Modelling Ferromagnetic Phase Transitions using the 2D Ising Model

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The Ising Model (or Lenz-Ising Model) is a model of Ferromagnetism based in statistical mechanics. It describes a magnetic medium as a lattice of discrete atomic spins, with the configuration and interaction between these spins determining the lattice's thermodynamic properties. By utilising Monte Carlo algorithms, the model can be used to calculate specific thermodynamic quantities and identify phase transitions of these mediums. The aim of this project was to implement the two-dimensional version of this model and determine the critical (or Curie) temperature T_c associated with the phase transition between a ferromagnet and a paramagnet. This was achieved by constructing an N x N lattice of randomised spins in Python, then applying the Metropolis algorithm to examine the behaviour of thermodynamic quantities over a substantial temperature range $(0K - 1000K)$. The result for the Curie temperature from this simulation was found to be in agreement with the Onsager solution for the 2D Ising model.

I. INTRODUCTION

The Ising model was first proposed by Wilhelm Lenz in 1920 and later solved by his student Ernst Ising in his 1924 PhD thesis, though it should be noted that this solution was for the 1-dimensional version of the model. [1] In general, the model describes a magnet as a graph/lattice of N^d spin sites, where d is the dimension of the system, and each spin is quantised as up or down. Mathematically, this means for each site in the lattice, S_i (where $i \in N$), the associated spin value $S_i \in \{|+1\rangle, |-1\rangle\}$. The system is treated as periodic, meaning the local arrangement of the spins repeats itself (in each dimension) at the boundaries of the lattice. The 2-dimensional approach is of particular interest due to its simplicity and ability to demonstrate phase transitions.

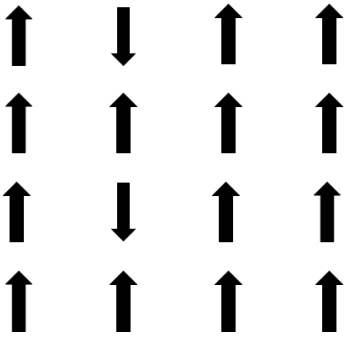

Figure 1. Visualisation of the 2D Ising Model for N = 4

Figure 1 demonstrates the model for a simple lattice, $|+1\rangle$ spins are represented by upward arrows and $|-1\rangle$ spins by downward arrows. A natural question that arises is how to determine the energy of this system. The approach based in statistical mechanics would be to sum over all the microstates of the system in question to determine its Hamiltonian function. A microstate being a possible spin configuration of the lattice.

For any two adjacent spins of the lattice $i, j \in N$, there is an associated exchange interaction J_{ij} and an external magnetic field that interacts with spin j denoted h_j. We can think of the interaction term arising due to each spin having an intrinsic magnetic field and the resulting effect this field has on the spin's neighbours. The magnitude of J_{ij} signifies how strong the tendency of spins i and j is to be anti-aligned, meaning one up and one down. The sign of J_{ij} relates to whether neighbouring spins tend to align or anti-align, the former indicating the medium is ferromagnetic. The external magnetic field has the effect of splitting the energies of spin states, this is known as the Zeeman effect. Named after the Dutch Physicist Pieter Zeeman who observed the splitting of spectral lines in the presence of magnetic fields, as documented in his 1897 paper "The Effect of Magnetisation on the Nature of Light". [2]

Thus, the energy of a configuration is given by the following Hamiltonian, (where μ is the magnetic moment):

$$H(S) = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - \mu \sum_j h_j S_j \qquad (1)$$

For simplicity, only the contribution of the exchange interaction was considered when calculating the energy of the lattice, the omission of this external field term should however be noted when comparing the accuracy of the results with other solutions. In the 2-dimensional model, each lattice site has 4 adjacent nearest neighbours, so we determine the energy associated with the site's interactions by summing over these 4 neighbouring spins. We will also assume

the exchange interaction is equal for all adjacent lattice sites:

$$E = -J \sum_{\langle ij \rangle} S_i S_j \tag{2}$$

Where $\langle ij \rangle$ signifies that the summation is limited to the nearest neighbouring spins. A consequence of this relation is that two adjacent sites that are aligned, i.e., both spin up ($\langle +1|$) will have a lower associated energy than two sites which are anti aligned (one up and one down). As the temperature of the system is increased, it is expected that more spins will flip due to the additional thermal energy introduced to the system. Thus, the spin-spin interaction energies will evolve, and consequently so will the net energy and net spin of the entire lattice; the latter of which will be referred to as the 'magnetisation' from here on.

