, \quad \text{Magnetisation} \quad (5)$$

$$\overline{\epsilon} = \frac{1}{N^2} \overline{\mathcal{H}}, \quad \text{Energy} \quad (6)$$

$$c = \frac{1}{N^2} \beta^2 \left(\overline{\mathcal{H}^2} - \overline{\mathcal{H}}^2 \right), \quad \text{Heat Capacity} \quad (7)$$

$$\chi = N^2 \beta \left(\overline{m^2} - \overline{|m|}^2 \right), \quad \text{Magnetic Susceptibility} \quad (8)$$

where $M = \sum_i \mu s_i$, and the expressions in eq.(7) and (8) follow from the relationship between equilibrium thermal fluctuations in a given thermodynamic quantity and its respective susceptibility.^[4] Another common result is that these fluctuations are maximal at the phase transitions.^[4] Hence, the simulated dependence of c and χ on temperature can be used to determine the critical temperatures of the phase transitions for various lattice sizes. An important point to make is that the absolute magnetisation of the lattice appears in eq.(5) and (8). This helps decrease the overall variance in the magnetisation at low temperatures, i.e., in the ordered phase. This is due to the possibility in those cases for the overall magnetisation of the lattice to abruptly flip completely, which would then lead to large errors in the statistical averages.

Once the equilibrium properties are obtained, the finite-size scaling of the Ising model is investigated. It is suggested^[6] that the critical temperature varies with linear lattice dimension N as:

$$T_C(N) = T_C(\infty) + aN^{-\frac{1}{\nu}}, \quad (9)$$

where a and ν are constants. The best fit to the data for each lattice size is found, and an estimate for the critical temperature of an infinite lattice with no externally applied field, $T_C(\infty)$, is derived and compared to Onsager's theoretical result.

Another important property of the Ising model, despite its simplicity, is that it predicts the presence of hysteretic behaviour of the magnetisation when the externally applied field H is varied smoothly. However, this phenomenon is difficult to derive analytically, so its existence is confirmed using the Monte Carlo approach.

3 Implementation and Performance

3.1 Implementation

A description of how the Metropolis algorithm was implemented, the relevant data collected, and then appropriately analysed, is now presented.

For simplicity, the Boltzmann constant, the exchange strength, and the magnetic moment are set to unity in all that follows: $k_B = J = \mu = 1$.

In the $H = 0$ case, Monte Carlo simulations were performed for a set of different temperatures $T \in [0.2, 5.0]$. The temperature is first set to $T = 0.2$, and a lattice with all spins set to $s_i = +1$ is initialised. Such a lattice corresponds to the equilibrium state at $T = 0$. It is evolved for a total of 25,000 time steps per lattice site. One time step per lattice site, i.e., N^2 time steps, is referred to as a single lattice sweep. The same lattice is then reused, evolving it for a further 25,000 sweeps at the next T value, and so on for all other temperatures. For each T the energy and absolute magnetisation per lattice site are recorded after each sweep, and plotted once the simulation has completed. These plots are then examined by eye to make sure that the system has evolved as expected. For instance, at low temperatures it is expected that the system will thermalise to a state with non-zero magnetisation due to the process of spontaneous symmetry breaking^[4], as observed in Figure 1.

