Ising Model

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This paper explores the implementation of the 2D Ising model using the Metropolis Monte Carlo algorithm in the programming language: Python. A 2D Ising model is built to analyze the scope of behaviors of ferromagnetic system and compare them to real phase transitions.

I. INTRODUCTION

A. Ising Model

The Ising model is a statistical model introduced in 1920 by physicist Willhelm Lenz to describe the properties of a ferromagnetic system undergoing phase transitions. It consists of a regular N-dimensional lattice where each node can take two states, which can be described with the values +1, -1 and we refer to them as up and down. This project examines the two-dimensional Ising model which uses a N × N lattice. Generally, computing and interpreting thermodynamic variables is rather ineffective because all possible states of the given system need to be taken into consideration when calculating the partition function. However, simplifications allow the Ising model to be easily implemented numerically.

Applying simplifications to our system does not affect our results, because in this case microscopic changes in a system do not affect its thermodynamic variables[1]. This property allows phase transitions to be classified within separate classes, each with the same parameters, equations and constants. As a result, the system is comparable to a ferromagnet and is called "Ising model". The approximations from the Ising model are hence used to understand phase transitions of ferromagnetic systems.

The simplifications include the assumption that the exchange energy term (J) is constant in all cases and is positive: $J > 0$. Consequently, the interaction is assumed to be isotropic: each atomic spin only interacts with its adjacent spins and neglects long-range interactions. For example, we could say that the forces are such that when two neighboring spins are the same (both +1 or both —1) the energy is -U, and when two neighboring spins are different (one is +1, the other —1) the energy is +U. The last simplification involves folding the lattice into a torus-shape to connect the lattice boundaries and allow spins from opposite edges to be considered neighbors. This ensures greater resemblance of an ideal infinite-size lattice.

B. Hamiltonian

The Hamiltonian of this system is defined as the sum of all spin interactions in the lattice. In our case, it represents the internal energy of a given configuration and it can be written as:

$$H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j - \mu \sum_j \sigma_j \tag{1}$$

Where the first and the second terms include nearest-neighbor interaction and the interaction with the external magnetic field respectively. J is the coupling constant between the spins, while σ_i and σ_j are values for the spins at corresponding positions, the magnetic moment is given by ν and represents the strength of the external magnetic field.

For this project coupling constant J is assumed to be positive as we only consider ferromagnetic behaviour. Note that for $J > 0$, the Hamiltonian will be minimised when spins align with their neighbours, which will be the preferred configuration. This represents the material being ferromagnetic. In case of a negative J, preferred configuration is with spins opposing each other, which corresponds to anti-ferromagnetic interactions.

The configuration probability $P_\beta(\sigma)$ represents the probability of a system being in a particular state (in equilibrium) and is given by the Boltzmann distribution with inverse temperature greater than zero:

$$P_\beta(\sigma) = \frac{\exp(-\beta H(\sigma)}{Z_\beta} \tag{2}$$

where the normalisation constant Z is a partition function given by:

$$Z_\beta = \sum_\sigma \frac{\exp(-H(\sigma))}{K_b T} \tag{3}$$

which refers to the function of a thermodynamic variable that describes properties of the overall thermodynamic system in equilibrium.

C. Ferromagnetism

In ferromagnetic materials, an increase in temperature causes entropy to compete with the tendency for its dipoles to align. Hence, above a certain point called the Curie temperature, a second-order phase transition takes place and the system can no longer maintain a spontaneous magnetization thus becoming paramagnetic. When material is cooled below the Curie temperature,

electron spins of atoms in microscopic regions (domains) become aligned.

Magnetic domains are always present in ferromagnetic materials due to the nature of bounding of atoms in the material. The magnetic field is strong in the domain because of the large net field strength, however randomly ordered domains cause the ferromagnetic material to be demagnetised. In the presence of an applied magnetic field, the domains may line up with each other, resulting in the material being more magnetized. Due to the nature of ferromagnetism, the domains remain aligned in absence of the applied field.

D. Phase Transitions

Phase transitions are transitions between different physical states of the same substance. During a phase transition of a given medium, certain properties of the medium change, often discontinuously, as a result of the change of external conditions, such as temperature, pressure, or others.

Phase transitions are divided into two broad categories. First-order phase transitions (discontinuous) are those that involve a latent heat. During such a transition, a system either absorbs or releases a fixed amount of energy per volume while temperature of the system remains constant. Examples are the melting of ice or the boiling of water. Second-order phase transitions (continuous) are characterised by a peaked or divergent heat capacity and infinite correlation length around a point in parameter space called the critical point. Correlation length describes how microscopic variables at a distance are related. Near the critical point, spin fluctuations become more correlated as spins are infinitely aware of their neighbors. Second-order phase transitions include transitions associated with an emergence of magnetism, superconductivity, superfluidity, orientational order, etc.

Second order phase transitions are also seen in magnetic systems, such as at the Curie point in ferromagnets, which indicates the transition between the paramagnetic phase and the ferromagnetic one. That means that below the Curie temperature, the system presents spontaneous magnetization in absence of an external magnetic field, whereas above it the system is not magnetized and only responds when an external magnetic field is applied.