II. PHASE TRANSITIONS

The measurement of interest in this investigation is the critical (or Curie) Temperature T_c associated with the phase transition between a ferromagnet and a paramagnet. Which of these two categories a material falls into depends on the behaviour of their constituent magnetic moments (spins) in relation to external magnetic fields. Ferromagnetism is defined by 'strong interactions between neighbouring dipoles, with a high degree of alignment even in a weak external magnetic field'. Whereas paramagnetism signifies 'partial alignment of electron spins/magnetic moments with the direction of the external field'. Therefore, the transition may also be referred to as the point of 'spontaneous magnetisation'. [3] It should also be noted that there is a third category materials may fall into, that being diamagnetic. Such mediums are defined by the absence of permanent magnetic moments and thus, were not crucial to this investigation.

It is useful to consider ferromagnetic phase transitions in a thermodynamic context to understand why they are of particular interest. Paul Ehrenefest classified phase transitions by the behaviour of a system's 'derivatives of free energy'. [4] Free energy meaning the part of a system's energy that is available to do work at a constant temperature, the energy itself is derived from the first law of thermodynamics [5] as shown in equation (3).

$$dU = dQ + dW \tag{3}$$

Where dU denotes the change in internal energy, dQ the change in thermal energy and dW the work done by the system. Equation (4) shows the free energy form of equation (3) as defined in the fundamental thermodynamic relation for a closed system [6]:

$$dF = -SdT - PdV \tag{4}$$

Here the Helmholtz free energy is represented with the conventional F. V and P are the volume and pressure of the system respectively. While S represents the entropy and T signifies the temperature.

A first order transition is characterised by a discontinuity in the first derivative of the system's free energy with respect to thermodynamic quantities like temperature or pressure. Whereas second order transitions refer to those that are continuous in this first derivative of free energy with respect to an external field, but discontinuous in the second derivative.

In the presence of a magnetic field, the free energy of a system is instead given by equation (5). As the work done on the system is due to the magnetic field, not changes in volume or pressure:

$$dF = -SdT - MdB \tag{5}$$

Where F is the free energy, M is the net magnetic moment of the system (magnetisation) and B the external magnetic field. All other variables are consistent with equation (4).
The magnetization of a material is therefore the first derivative of free energy with respect to an applied magnetic field (at constant temperature):

$$M = -\left.\frac{\partial F}{\partial B}\right|_T \tag{6}$$

The magnetic susceptibility of a material, χ is defined as the tendency of a material to become 'magnetised' in an external magnetic field. Magnetised meaning the state in which the constituent magnetic moments (or spins) are strongly aligned. This gives the following relation with the magnetisation:

$$\chi = \lim_{B \to 0} \frac{\mu_0 M}{B} \tag{7}$$

Where μ_0 is the permeability of free space, $4\pi \times 10^{-7} Tm/A$ [7]
Therefore, by first principles, the susceptibility represents the second derivative of free energy with respect to the magnetic field:

$$\chi = \mu_0 \frac{\partial M}{\partial B} = -\mu_0 \frac{\partial^2 F}{\partial B^2}\bigg|_T \tag{8}$$

From these relations, it can be deduced that ferromagnetic phase transitions are second order in this classification scheme. As the magnetisation will decrease continuously to zero as the temperature exceeds the Curie temperature, while magnetic susceptibility evolves discontinuously with temperature. The internal energy of the lattice $E(T)$ behaves in a continuous manner like that of magnetisation, while the derivative of this energy with respect to temperature (the specific heat capacity $C(T)$) mirrors the behaviour of magnetic susceptibility. This is because internal energy quantities are also derivatives of free energy with respect to temperature. Hence, by evolving the Ising lattice over a range of temperatures, the Curie temperature could be identified from the point of discontinuity in magnetic susceptibility and specific heat capacity. This can be achieved by applying the Metropolis algorithm to the lattice's spin configuration.

III. DETAILED BALANCE

To understand the operations of the Metropolis algorithm, its two primary statistical postulates should be considered, the first of which is the concept of detailed balance. Suppose we have a system of spins confined to the canonical ensemble, meaning the system is in thermal equilibrium with a temperature bath while temperature and volume (or pressure) remain constant, but with varying energy. The probability of occupying a state with energy E_i is given by:

$$P_i = \frac{1}{Z} e^{-\beta E_i} \tag{9}$$

Where Z=$\sum_i e^{-\beta E_i}$ is the partition function associated with a canonical ensemble. $\beta = k_B T$, with k_B = Boltzmann's constant ($1.3806488 \times 10^{-23} JK^{-1}$) [8] T again representing the systems temperature (K).