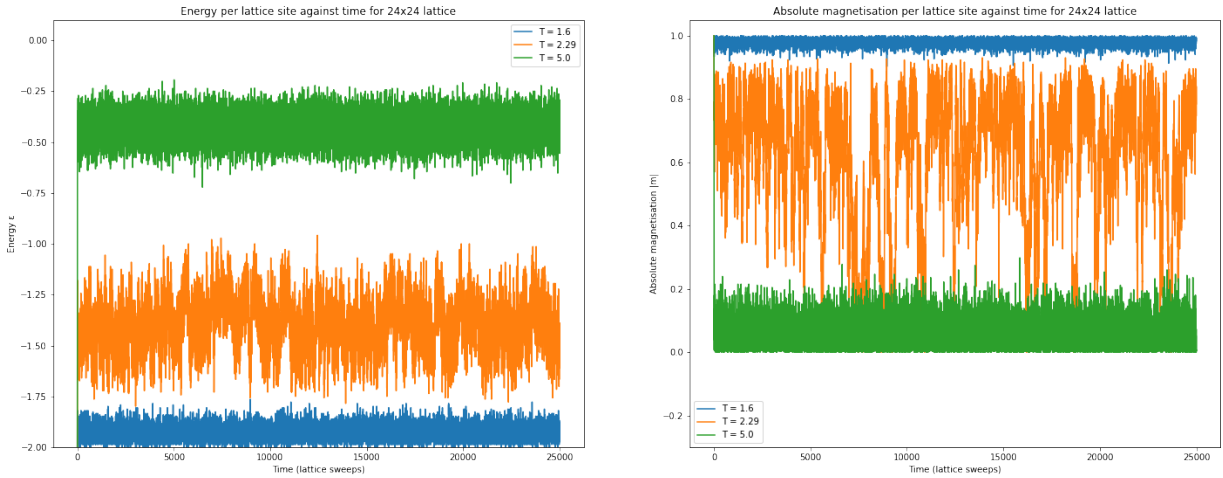


Figure 1: Plots of the energy (left) and absolute magnetisation (right) per lattice site against the number of lattice sweeps for a Monte Carlo simulation of the zero field Ising model with lattice size 24×24 at different temperatures. For $T = 2.29$ the system seems to thermalise much later compared to $T = 1.6$ and $T = 5.0$, namely around the 5,000th lattice sweep.

Once the behaviour of the system is deemed appropriate for the respective temperatures, the plots are used to determine how long it takes for equilibrium to occur. This is crucial, for it is important to only use the energy and magnetisation data sampled during equilibrium to calculate the relevant quantities in eq.(5)-(8). This time scale is called the equilibration time τ_{eq} of the system, and it will depend on the specific temperature at which the simulation is being performed. For example, from the plots of absolute magnetisation in Figure 1 equilibrium is seen to be reached much quicker for the $T = 1.6$ and $T = 5.0$ compared to $T = 2.29$. This is because the latter is near

the critical point of the system where fluctuations are large, and this in hand leads to the phenomenon of “critical slowing down”.^[5] This is a property of the specific Monte Carlo method used, i.e., the Metropolis algorithm, and more advanced algorithms do not suffer from this issue. Nonetheless, for the current simulations, an equilibration time of $\tau_{\text{eq}} \approx 5,000$ lattice sweeps at zero external field was judged sufficient for all temperatures.

The average properties of the system can now be found using the appropriate subset of the recorded data. However, the measurements of a given property after one lattice sweep and the next may not be statistically independent. Thus, in order to find true averages, only measurements separated by some number of lattice sweeps should be considered. This separation is found using the decorrelation time τ_{dec} of the simulation, which is a measure of how long it takes the system to get from one state to another, in which the number of spins which are the same as in the first state is no more than what one would expect to find by chance. The decorrelation time for a given property of the system, say the magnetisation $m(t)$, can be estimated from its autocovariance^[6]:

$$A(\tau) = \overline{m(t)m(t+\tau)} - \overline{m(t)} \times \overline{m(t+\tau)}, \quad (10)$$

where the averages are performed over the equilibrium samples. The autocorrelation as $\chi(\tau) \equiv \frac{A(\tau)}{A(0)}$, and is used to find the decorrelation time as the smallest time lag for which $\chi(\tau)$ is below $\frac{1}{e}$. As with the equilibration time, τ_{dec} will depend on the specific temperature of the simulation, with largest values occurring near the phase transition, again due to the phenomenon of critical slowing down.

Finally, once the decorrelation time is found for each temperature, the magnetisation and energy datasets are averaged over, sampling only values separated by $2\tau_{\text{eq}}$ lattice sweeps. To estimate the error in χ and c , the “jackknife” method^[5] is used, rather than simple error propagation since the quantities m^2 and $|m|$, or \mathcal{H}^2 and \mathcal{H} , are not statistically independent.

