

MAS3091

Computation and Simulation of The Ising Model

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December 2023



Abstract

The Ising model, a cornerstone in the field of statistical physics, provides a powerful framework for understanding phase transitions and collective behaviour in magnetic systems. In this report, we delve into the fundamental concepts of the model, derive key physical quantities, and employ computational techniques to simulate its behaviour. As well as this, we extend our investigation to explore theoretical lattices beyond the conventional square lattice, with a particular focus on the triangular lattice.

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1 Introduction

History of the Ising Model:

The model was invented by the German physicist Wilhelm Lenz. While at Hamburg in 1920 Lenz gave the model to his student Ernst Ising to explain the existence of ferromagnetism on the basis of his prior publication. Ising started his dissertation on the investigation of ferromagnetism, summarised in a short paper written in 1924 and published in 1925.

Significance in Statistical Mechanics:

The Ising model is one of the most renowned concepts in statistical mechanics and holds significance due to its foundational role in uncovering key principles of phase transitions and critical phenomena. The model is unique in being analytically and exactly solvable in one and two dimensions, whilst also being the simplest theoretical description of ferromagnetism [1]. It can be used in a vast range of fields, such as for modelling real materials, ferromagnetism, and liquids and gases, as well as being a model of a material undergoing phase transition. However, above certain temperatures, known as the critical temperature, the model loses its magnetisation and becomes demagnetised [2].

Goals:

In our research, we aim to create a simulation using various Monte Carlo approximation methods, with a particular focus on the Metropolis-Hastings Algorithm. Using this simulation we will explore the conditions required to obtain a phase transition and reading an ordered configuration state. Thus, we will compute and describe the relationships between energy and temperature, specific heat and critical temperature.

1.1 Introduction to Fundamental Ideas

Suppose we can observe an $N \times N$, lattice where each vertex is an atom with a free electron in its outer shell. Each edge of the lattice represents an interaction between electrons.

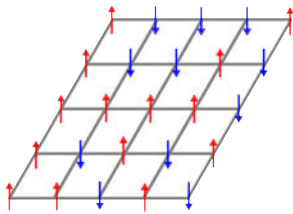


Figure 1: Square lattice

Each vertex of the lattice represents magnetic dipole moments of atomic spin which are pointed in the positive or negative direction, and are restricted to interact with their **nearest neighbours**. These points on the lattice consist of discrete variables $\sigma \in \{+1, -1\}$. The two-dimensional, $N \times N$ lattice is a fundamental model for displaying **phase transition**.

Hamiltonian Function:

Building on our initial definition of the model, we can begin to compute the energy of each lattice spin by using the Hamiltonian function.

Definition 1 (Hamiltonian function) For any two adjacent sites i, j within the lattice, there exists an interaction between these sites J_{ij} . The energy of a configuration σ is represented by the expression

$$H(\sigma) = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j - \sum_j h_j \sigma_j \quad (1)$$

Where h is the external magnetic field interacting with the lattice.

The factor of one half is to ensure that an interaction J_{ij} between lattice sites is not counted twice within the energy calculation.

Configuration Probability and the Boltzmann Distribution:

Definition 2 (Configuration probability) The probability that the system is in a state with configuration σ and follows the Boltzmann Distribution

$$P(\sigma) = \frac{\exp\{-\beta H\}}{Z}, \quad \beta = (k_B T)^{-1} \quad (2)$$

The Boltzmann constant, $k_B = 1.380649 \times 10^{-23} J \cdot K^{-1}$

The variable Z is known as the partition function such that

$$Z = \sum_{\sigma} \exp\{-\beta H\} \quad (3)$$

Phase Transition from Disordered to Ordered States:

The behaviour of the system varies as a function of temperature, by treating temperature as an independent variable we can study phase transition. This follows for the application to ferromagnetism, the material is magnetised when all the spins are aligned (pointed in the same direction) [3].

- **High temperature:** Thermal fluctuations dominate over the spin-spin interactions, causing disruption to the long range order of the system. Therefore no phase transition can occur.
- **Critical temperature:** We reach a point whilst decreasing the temperature that we can now attain a phase transition. We will see the precise analytic solution of the critical temperature in (Section 2.6).
- **Low temperature:** Thermal fluctuations become less significant compared to the energy associated with the spin-spin interactions, spins align to minimise free energy. The alignment of the spins is the phase transition from disorder to order.