The principle of detailed balance is that for a kinetic system in a state of equilibrium, a process is said to occur at the same average rate as the reverse process. In the context of the Ising picture, this means that the evolution of the system from one microstate to another occurs at the same rate as the backwards evolution between these two states. Consider the probability of the lattice going from a given energy state μ to state υ, which we denote $P(\mu \to \upsilon)$. The probabilities of occupying E_μ and E_υ are P_μ and P_υ respectively. Therefore, according to detailed balance, the following relation must hold:

$$P_\mu P(\mu \to \upsilon) = P_\upsilon P(\upsilon \to \mu) \tag{10}$$

Of course, an N = 50 lattice will have an immense number of possible microstates, as the amount of configurations scales with the number of lattice sites. The probability of any given microstate, P_i will depend on many factors, for example how energetically favourable its occurrence is. Thus, we expect a large collection of different probabilities associated with each microstate.

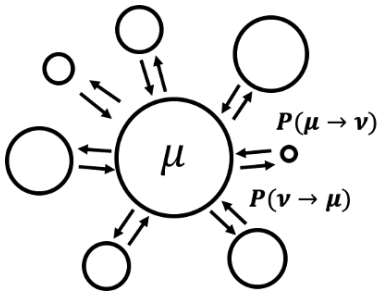

Figure 2. Visualisation of varying probabilities of a system's microstates

Figure 2 illustrates this concept by representing the probability of a given microstate by the size of its corresponding circle. From this we can deduce the following relation for a system in equilibrium:

$$\sum_\mu P_\mu P(\mu \to \upsilon) = \sum_\upsilon P_\upsilon P(\upsilon \to \mu) \tag{11}$$

For the purpose of the Metropolis algorithm, it is useful to express this relation in a way that can be computed using a common mathematical distribution, while accounting for the relative likelihood of a given state occurring. This is achieved through a technique known as importance sampling, in which one probability distribution is used to approximate values from a different distribution of interest. In this case, the canonical ensemble allows the detailed balance ratio to be written as a Boltzmann distribution for the energy difference between two given states:

$$\frac{P(\mu \to \upsilon)}{P(\upsilon \to \mu)} = \frac{P_\upsilon}{P_\mu} = e^{\beta(E_\upsilon - E_\mu)} \tag{12}$$

IV. ERGODICITY

Another key principle of the Metropolis algorithm is the concept of ergodicity, one of the two primary postulates of statistical mechanics. The ergodic hypothesis states that "a macroscopic system in equilibrium is assumed to progress in time through phase space so that it visits every allowed volume of phase space with equal probability". [9] Meaning that for a macroscopic quantity of a system, the average of one state over an infinitely large time period will be equal to the average over an infinite number of possible states at the same time:

$$\langle Q \rangle_{time} = \langle Q \rangle_{ensemble} \tag{13}$$

In relation to the Ising model, this postulate means that any path may be taken to reach the lattice's equilibrium state, at which point detailed balance would be satisfied. The average of the quantities of interest (such as lattice energy and magnetisation), if measured for an ensemble of different spin configurations will be equivalent to that of a single configuration evolving over a sufficiently large time period.

V. THE METROPOLIS ALGORITHM

In a 1948 conference at Cornell, Lars Onsager claimed to have (along with Bruria Kaufman) found an analytical solution for the 2D Ising model, presenting his solution for the spontaneous magnetisation, M_0 to those in attendance. [10] The solution was as follows:

$$M_0 = (1 - k^2)^{\frac{1}{8}} \tag{14}$$

Where $k = 1/(\sinh 2H \sinh 2H')$, with $H = H' = J/k_B T$ assuming J is isotropic, meaning equal in all directions throughout the lattice. The result holds true for $0 < k < 1$, with $T < T_c$.