For the case of a non-zero externally applied magnetic field, $H \neq 0$, the simulation was performed slightly differently. For a specific temperature T , a starting lattice with all spins set to $s_i = +1$ was initialised. This was then evolved at different values of H for 5 Monte Carlo sweeps each, starting at $H = 1$, going to $H = -1$ and then back to $H = 1$, in increments of $\Delta H = 0.01$. The magnetisation (not its absolute value) per lattice site was recorded after each sweep, and its average for each H -field value was found using the 5 samples.

3.2 Performance

At various points throughout the implementation of the Monte Carlo simulation appropriate decisions were made to ensure the code runs as efficiently as possible. These include:

- Explicitly calculating the total lattice energy and magnetisation only once at the start of the simulation, and finding the values of these properties at later points by simply evaluating the changes in them at every single-spin-flip operation. Specifically, the change in the total magnetisation of a lattice when flipping the spin at, say, lattice site i is $\Delta M = -2\mu s_i$, where s_i is the initial spin value. Similarly, the

change in total energy is $\Delta\mathcal{H} = 4J(z - 2) - H\Delta M$, where z is the number of sites neighbouring to i which initially had the same spin as s_i .

- Reusing the same lattice (in the $H = 0$ case) when going from simulating the evolution of the system at one temperature to the next. This greatly reduces the number of lattice sweeps required for the system to thermalise, meaning that computer time can instead be used to acquire more equilibrium measurements.
- To find the acceptance ratios from eq.(4) in the Metropolis algorithm, certain exponentials have to be evaluated if $\Delta\mathcal{H} > 0$. This is likely the slowest part of the algorithm since such calculations on computers are carried out using a polynomial expansion of e^x which involves many floating-point multiplications and additions. Thus, rather than doing this for each single-spin-flip operation, the performance of the program is improved by calculating the relevant exponentials once at the start of the simulation, and later simply accessing them when required.

Overall, the algorithm implemented with the performance boosts above is capable of running 1,000 lattice sweeps of a 64×64 system for $4.38 \text{ s} \pm 17.4 \text{ ms}$. This was measured using the `%timeit` IPython magic command.

4 Results and Analysis

4.1 $H = 0$

The Monte Carlo simulation described in the previous sections was performed for 7 different lattice sizes: $N = 4, 8, 12, 16, 24, 32, 64$. For $N = 4$ the results from the simulation were compared to those found by the partition function approach mentioned in section 2, in order to ensure the validity of the algorithm. The results for the other lattice sizes were used to investigate the behaviour of the magnetisation, energy, heat capacity, magnetic susceptibility, and entropy per lattice site, as well as the finite-size scaling of the model.

4.1.1 Validity Tests for $N = 4$

For $N = 4$ the mean magnetisation, energy, and heat capacity per lattice site were found at different temperatures using the two numerical methods described in section 2. For the partition function approach, the following expressions were used to find the relevant properties^[4]:

$$\overline{|m|} = \frac{1}{N^2} \sum_{\{s_i\}} \left[|M(\{s_i\})| \frac{\exp(-\beta\mathcal{H}(\{s_i\}))}{Z} \right], \quad (11)$$

$$\bar{\epsilon} = \frac{1}{N^2} \sum_{\{s_i\}} \left[\mathcal{H}(\{s_i\}) \frac{\exp(-\beta\mathcal{H}(\{s_i\}))}{Z} \right], \quad (12)$$

$$c = \frac{d\bar{\epsilon}}{dT}. \quad (13)$$

The results from these two methods are provided in Figure 2, and can be seen to agree. Hence, one can conclude that the Monte Carlo Metropolis algorithm has been implemented correctly.