This can also be derived from the Boltzmann distribution. At high temperatures, due to the inverse proportionality we have a small value for β thus the probability of an ordered state

becomes exponentially small. This is why we do not attain phase transitions at high temperature for disorder to order. Note that if we defined phase transition as being the transition from disordered states to ordered states then the relations for high and low temperature would be flipped.

1.2 Monte Carlo Approximation Methods for Numerical Simulation

Introducing the Metropolis Algorithm

Among other algorithms such as the *Wolff algorithm* [4] and *Glauber dynamics* [5], we will most frequently utilise the Metropolis algorithm which is defined in Theorem 3.

Definition 3 (Metropolis-Hastings Algorithm) The Metropolis algorithm is the most commonly used Monte Carlo approximation in simulations of the Ising model.

The algorithm generates a sequence of sample values in such a way that, as increasingly more sample values are produced, the distribution of values more closely approximates a desired probability distribution.

Remark: The Metropolis algorithm [3] is an example of a **Markov Chain Monte Carlo algorithm** (*MCMC*) meaning that the probability of each event depends only on the state attained in the previous event. The desired distribution, for the example of the Ising model, would be the Boltzmann distribution introduced in Definition 2.

2 Computations

As a preliminary to our simulation, we must define and derive various physical quantities.

2.1 Mean Energy

The mean energy of the system can be calculated by taking the derivative of the partition function (2) with respect to β .

$$\frac{\partial \ln(Z)}{\partial \beta} = \frac{1}{Z} \sum_{\sigma} -H(\sigma) \exp \{-\beta H(\sigma)\} = -\bar{H}$$

Within our simulation however, we are able to calculate the mean energy of our system, by using our previously defined **Hamiltonian function** (1) by which we calculate the energy of one particular point on the square lattice.

$$H(\sigma) = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j - \sum_j h_j \sigma_j$$

Assuming a ferromagnetic system ($J = 1$) and no external magnetic field ($h = 0$), our energy calculation simplifies to:

$$H(\sigma) = -\frac{1}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

Thus, to calculate the mean energy, we take the sum of the energy over all points on the lattice of dimension $N \times N$ and divide by N . This can be represented by the following expression:

$$\overline{H} = -\frac{1}{2} \left\langle \sum_{\langle i,j \rangle} \sigma_i \sigma_j \right\rangle \quad (4)$$

2.2 Variance

Interestingly, if we differentiate the mean energy with respect to β again (i.e. the second derivative of the partition function with respect to β), we are given the variance of the energy:

$$\frac{\partial^2 \ln(Z)}{\partial \beta^2} = \text{Var}(H) \quad (5)$$

Proof 1

$$\begin{aligned} \frac{\partial^2 \ln(Z)}{\partial \beta^2} &= \frac{1}{Z} \sum_{\sigma} -H(\sigma) \exp \{-\beta H(\sigma)\} \\ &= \frac{1}{Z} \sum_{\sigma} H^2(\sigma) \exp \{-\beta H(\sigma)\} + \frac{1}{Z^2} \frac{\partial Z}{\partial \beta} \sum_{\sigma} H(\sigma) \exp \{-\beta H(\sigma)\} \\ &= \sum_{\sigma} H^2(\sigma) p(\sigma) + \frac{1}{Z} \frac{\partial Z}{\partial \beta} \sum_{\sigma} H(\sigma) p(\sigma), \quad : p(\sigma) = \frac{1}{Z} \exp \{-\beta H(\sigma)\} \\ &= (H^2) - (\overline{H})^2 \\ &= \text{Var}(H) \end{aligned} \quad \blacksquare$$

2.3 Mean Magnetisation

Similarly to the calculation of mean energy, for an $N \times N$ lattice, we can take the net magnetisation of the lattice.

$$M = \sum_{i=1} \sigma_i \implies \overline{M} = \left\langle \sum_{i=1} \sigma_i \right\rangle \quad (6)$$

Such that σ is the magnetisation of a single point on the lattice where $\sigma \in \{+1, -1\}$.