From the Onsager solution, the relationship for the Curie temperature is given by equation (15) [11]:

$$T_c = \frac{2J}{k_B \ln(1 + \sqrt{2})} \tag{15}$$

For the purpose of computing a numerical solution, the Metropolis algorithm is a simple way to produce a canonical ensemble for this system. A brute force approach would require calculations for the partition function and thermodynamic quantities for every possible spin configuration of the lattice. Consider that a 2D lattice of N spin sites will have 2^{N^2} possible states and the thermodynamic limit requires $N \to \infty$. The resulting number of calculations would be too large, making this approach impractical. The immediate benefit of the Monte Carlo simulation is that it can reduce the number of calculations needed and thus, requires less computing power. The Metropolis algorithm achieves this by sampling select states, then estimating the corresponding thermodynamic variables as an ensemble average.

It should be noted that the sampled states are not randomly selected. The probability of a state occurring is factored into the sample, as it would be inefficient to sample states that are physically unlikely to occur, such as spin configurations that are energetically unfavourable.

The algorithm has the following steps:

1. Call the current spin configuration state i
2. Randomly select a lattice site with spin S_n and calculate the energy associated with its nearest neighbours,
3. Perform a trial move, flipping the spin S_n ($S_n = -S_n$).
4. Call this new configuration of the lattice state f and calculate the new energy of spin S_n associated with its nearest neighbours
5. Calculate the change in energy, ΔE between states E_i and E_f
6. If $\Delta E \leq 0$, accept the trial with probability 1
7. If $\Delta E > 0$, accept the trial with probability $e^{-\beta \Delta E)}$
8. If the trial is not accepted, flip spin S_n back ($S_n = -S_n$).
9. Return to step 1 until the desired number of iterations is reached

VI. METHODOLOGY

To apply the Metropolis algorithm, an initial lattice was first generated. Though a random arrangement of spins is required, for reasons that will become obvious,

a random ratio of $|+1\rangle$ spins to $|-1\rangle$ spins is not desired, at least initially. Consider an initial 2D lattice with N = 50, where the majority of spins begin as $|+1\rangle$. By definition, the magnetisation of the lattice is:

$$M = \sum_{i}^{50^2} S_i \tag{16}$$

Thus, it is expected that the magnetisation (net magnetic moment) will be positive. Once a sufficient number of iterations of the algorithm are carried out, enough sites will have flipped such that the system reaches a state of equilibrium. This is marked by a roughly equal proportion of $|+1\rangle$ and $|-1\rangle$ spins, due to equal rates of spins flipping in both directions ($|+1\rangle \leftrightarrow |-1\rangle$). This initial configuration is only necessary to judge whether the algorithm's computation is correct.

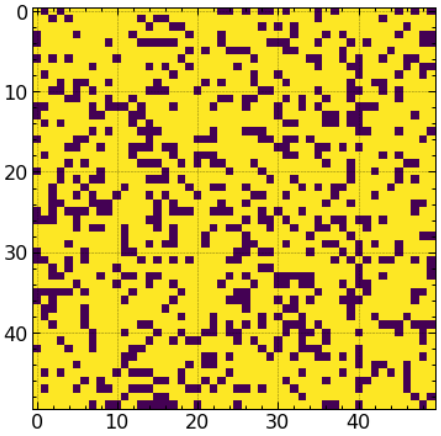

Figure 3. Randomly generated lattice configuration for N = 50, with 75% of spins in state $|+1\rangle$ (yellow).

As shown in Figure 4, the average spin of the lattice, (which is the magnetisation divided by N^2), tended towards zero, indicating a state of equilibrium was achieved after approximately 5000 iterations of the algorithm. The validity of detailed balance, and thus the algorithm itself, is contingent on the system being in equilibrium. Hence this factor must be considered when calculating thermodynamic quantities from the ensemble, as the algorithm's selection probabilities for trial moves are derived from detailed balance.

Consider the case where a single spin is flipped, causing the lattice to evolve from a state i to a state f. If the energy difference between these states,

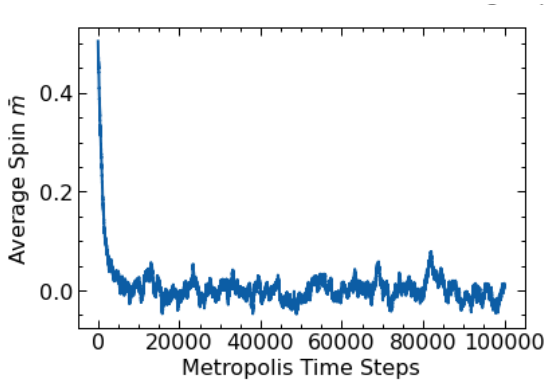

Figure 4. Graph of average spin for 100,000 iterations of the Metropolis algorithm, with $J = 1 \times 10^{-21}$ and $T = 300K$