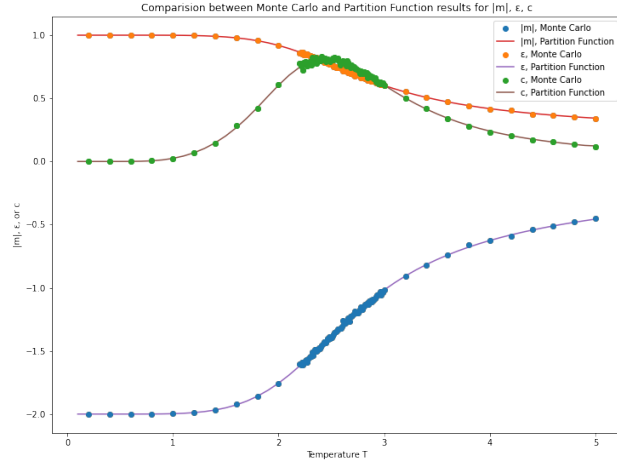


Figure 2: Plot showing the comparison of the mean absolute magnetisation $|m|$, energy ϵ and heat capacity c at different temperatures found using two numerical methods for a 4×4 lattice. The solid lines represent the results from explicitly finding the partition function for the system, whereas the dots - from a Monte Carlo simulation. Errors are also plotted for the latter approach but are too small and hence not visible.

4.1.2 Results for Larger Lattices

For the remaining lattice sizes, the first step in the analysis involves comparing the decorrelation times, defined in section 3. The results are plotted in Figure 3. It is observed that τ_{dec} peaks for all N near where the supposed phase transition is, as expected from the critical slowing down of the Metropolis algorithm. Moreover, the decorrelation times peak to higher values for larger lattices. In fact, τ_{dec} is expected to actually diverge in the thermodynamic limit of $N \rightarrow \infty$,^[5] the same way the heat capacity c and magnetic susceptibility χ should, for the critical fluctuations become infinitely large for an infinite system. This clearly does not happen for our finitely-sized systems, but the expected behaviour is nonetheless exhibited. In addition, the decorrelation times for the energy data are in general smaller than for the absolute magnetisation. This is likely related to the fact that it is specifically the magnetisation that is used as the order parameter for ferromagnetic systems.

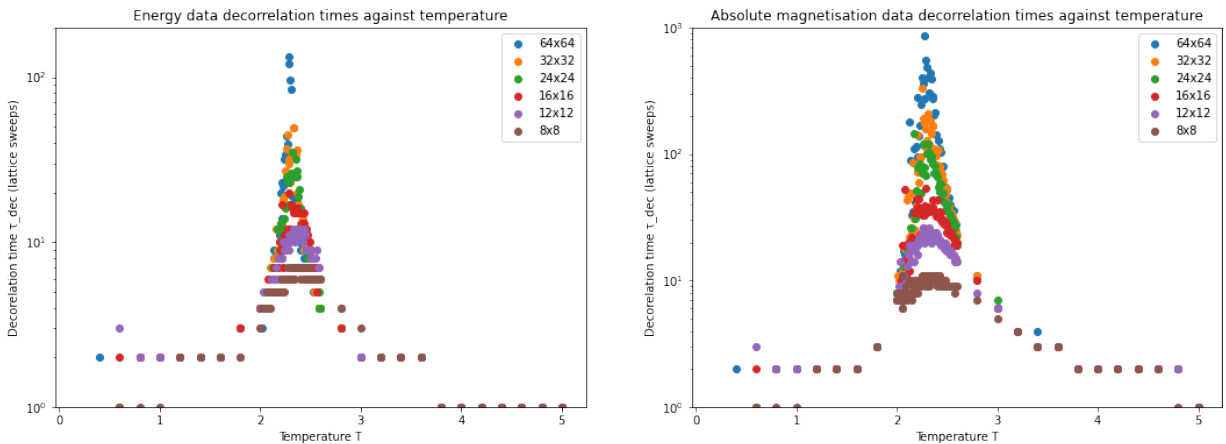


Figure 3: Plot showing the decorrelation times for energy (left) and absolute magnetisation (right) data of Monte Carlo simulations for various lattice sizes. The vertical axis is logarithmic in both plots to allow for better distinction of the results for different N . The τ_{dec} peak at the critical point, doing so to higher values for larger lattices. This is related to the critical slowing down phenomenon of the Metropolis algorithm used to simulate the system.

Next, the energy and absolute magnetisation per lattice site are compared for the different lattice sizes. The results from the simulations are plotted in Figure 4, along with Onsager’s analytic solutions for the two quantities.^[7] The Monte Carlo data visibly approaches the true solution for increasing N . Notably, the order parameter of the system $|m|$ changes continuously from zero in the high-temperature disordered state to a non-zero value in the low-temperature ordered state, showing that the phase transition is of second-order. The errors are also plotted, but are too small to be distinguishable from the data points themselves.