2.4 Derivation of the Specific Heat

To find the equation for the specific heat of the system, we differentiate the mean energy \overline{H} , with respect to temperature T .

$$C = \frac{\partial \overline{H}}{\partial T} = k_B \beta^2 \text{Var}(H)$$

Remark: We find that this result is closely related to the variance, which is interesting since the variance is the second derivative of the mean energy with respect to β . This means that if we find the variance of the system, we are able to estimate its specific heat [3].

Proof 2

$$\begin{aligned}
 C &= \frac{\partial \bar{H}}{\partial T} = \frac{\partial}{\partial T} \left(-\frac{\partial \ln(Z)}{\partial \beta} \right) \\
 &= \frac{\partial \beta}{\partial T} \frac{\partial}{\partial \beta} \left(-\frac{\partial \ln(Z)}{\partial \beta} \right) \\
 &= -\frac{1}{k_B T^2} \left(-\frac{\partial^2 \ln(Z)}{\partial \beta^2} \right) \\
 &= \frac{1}{k_B T^2} \text{Var}(H) \\
 &= k_B \beta^2 \text{Var}(H)
 \end{aligned}$$

■

2.5 Magnetic Susceptibility

The magnetic susceptibility is defined as a ratio of the magnetisation of the system. Mathematically, it can be represented as

$$\chi = \frac{\partial \langle M \rangle}{\partial T} \quad (7)$$

Such that $\langle M \rangle$ is the mean magnetisation (6) and T is the absolute temperature of the system. This expression for χ can also be represented as

$$\chi = \beta \sum_{\langle i,j \rangle} \langle \sigma_i \sigma_j \rangle = \beta \sum_{\langle i,j \rangle} \langle M \rangle \quad (8)$$

This is the calculation that will be used in Section 3.2.2 when we simulate the relationship between magnetic susceptibility and temperature.

2.6 Critical Temperature

For the *isotropic* case $J = J^*$ (where the spin-spin interactions are uniform and identical in all directions), the relation for critical temperature T_c is:

$$\frac{k_B T_c}{J} = \frac{2}{\ln(1 + \sqrt{2})} = 2.269 \quad (9)$$

3 Simulation

3.1 Visualising Phase Transition

In this section, we will begin to study the simulation of the two dimensional Ising model using previously described Monte Carlo integration methods, such as the Metropolis algorithm(3). As well as this, we will construct plots based on computations of our desired physical quantities with the goal of displaying evidence of phase transition at the Curie temperature, or more commonly the **critical temperature**.

3.1.1 Initial Model

We can construct an initial simulation of the Ising model by generating a defined $N \times N$ lattice consisting of spin states $\sigma \in \{+1, -1\}$ [6]. We will represent these states of magnetic spin via colours of black and white.

A common method of generating a random array of $+1$ and -1 values would be to utilise a simple Gibbs sampling method [3]. Alternatively, we can generate random values numerically using NumPy [7] in Python.

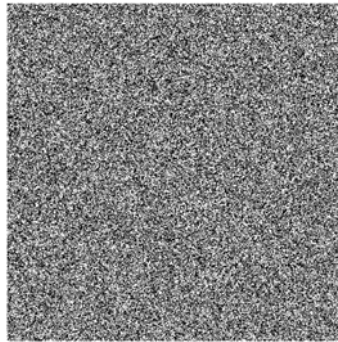


Figure 2: Initial lattice of dimensions 500×500

The lattice in Figure 2 will be the foundation of our simulations and computations going forward.

3.1.2 Application of the Metropolis Algorithm

We can use our previous knowledge of the Metropolis algorithm (3) to simulate our above lattice undergoing **phase transition**. The goal of this simulation would be to reach a ferromagnetic state such that all the spins are pointing in the same direction.

To simplify our simulation, we will mitigate the effect of an external magnetic field, h within our energy calculation. Thus, our expression for the Hamiltonian function(1) becomes:

$$H(\sigma) = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \quad (10)$$



(a) Initial lattice (b) 2000 iterations (c) 3000 iterations (d) 4000 iterations (e) 10000 iterations

Figure 3: Initial 500×500 lattice undergoing increasing iterations of the Metropolis algorithm.