$\Delta E \leq 0$ then the evolution to state f is said to be energetically favourable, as the overall system is moving to a state of lower energy. This is a direct consequence of the first and second laws of thermodynamics, which signify energy conservation and entropy increase [5]. Thus, the flip is accepted with probability $P(i \to f) = 1$. However, in the case that $\Delta E > 0$, due to state f being of a higher energy than state i, this is less energetically favourable and hence, a less probable outcome. Therefore, the algorithm proposes the opposite probability relation, $P(f \to i) = 1$. Substituting this probability into equation (12) for detailed balance:

$$\frac{P(i \to f)}{1} = P(i \to f) = e^{-\beta \Delta E} \tag{17}$$

The result of applying these probabilities over many iterations was of course, an ensemble of states. The natural approach of statistical mechanics was to then calculate averages of thermodynamic variables over the ensemble. The algorithm seeks to preserve the validity of these averages, as they are less likely to be affected by the inclusion of states that are unlikely to occur.

There were two primary thermodynamic quantities that were determined from the ensemble for the purpose of identifying the phase transition, total energy E, and magnetisation M of the lattice. As the ferromagnetic phase transition is second order, these variables are continuous, and thus were not ideal quantities to identify the critical temperature from. For this purpose, quantities which vary discontinuously with temperature are desired, as the point of discontinuity marks the temperature at the point of transition. Therefore, the variance of the two aforementioned quantities were calculated. These variances were then used to determine the specific

heat capacity C and magnetic susceptibility χ respectively for each configuration (equivalent to the partial derivatives of E and M with respect to temperature). We express these variables as a function of temperature:

$$E(T) = \frac{1}{N^2}\sum_i E_i \tag{18}$$

$$M(T) = \frac{1}{N^2}\sum_i S_i \tag{19}$$

$$C(T) = \frac{1}{N^2}\frac{1}{k_B T^2}(\langle E^2\rangle - \langle E\rangle^2) \tag{20}$$

$$\chi(T) = \frac{1}{N^2}\frac{1}{k_B T}(\langle M^2\rangle - \langle M\rangle^2) \tag{21}$$

The mean values and variances were generated from the ensemble at a given temperature T, so applying the Metropolis algorithm for varying temperatures generated many ensembles over the desired range. The thermodynamic quantities from each ensemble were then plotted over this temperature range. Note that for each application of the algorithm, it was necessary to exclude the first few thousand iterations from the data. As the algorithm required at least 5000 iterations to reach equilibrium, where detailed balance holds true. For convenience, a slice of the final 10,000 thousand or so iterations of the ensemble were taken.

Several other variables had to be initialised before running the algorithm. The exchange interaction, J was taken to be 1×10^{-21}, as a value similar in magnitude to the Boltzmann constant produced energy values that were of a convenient size for graphing purposes. An initial temperature range of $0K$ to $5000K$ was used to show the general behaviour and then $0K$ to $500K$ to more precisely identify T_c , as equation (15) predicts a Curie Temperature of $164K$ for the chosen value of J. Ensembles were generated at regular $2.5K$ intervals over this temperature range. Ideally smaller increments are desired to produce smoother curves and to visually represent discontinuities, but this choice was due to limitations of the computing power available. The number of sites per dimension of the lattice, N was taken to be 15, again due to these limitations.

VII. RESULTS

As shown in Figure 5, the total energy of the lattice increases rapidly with temperature up to $200K$, before

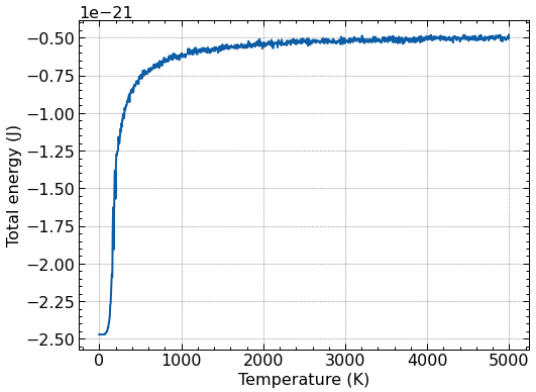

Figure 5. Plot for the total energy of the $N = 15$ lattice between $0K$ and $5000K$.