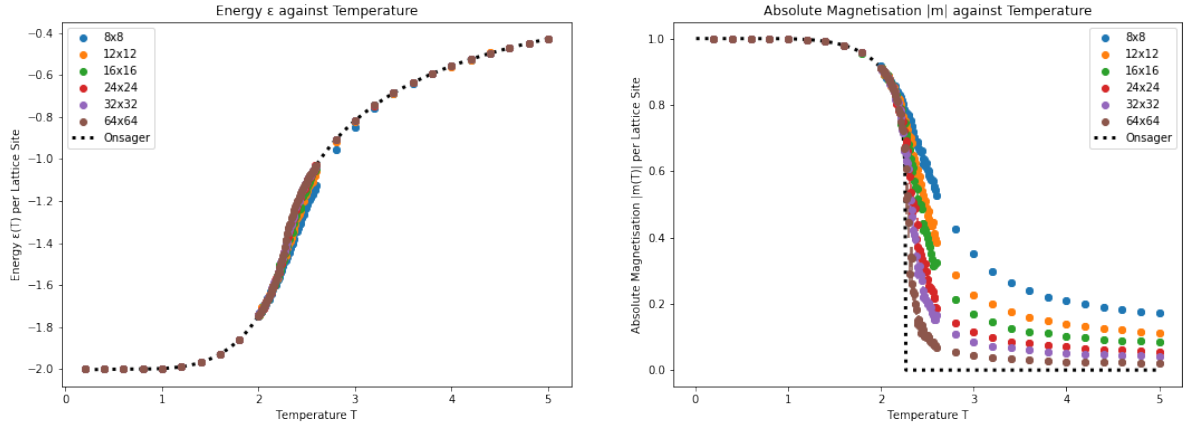


Figure 4: Plots showing the energy ϵ (left) and absolute magnetisation $|m|$ (right) per lattice site for various lattice sizes. The analytic solutions provided by Onsager (1944) are also plotted on each plot using black dotted lines. The Monte Carlo data approaches these analytic results for both energy and magnetisation, the former happening quicker, i.e., for smaller lattice sizes. The errors, are also plotted, but are too small to be distinguishable from the data points.

Moving on, the heat capacities and magnetic susceptibilities per lattice site between the various N are compared. The results are plotted in Figure 5, along with the analytic solution for heat capacity.^[7] The two properties peak, as expected, at the supposed phase transition, reaching higher values for larger lattices. This agrees with the theory since both the heat capacity and the magnetic susceptibility are expected to diverge at the critical temperature in the thermodynamic limit. Moreover, the Monte Carlo simulation data for the heat capacity is in great agreement with the analytic solution, becoming better as N increases, as is to be expected.

Table 1: Best estimates for parameters from least squares fit of finite-size scaling relation for $T_C(N)$

	heat capacity	magnetic susceptibility
$T_C(\infty)$	2.259 ± 0.057	2.260 ± 0.053
a	0.57 ± 0.95	1.7 ± 1.3
ν	1.2 ± 1.4	1.1 ± 0.5

Once the heat capacities $c(T)$ and magnetic susceptibilities $\chi(T)$ are obtained, estimates of the critical temperature for each lattice size can be determined by finding where $c(T)$ and $\chi(T)$ peak. However, the errors in the data points near these peaks are significant (as is visible in the width of the scatter plots in Figure 5). Hence, instead the range of temperatures near the peak where we would expect the true critical temperature to be should be found. This

is achieved by considering the data points furthest away from the peak, whose values agree with the peak value to within the error bounds. The critical temperature is then estimated as the midpoint of this range. The results, on separate plots for estimates from $c(T)$ or $\chi(T)$ data, for the different lattice sizes are given in Figure 6, along with the best