Firstly, we must define the steps to undergo the Metropolis algorithm in the example of our model.

Definition 4 (Metropolis Algorithm: Steps) To undergo the Metropolis algorithm with the example of The Ising model, we must undergo the following steps:

1. Call the current lattice state μ .
2. Choose a random point on the lattice $\sigma_i \sigma_j$ which we can refer to as v . The probability such that we accept this new state v is $P(\mu \rightarrow v)$.
3. Through calculation via our simplified Hamiltonian(10),
 - If $H_v > H_\mu$, $P(v \rightarrow \mu) = 1$,
 $P(\mu \rightarrow v) = \exp\{-\beta(H_v - H_\mu)\}$ By which our desired distribution is the Boltzmann probability(2).
 - Else:
 $H_\mu > H_v$, $P(\mu \rightarrow v) = 1$. Via the law of total probability.
4. Flip the spins, i.e. change to state v with the given probabilities defined above.
5. Repeat from Step 1. until we appear to reach an ordered state, or equilibrium state.

The rate at which we reach an ordered state will depend on the temperature of the system. Furthermore, whether or not we reach a state of ferromagnetism will depend on the number of algorithm iterations. We can apply the steps of the Metropolis algorithm to our initial lattice in Figure 2 with constant temperature.

With regard to Figure 3, we are assuming the model is ferromagnetic ($J = 1$), there is no external magnetic field ($h = 0$), and we are maintaining a constant temperature ($\beta = 10$).

We can observe that as $n \rightarrow \infty$, or as the number of iterations greatly increases, the simulation begins to show evidence of phase transition occurring from a random, disordered state to a ferromagnetic, ordered state. Although the model appears to be ferromagnetic, we will *almost* reach a state of equilibrium and, unless we run our simulation $n = \infty$ times, it is extremely difficult to give a clear example of the model reaching equilibrium.

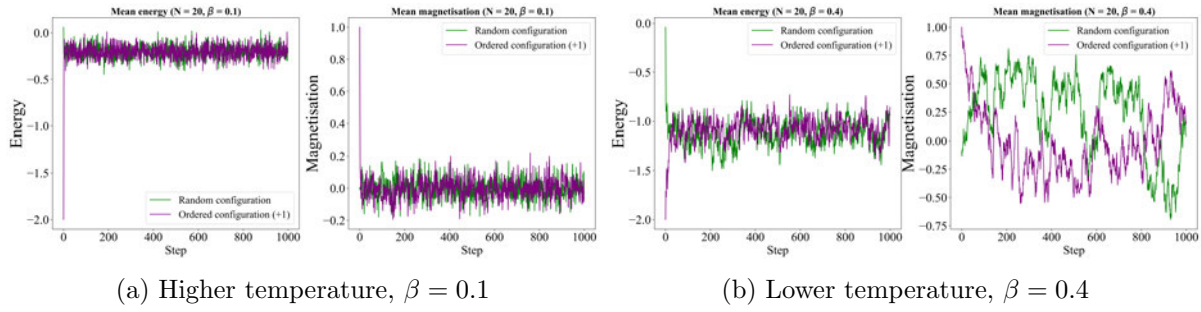


Figure 4: Relationship between mean energy and mean magnetisation

3.2 Plotting Physical Quantities

Using our previously defined physical quantities in Section 2, we aim to:

- Display the influence of temperature on reaching an ordered state.
- Display the model undergoing phase transition at the critical temperature.

3.2.1 Fluctuating Temperature and its Effect on Ordered States

To display the relationship between temperature and reaching an 'equilibrium' or ordered state. We must first compute the mean energy and mean magnetisation of the system. Our hypothesis is that, at low temperatures, the individual spins on the lattice will align to minimise free energy and we will reach an ordered state. In our simulation [8], we will compute the mean energy and mean magnetisation beginning with two lattices: one of random configuration, and one beginning in a ferromagnetic state. This is with the intention of better displaying phase transition between varying ordered states.