the rate of energy increase begins to decrease, eventually beginning to level off between $4000K$ and $5000K$. This trend was expected based on the equation of interaction energies of neighbouring spins (2). Close to $0K$, the lattice began with a high degree of spin alignment. As the temperature was increased, more energy was introduced into the system, and so thermal effects became increasingly significant. The additional thermal energy caused more spins to flip, resulting in more neighbouring spins becoming anti-aligned. As implied by equation (2), anti-aligned spin pairs will have a higher interaction energy than pairs that are aligned, so the resulting effect is that the total energy of the lattice increases with temperature. At the point of ferromagnetic phase transition, there is a shift to a very low level of spin alignment associated with paramagnetism, so this point should correspond to the point where the slope of energy with respect to temperature is steepest and increasing. In Figure 5, this point seems to lie at a temperature between $100K$ and $200K$.

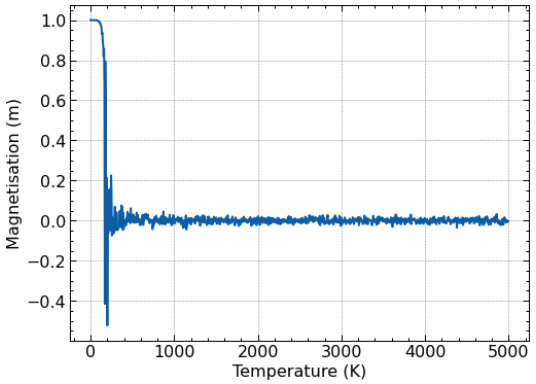

Figure 6. Plot for the Magnetisation of the $N = 15$ lattice between $0K$ and $5000K$.

The magnetisation of the lattice, as shown in Figure 6, starts off as approximately 1.0 at $0K$, then oscillates, rapidly approaching zero between $100K$ and $200K$, remaining constant up to $5000K$. This is consistent with the behaviour predicted by the initial state of the lattice and equation (16). Initially, 75% of the spins were in state $|+1\rangle$, which is expected to yield a net magnetic moment of 1.0 for the entire lattice. As temperature was increased and more spins flipped to state $|-1\rangle$, the magnetic moments began to cancel each other out, causing the net spin to decrease to zero. A paramagnet is said to have a low degree of alignment even in an external magnetic field, so beyond the critical temperature, the magnetisation of the lattice should be relatively close to zero.

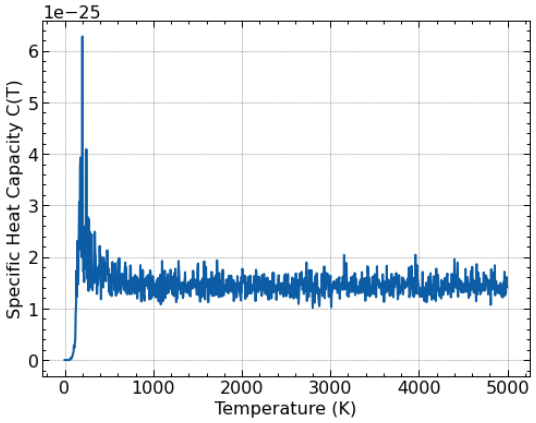

Figure 7. Plot for the Specific heat capacity of the $N = 15$ lattice between $0K$ and $5000K$.

As stated previously, for the chosen value of the exchange interaction, equation (15) of Onsager's solution for the 2D Ising model predicts the Curie temperature to be approximately $164K$. Both specific heat and magnetic susceptibility are second derivatives with respect to the system's free energy, given the ferromagnetic transition is second order, it is expected that the temperature at the point of phase transition should be marked by a discontinuity in the behaviour of both quantities. As shown in Figure 7 and Figure 8, the expected discontinuity corresponds to the sudden spikes in specific heat capacity and magnetic susceptibility respectively at $100K < T < 200K$. As expected, both specific heat capacity and magnetic susceptibility level off after this discontinuity, as the lattice has become paramagnetic, with a high degree of anti-alignment of spins.