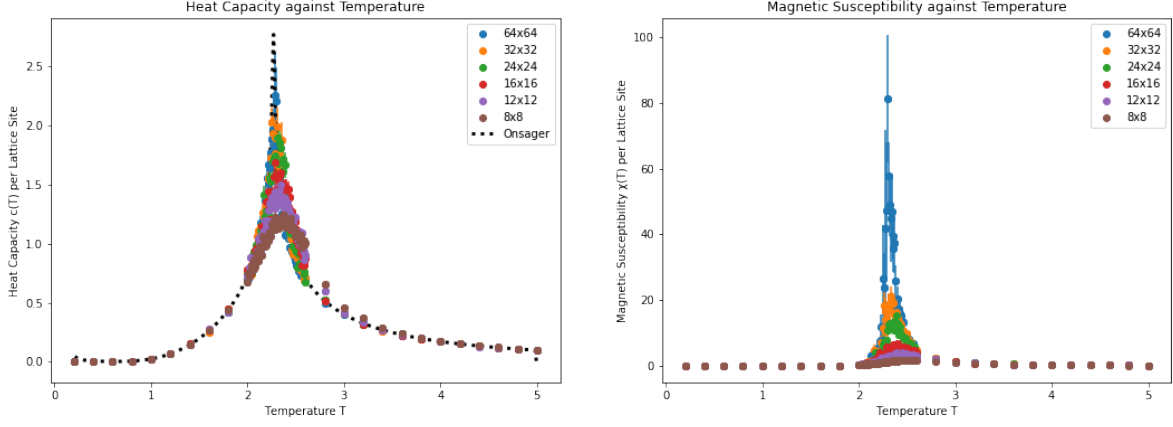


Figure 5: Plots showing the heat capacity $c(T)$ (left) and zero field magnetic susceptibility $\chi(T)$ (right) per lattice site for various lattice sizes. The analytic solution for $c(T)$ by Onsager is also plotted on the left with a black dotted line. The Monte Carlo data for both $c(T)$ and $\chi(T)$ peak at the supposed critical point, as expected, and $c(T)$ agrees very well with the theoretical result, this agreement improving with larger lattice dimension N . However, for larger N the errors in the data points also increase due to the increasing decorrelation length. Hence, the true peak positions, and thereby the values of $T_C(N)$, become more uncertain.

non-linear least squares fit of the proposed finite-size scaling relation from eq.(9). The best estimates of the parameters $T_C(\infty)$, a , and ν are given in Table 1. Both datasets seem to underestimate $T_C(\infty)$, although they nonetheless agree with the analytic result $T_C(\infty) = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$ to within one standard deviation. One should note that the errors in the other two model parameters a and ν are relatively large, so there are likely many reasonable fits to the data.

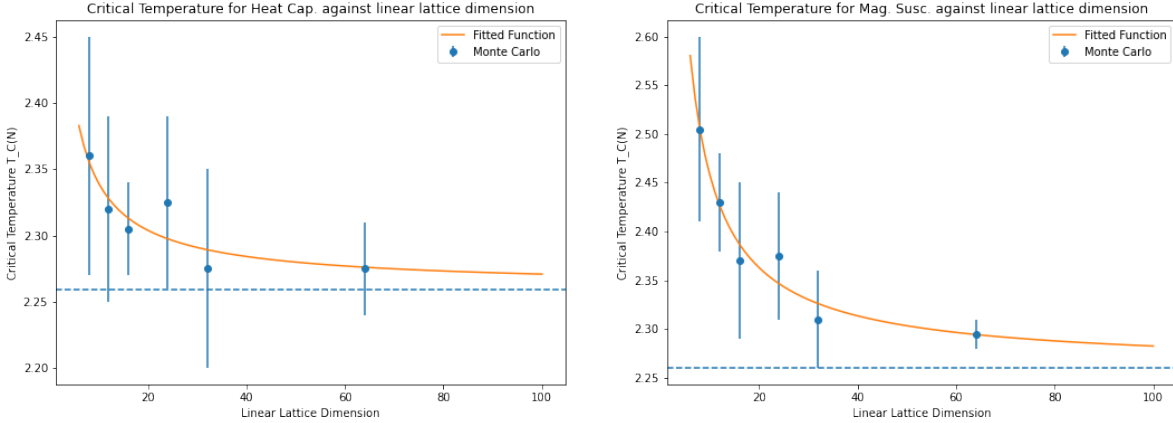


Figure 6: Plots of the critical temperatures $T_C(N)$ estimated from the peak positions of the Monte Carlo data for heat capacity (left) and zero field magnetic susceptibility (right). The best non-linear least squares fit for both datasets is also plotted with an orange solid line, along with the relevant horizontal asymptote corresponding to the critical temperature in the thermodynamic limit $T_C(\infty)$. The Monte Carlo estimates of $T_C(N)$ agree with the proposed exponential finite-size scaling relation to within their errors.