E. Lars Onsager's Exact Solution

The one-dimensional Ising model was solved by Wilhelm Lenz's student Ernst Ising[2]. Consequently, the two-dimensional model with no external field for the infinite square lattice was analytically solved by Lars Onsager in 1944[3], showing that the model undergoes a phase transition at the critical temperature given by:

$$T_c = \frac{2J}{K_b \ln(\sqrt{2}+1)} \tag{4}$$

The spontaneous magnetization that occurs at temperatures lower than T_{crit} was shown to be:

$$M = [1 - \sinh^{-4} \frac{2J}{K_b T}]^{\frac{1}{8}} \tag{5}$$

Onsager's exact solution allows us to compare and prove the validity of approximations.

F. Critical Phenomena

Critical phenomena refer to the collective name of critical points. Generally, most of them are deduced from the divergence in correlation length. The critical phenomena include scale relations, which involve linear transformations - enlarging and shrinking objects - by scale factors, universality, critical exponents from power-law divergences and fractal nature.

The behavior of physical values near a second phase transition can be described through critical exponents in the Ising model. It is known through observations that the thermodynamic properties of the system near a phase transition do not depend on changes in microscopic characteristics of the physical system. However they do depend on general features such as dimensionality and symmetry. This phenomenon is known as universality and is a prediction of the renormalization theory of phase transitions - a apparatus that permits investigation of the changes of physical system viewed at varying scales.

As briefly mentioned earlier, at zero temperature, the system can take either +1 or -1. At higher (but still below the T_C) temperature, the state is still globally magnetized but clusters of the opposite begin to resurface. As the temperature keeps increases, the clusters begin to contain clusters in within and their size, which is related to the correlation length, increases to infinity until it divergence takes place at T_{Crit}. This suggests that the entire system is made up of several clusters and there is no global magnetization. Above the T_{Crit}, the system is now globally disordered containing ordered clusters inside.

Note to the importance of critical points, critical exponents can be calculated by power-law fitting near T_{Crit} magnetisation of the ferromagnetic system. Here β is the critical exponent evaluated via the Monte Carlo simulations of lattice models. The accuracy of this first principle method depends on available computational resources, which determine the ability to go to the infinite volume limit and to reduce statistical errors.

$$M_s(T)/M_0 = A[(T_{crit} - T)/T_{crit}]^{\beta} \tag{6}$$

The exact values of critical exponents are:

Exponents		values
Magnetic order parameter	β	0
Magnetic Susceptibility	γ	1/8
Heat Capacity	α	7/4

G. Metropolis Monte Carlo Algorithm

The metropolis algorithm is the most commonly used Markov chain Monte Carlo method to calculate Ising model estimations. It consists on obtaining a sequence of random samples from a probability distribution from which direct sampling is difficult, especially when the number of dimensions are high. This sequence is used to approximate the distribution or to compute an integral (expected value).

The Metropolis-Hastings Monte Carlo algorithm receives an input which in our case is a $N \times N$ square lattice - which have the possible states +1 and -1 - and temperature. A point on the lattice will be randomly chosen and its energy difference, δE, between the spin at the site and the flipped spin at the same site is calculated as selection probabilities $g(\mu, \nu)$ which represent the probability that the new state ν (flipped state) is selected by the algorithm out of all states, given that one is in state μ.

It then uses acceptance probabilities $A(\mu,\ \nu)$ which involve examining the selection probabilities $g(\mu, \nu)$ to determine whether the spin will be flipped into new state ν, or remain as state μ. In detail, if the $\delta E \leq 0$, which means the flipped state is energetically more stable, the spin is flipped and new state ν is accepted. If $\delta E \leq 0$,the spin may still be flipped into new state ν, if a randomly chosen point is lower than the Boltzmann distribution for the δE. This is to satisfy detail balance: at equilibrium, each elementary process is in equilibrium with its reverse process.These changes are saved and other random lattice points are picked and checked until the total number of steps is reached and the final lattice is printed out. The printed lattice is often ferromagnetic, in which all sites point in the same direction.

H. Calculating Observables

With simulations of the system running, properties can be investigated by calculating observables and their dependence on the temperature of the system. The average energy per spin is determined by:

$$< E >=< \sum_{<i,j>} H_i j >= \frac{1}{2} < \sum_{i,j} H_i j > \qquad (7)$$

the 1/2 considers that every pair is counted twice in the sum. $\langle E \rangle$ should be a continuous function of temperature, with a point in inflection at T_{Crit}, and should approach 0 after this point, signifying that a phase change has occurred and the materials has become disordered and paramagnetic.