Narrowing the temperature range to $0K < T < 500K$ and examining the spike in magnetic susceptibility, the

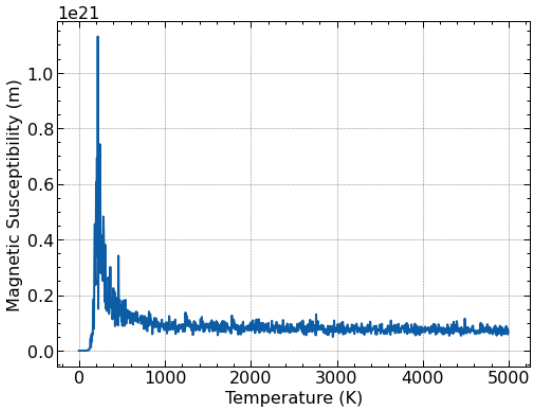

Figure 8. Plot for the Magnetic Susceptibility of the $N = 15$ lattice between $0K$ and $5000K$.

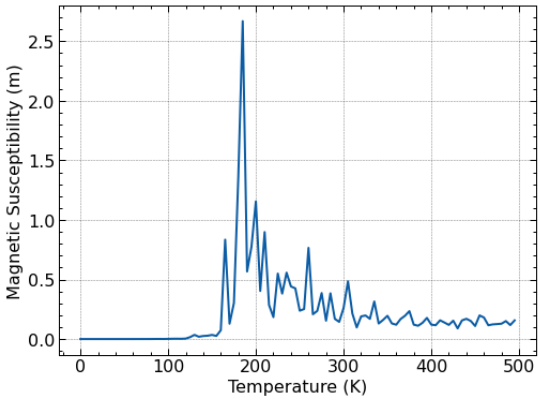

Figure 9. Plot for the Magnetic Susceptibility of the $N = 15$ lattice between $0K$ and $500K$.

Curie temperature T_c was found to be approximately $170K \pm 10K$. This is shown in Figure 9 by the point at which the large spike first occurs. The associated systematic error was calculated using the scale of the graph's axis for the simulated data.

VIII. CONCLUSION

The purpose of this project was to simulate the two-dimensional Ising model and use Monte Carlo methods to identify the critical (Curie) temperature T_c associated with the ferromagnetic phase transition. The Metropolis algorithm successfully identified the critical temperature to be approximately $170K \pm 10K$, as the Onsager solution predicts T_c to be $164K$ for $J = 1 \times 10^{-21}$, which lies in the range of the simulated result. This suggests that the model was accurately represented by the Python code and the algorithm was successfully implemented, despite the limitations of the available computing power.

Four thermodynamic variables were observed in the course of the investigation, all of which behaved in a manner consistent with the second order classification of the ferromagnetic phase transition. The first derivatives of free energy, total energy and magnetisation, exhibited continuous relationships as a function of temperature. While the second derivatives of free energy, specific heat capacity and magnetic susceptibility, both demonstrated discontinuities at a similar temperature point. All the dependent variables being in agreement with the Ehrenfest classification scheme further supports the validity of the result for the critical temperature.

The majority of the uncertainty in the observed result for this temperature arises due to random error. Working within the confines of detailed balance, and statistical mechanics as a whole, requires large numbers of iterations/microstates to obtain accurate results. However, taking such a large number of measurements will result in more opportunity for random errors to arise and affect a measured quantity. This can be observed by repeated simulations of the algorithm for the same initial values such as J, as slight fluctuations in the dependent variables' plots are observed. In theory, the effect of such errors could be offset by reducing the increments of the temperature range and generating larger ensembles. As this could produce smoother behaviours of these variables with temperature and reduce the statistical weight of anomalous measurements. Though, as stated previously, this was not feasible due to the technical limitations of this project.

Another source of uncertainty arises from the scale of the plot for magnetic susceptibility, which was used to identify the critical temperature. This is of course, a systematic error and so there is no obvious way to avoid this uncertainty. Though the scale only entails an percentage error of 6% on the obtained result for T_c, it would be advisable to use additional Python code to identify this point on the plots more precisely. An approximate value for T_c could even be obtained from all four graphs and then calculated as an average of these estimates.

Additionally, there are a number of factors that limit how we may interpret the final result, as the 2-dimensional Ising model utilised here differs from physical magnets in a number of ways. For instance, the assumption of the exchange interaction J being isometric, the omission of an external magnetic field or the existence of a magnet as a 2D medium. These assumptions are valued more for their simplicity and usefulness in simulating phase transitions, despite how they differ from the physical reality of magnetic mediums. Though these differences should be considered when comparing the results to the behaviour of physical magnets in nature, the replication of Onsager's solution in this investigation provides further evidence for the validity of the 2D Ising model in identifying ferromagnetic phase transitions.

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