We can observe from Figure 4 that at low temperatures, we remain in an ordered configuration of net zero magnetisation. Conversely, at high temperatures, the energy of the system increases and we tend to a disordered configuration, despite already beginning in an ordered state.

Remark: As previously described within Definition 2 (Boltzmann Distribution), the temperature of the system follows a thermodynamic beta. This means that the relationship between absolute temperature and β is inversely proportional. $\beta = (k_B T)^{-1}$.

3.2.2 Phase Transition at the Critical Temperature

As stated in Definition 9, the **critical temperature** of the Ising model is $T_c = \frac{2}{\ln(1+\sqrt{2})} = 2.269$. A ferromagnetic material becomes magnetised when the temperature, T is below the critical temperature [9]. Thus when the temperature is low, as previously shown in the above plots, most spins acquire the same orientation, i.e. we reach an ordered state. As well as this, to fluctuate from an ordered to a disordered state, we have a phase transition at the critical temperature.

Next, we will now fluctuate the temperature to show that, as we approach the critical temperature, we can observe a phase transition. Using our physical quantities described in Section 2, we can observe the following relationships.

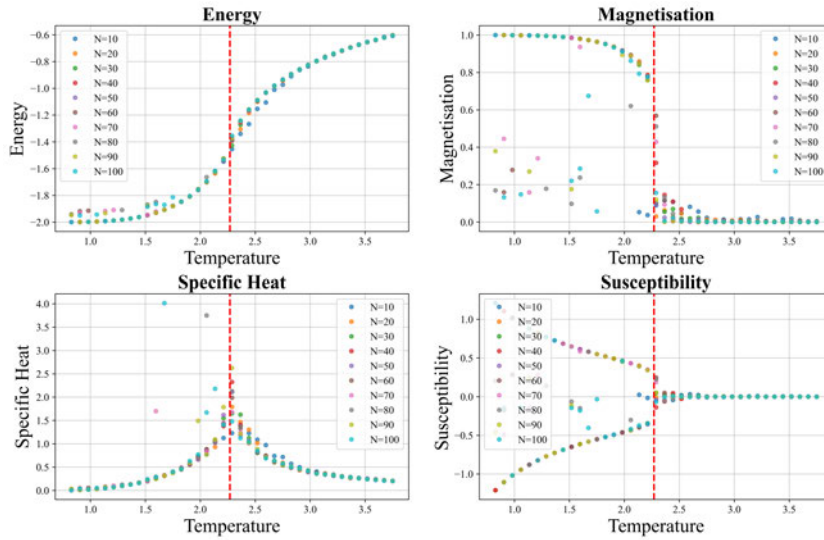


Figure 5: Mean energy (\overline{H}), mean magnetisation (\overline{M}), specific heat (C), and magnetic susceptibility (χ) plotted against varying temperature approaching critical temperature, $T_c = 2.269$

Remark: In our computation, we are simulating at varying lattice dimensions. As Figure 5 suggests, we are simulating from $N = \{10, 20, \dots, 100\}$ for an $N \times N$, two-dimensional lattice. This is in order to display that phase transition is invariant to lattice dimension. These are the findings of 5 per quantity:

- **Energy:** Non-linear relationship that displays an energy decrease at the critical temperature. As well as this, the critical temperature remains constant despite an energy fluctuation.
- **Magnetisation:** Quickly reaches 0 net magnetisation after undergoing phase transition from an ordered to disordered state as temperature is increasing (Section 3.2.2).
- **Specific heat:** Conversion at the critical temperature.
- **Magnetic susceptibility: Recall:** The susceptibility is a ratio of the magnetisation. Thus, like the magnetisation plot, the susceptibility will also converge at the critical temperature with a value of 0.

4 Proof in Square Lattice Dimensions

One-Dimension:

Ising carried out an exact calculation for the special case of a one-dimensional lattice. His analysis showed that there was no phase transition to a ferromagnetic ordered state at any finite temperature [1]. The one-dimensional model can be thought of as a linear horizontal lattice, where each site only interacts with its left and right neighbour. The system is disordered, for any positive β , the correlations $\langle \sigma_i \sigma_j \rangle$ decay exponentially in $|i - j|$:

$$\langle \sigma_i \sigma_j \rangle_\beta \leq \exp\{|i - j|\}$$

A recently relevant application of the one-dimensional Ising model is the spread of diseases, more specifically being used to model the speed of contamination. The 'spin' in this context are infected or non infected people [1].