As a final result of the analysis for $H = 0$, the entropy per lattice site is obtained from the heat capacity data using the following integral approximated as a Riemann sum:

$$s(T) = \int_0^T \frac{c(T)}{T} dT, \quad (14)$$

where the Third Law of Thermodynamics is used to set $s(0) = 0$.^[4] The plots of entropy against temperature for the different lattice sizes, along with the analytic solution^[7], are given in Figure 7. The entropy increases from low to high values when the system passes through the critical point, i.e., when it transitions from an ordered to a disordered state, which agrees with the expected thermodynamic behaviour. Moreover, the Monte Carlo data for each N does agree overall with the analytic solution, although there are some deviations, likely due to the simple estimation method of the integral in eq.(14). Nonetheless, $s(T)$ does seem to approach $\ln(2) \approx 0.693$ as $T \rightarrow \infty$, as one would expect, for the Ising model is a two-state system.

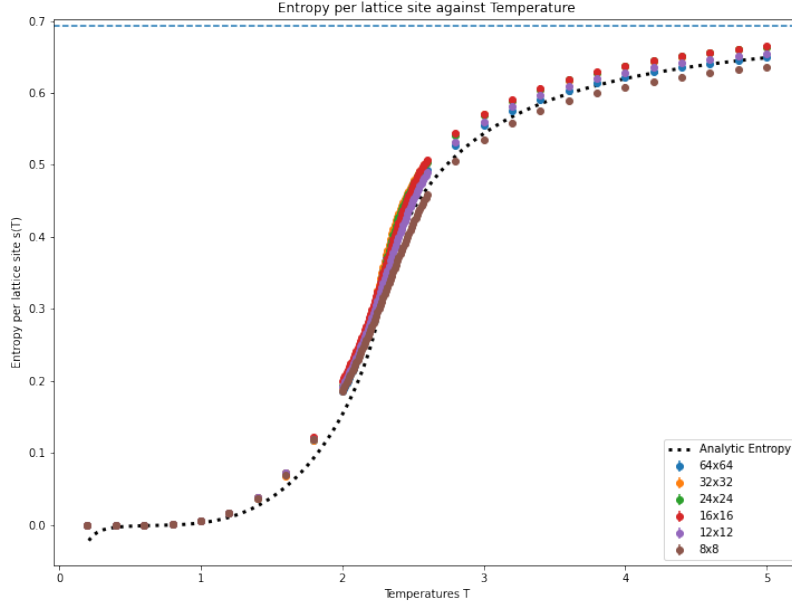


Figure 7: Plot of the entropy $s(T)$ per lattice site for various lattice sizes. The errors, albeit too small to be visible, are found by error propagation for sums of independent measurements, since the entropy integral is being approximated as a Riemann sum, and the values of $c(T)$ for different temperatures can be assumed to be statistically independent. The analytic solution is plotted with a dotted black line, and the asymptotic limit of $s(T) \rightarrow \ln(2)$ as $T \rightarrow \infty$ is shown with a dashed blue line.

4.2 $H \neq 0$

For the case of a non-zero externally applied magnetic field, the hysteretic behaviour of the model is analysed, as described in section 3, for a range of different temperatures from $T = 0.5$ to $T = 5.0$, and a lattice size of 32×32 . The resulting curves of mean magnetisation per lattice site against H -field value are plotted in Figure 8. Hysteresis is observed for temperatures near/below the critical temperature, whereas for higher temperatures the flipping of magnetisation simply occurs at $H = 0$. The hysteresis effects are noticeably more pronounced at lower temperatures. This is to be expected since at high values of inverse temperature β , the acceptance ratios in eq.(4) are low for positive energy changes, and hence high field strengths are required to make $\Delta\mathcal{H} < 0$ and thereby flip the total magnetisation of the lattice. Moreover, the flipping of the magnetisation is more abrupt at lower temperatures, as can be inferred from the square-like shapes of the hysteresis loops. Overall, it can be concluded that the Ising model does indeed exhibit hysteretic behaviour in the presence of an external magnetic field.