Two-Dimensions:

Ising wrongly predicted that a phase transition does not occur in higher than one-dimension. In 1936, Rudolf Peierl showed that the two-dimensional version must have a phase transition at finite temperature. Finally in 1944, the two-dimensional Ising model without an external field was solved analytically by Lars Onsager by a transfer-matrix method. [1][10]

Kramers and Wannier were also able to show that the high-temperature expansion and the low-temperature expansion of the model are equal up to an overall rescaling of the free energy. This allowed the phase transition point in the two-dimensional model to be determined exactly, under the assumption that there is a unique critical point.

Three-Dimensions:

As in two dimensions, Peierl's argument shows that there is a phase transition, however many theoreticians have searched for an analytical three-dimensional solution for many decades, which would be analogous to Onsager's solution in the two-dimensional case. Such a solution has not yet been found, although there is no proof that it may not exist.

5 Triangular Lattice

Constructing the Model:

Recall: For the Ising model on a square lattice, we suppose we have a series of atoms, with a free electron in their outer shells, on the vertices of a square $N \times N$ lattice, with each edge representing an interaction between electrons.

For the triangular lattice, we follow this same general theory, however now the atoms sit on the vertices of a triangular lattice, with each of these spins having three body interactions from their **next-nearest neighbours**.

Remark: We solve our triangular lattice model using the same Hamiltonian function introduced in Section 1.1.

5.1 Phase Transitions

Restricting Nearest Neighbours:

Recall: The Ising model on a square lattice restricts atoms to only interact with their **nearest neighbours**, allowing for this model to exhibit phase transitions.

However, if we apply this theory to the triangular lattice, the system becomes what we describe as **frustrated**.

Definition 5 (Geometrical Frustration) A phenomenon in condensed matter physics where, for antiferromagnetic couplings, the system is unable to find a **unique ground state**.

In order to visualise this concept, if we imagine three spins on the vertices of a triangle. Once two of these spins align anti-parallel, the third is frustrated as its two possible orientations (up or down) give the same energy, hence it cannot simultaneously minimise its interactions with both of the other two.

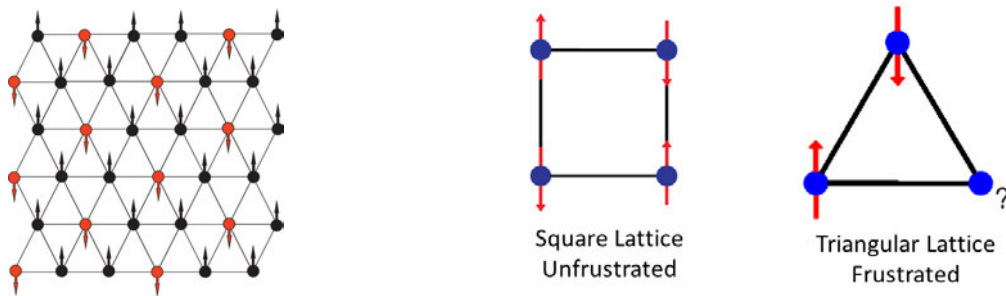


Figure 6: Triangular lattice structure [left] and its geometrical frustration visualised [right].

Due to the system being frustrated, as the temperature approaches zero:

- The process of atoms aligning proceeds much slower than in ordinary frustrated systems.
- The **residual entropy** does not disappear [11].

As a result of this, when atoms are restricted to their nearest neighbours and the system is frustrated, the spin ordering of the atoms is strongly suppressed and thus the Ising model on a triangular lattice does not exhibit phase transitions at any finite temperatures.

The question is whether we can alter our model in order to allow for phase transitions.

Achieving Phase Transitions:

Suppose that we adapt the way we construct our model by no longer restricting atoms to only interact with their nearest neighbours, yet we now allow them to interact with their next-nearest neighbours. Doing this, as well as adding an **external magnetic field**, subsequently stabilises the spin state of the atoms, and as a result the system exhibits phase transitions [12].

5.2 Applications of the Triangular Lattice Model

Universality:

Definition 6 (Universality) An aspect of critical phenomena where, under the correct conditions, several systems can operate under the same general theory.

The Ising model is a particularly perfect example of **universality**. Due to the model's general simplicity and versatility, it can be used in many different fields of condensed matter physics.

Applications:

- **Two dimensional triangular lattice:** Can be used to describe a variety of real materials such as $Ca_3Co_2O_6$, $CsCoCl_3$, $CsCoBr_3$, FeI_2 , with each of these materials exhibiting multistage magnetism behaviours [12].
- **Three dimensional triangular lattice:** Is experimentally relevant in a range of systems which include artificial dipolar magnets, real materials (such as $Ba_3CuSb_2O_9$), and frustrated Coulomb liquids [11].

Remark: There are also a vast amount of applications for the square lattice Ising model, with it being used for a variety of simulations in fields such as spin glasses, alloys, and lattice gases [13].

6 Conclusion

The Ising model is an extensive area of condensed matter physics with research and discoveries continuing daily. During this report, we have explored the fundamentals of the model and the theory behind it, defining key concepts such as the Hamiltonian function, the Boltzmann distribution, as well as introducing the Metropolis-Hastings algorithm. We also delved into computation of the model, exploring specifically the mean energy, variance, mean magnetisation, specific heat, and magnetic susceptibility, as well as using these ideas to simulate our model. We then expanded our model by looking at alternative dimensions and lattice structures, specifically the triangular lattice.

Although this report has investigated a range of subjects, it is important to be aware that there is limit to how much is covered, and thus the reader is strongly encouraged to continue their own research into the topic.

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A Acknowledgements

██████████ 1, 2.6, 4, 6

James ██████████: 1.1 - 1.2, 2.1, 2.3, 2.5, 3, 6

██████████ 2.1 - 2.2, 2.4, 5, 6

B Group Meeting Log

All group meetings were held in the Phillip Robinson Library.

All members were present at each meeting.

Week 1

- *25/09/23, 10:00 – 13:00*
- Understanding topic and background reading.
- Allocating roles for research.

Week 2

- *02/10/23, 10:00 – 13:00*
- Planning the simulation and writing draft code in Python.
- Further independent research.
- Solidifying roles for independent research.

Week 3

- *09/10/23, 10:00 – 13:00*
- Discuss outcome of meeting with supervisor (further computations for the simulation).
- Planning presentation structure.
- Continued independent research.

Week 4

- *16/10/23, 10:00 – 13:00*
- Ensured that each member of the group was using a consistent layout within the presentation.
- Found various sources prior to the lecture presented by Library staff.
- Constructed the first draft of the presentation.

Week 5

- *23/10/23, 10:00 – 13:00*
- Modified presentation based on supervisor feedback.
- Constructed the second draft of the presentation with a continued focus on mathematical accuracy.
- Sent the second draft to our supervisor, awaited feedback, and then constructed a third draft.
- *26/10/23, 13:00 – 14:00*
- Rehearsed the presentation based on the third draft ensuring timings were correct and small inconsistencies in our own presentation styles were mitigated.

Week 6

- *30/10/23, 8:45 – 9:45*
- Final rehearsal of the presentation before the examination.

Week 7

- *13/11/23, 10:00 – 13:00*
- Studied L^AT_EX formatting, as a group, for the design of the poster as well as the report.
- Planned the video presentation and constructed the first draft of the poster.

Week 8

- *20/11/23, 10:00 – 13:00*
- Finalised our poster after supervisor feedback.
- Individually curated notes and a plan for the video presentation.

Week 9

- *27/11/23, 10:00 – 13:00*
- Recorded the video presentation and finalised our poster after our advisory session.
- Assigned individual research based on chapters in the report.

Week 10

- *04/12/23, 10:00 – 13:00*
- Worked on separate sections of report following advisory session.

Week 11

- *11/12/23, 10:00 – 13:00*
- Continued working on the report.
- Sent supervisor draft to finalise and submit on 15/12/23.
- *14/12/23, 10:00 – 13:00*
- Adjusted report based on supervisor feedback.