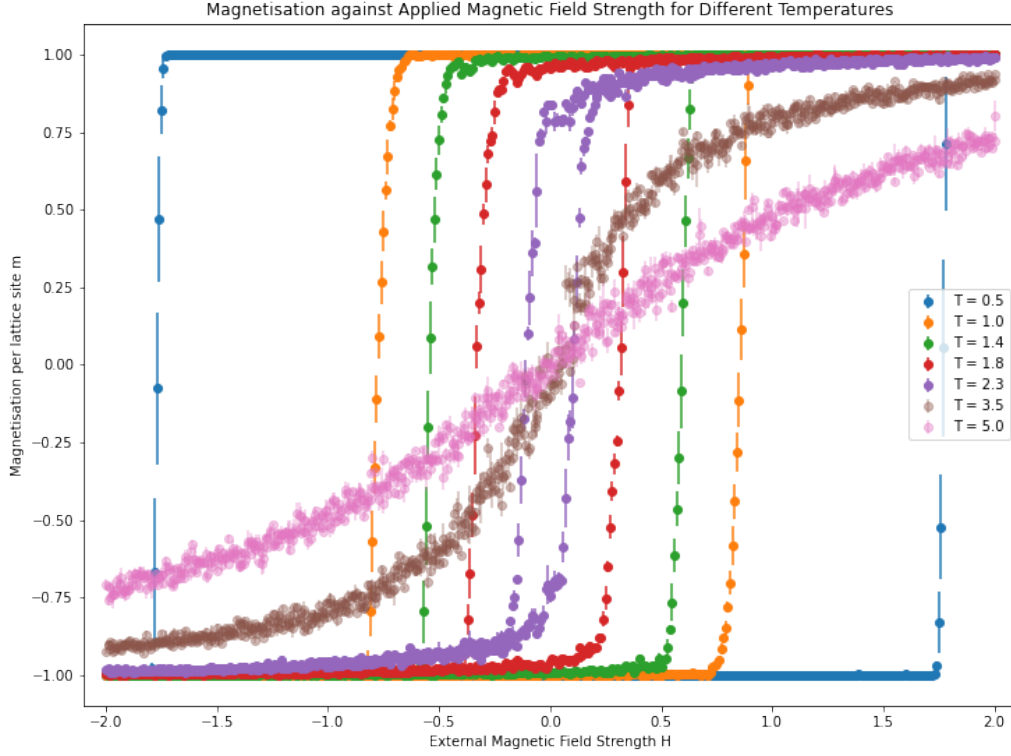


Figure 8: Plots of the hysteresis curves of magnetisation per lattice m site against applied magnetic field strength H for different temperatures. The curves for high temperatures $T = 3.5$ and $T = 5.0$ are plotted using transparent dots in order to allow better visibility of the hysteresis loops at lower temperatures. The Monte Carlo simulations were performed for a 32×32 lattice.

5 Conclusion

In summary, the Monte Carlo method, implemented through the Metropolis algorithm, successfully simulates the behaviour of the 2-dimensional Ising model of ferromagnetism. The equilibrium properties of the system with no external field applied, namely energy, absolute magnetisation, heat capacity, and entropy, agree well with Onsager's analytic results for an infinite lattice, this agreement becoming better for simulations of larger lattices. Specifically, the critical temperature of the continuous phase transition in the thermodynamic limit was estimated to be $T_C(\infty) = 2.259 \pm 0.057$, which matches the theoretical value $T_C = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$. Moreover, the zero-field magnetic susceptibility, as well as the hysteretic behaviour of magnetic systems when an external field is present, were also observed to exhibit the expected behaviour.

Overall, it can be concluded that Monte Carlo simulations are indeed a very useful tool for solving problems which are difficult to handle analytically, and the 2-dimensional Ising model is an illustrative example of this.

Word Count: 3131

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