The average magnetization per unit spin is given by:

$$< M >= \frac{1}{N^2} \sum_{(i,j)} \sigma_i j \qquad (8)$$

By plotting the average magnetisation per spin after each implementation of the Metropolis algorithm against the number of iterations, the average magnetisation should be seen to approach a constant value signifying that equilibrium has been achieved, and the minimum number of iterations required to achieve is thus determined, which will help to increase the efficiency of the algorithm. The magnetisation can also be used to show that a phase transition has occurred in the material and approximate the Curie temperature T_C . By plotting the average magnetisation after equilibrium has been reached against a series of values of temperature, a phase transition should be observed at T_C . The magnetisation should be 1 or -1 initially as it is ferromagnetic, but after T_C it should be zero, since it becomes paramagnetic [4].

The formulas for calculating Specific Heat Capacity (C_ν) and Magnetic susceptibility (χ) are given as:

$$C = \frac{< E^2 > - < E >^2}{K_b T^2} \qquad (9)$$

$$X = \frac{< M^2 > - < M >^2}{K_b T^2} \qquad (10)$$

For both plots of C_ν against temperature and χ against temperature, they should exhibit a discontinuity at T_{Crit}, which would indicate that the phase transition that has occurred is of second order.

II. METHODS

A. Simulation

We chose the transition probability to be Boltzmann distribution. We also chose states which our system passes through based on this transition probability.

1. *Absence of magnetic field, ν = 0*

For 90 uniformly distributed temperatures in the range 0.5 - 3.4 (adimensional units), an initial ferromagnetic (all +1 spins) matrix of size 50 × 50 was created in which the metropolis algorithm was implemented per 100 sweeps for equilibration. Consequently, the average magnetization and total energy of every 100 steps for 900

sweeps was calculated and was followed by their averages. This program was run 5 times for each temperature and the average of the 5 runs was computed.

With the average magnetization and total energy for temperatures 0.5 - 3.4, parameters which experience divergences such as heat capacity and magnetic susceptibility were calculated to deduce the T_{Crit} of the system. The T_{Crit} value corresponds to the peak (divergence) of $\langle\chi\rangle$ plotted against temperature.

2. *Forking Graph*

The forking graph of magnetization is produced by initializing a random lattice of size 50×50 with no magnetization strength for values in temperature range: 0.5-3.4. Just like mentioned before, the metropolis algorithm is implemented per 100 sweeps for equilibration but instead of taking their average, the values are plotted against temperature to produce the forking graph.

3. *Presence of magnetic field*

A constant value of temperature 1.5 is assumed for this simulation followed by the same initial conditions set for the lattice used without the magnetic field (50×50 size and ferromagnetic). With these conditions, every value of ν in the range 0.1 to 2.0, the Metropolis Algorithm is run for 100 sweeps for equilibration. Consequently, the average magnetization of every 100 sweeps for a total of 900 sweeps is recorded and their averages are calculated.

B. Coarse-grained modelling

Coarse-grained modelling is an efficient method for simulating complex systems using their simplified representation. In this project, the coarse-grained Ising model is used to study properties of a ferromagnetic system near the critical point and to prove the near-critical phenomena.

The initial conditions for the lattice are set to size 729 $\times$ 729 (for more illustrative results) and the absence of a magnetic field. For every value in the temperature range of $T_{Crit} - 0.3$, T_{Crit} and $T_{Crit} + 0.3$, the matrix conducts 1000 sweeps and its states are recorded. Coarse graining is conducted and the matrix is divided into N $\times$ N - N=3 in this project - equal matrices. A new matrix of the initial matrix divided by the N is set up where each spin represents the dominant mode of the corresponding N $\times$ N matrix in the initial matrix. This process is repeated 4 times and each new state is recorded.

C. Fit for Critical Exponents

Near T_{crit} the magnetisation obeys a power law,

$$M_s(T)/M_0 = A[(T_{crit} - T)/T_{crit}]^{\beta} \tag{11}$$

Least-squares fitting algorithm provided by the NumPy package from Python is used to find the value for the parameter β, which represents a critical exponent for magnetisation.

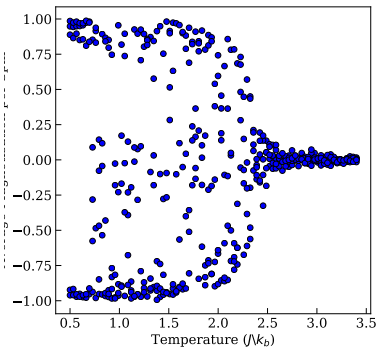


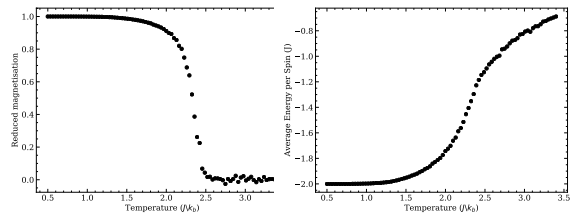
FIG. 1: Average magnetisation per spin obtained from 5 iterations of the Metropolis algorithm, each starting with random configuration for 50×50 lattice and given enough time to reach equilibrium. Eventually, each lattice, starting either from -1 or +1, with the exception of small fluctuations reaches disordered (symmetric) state, resulting in a characteristic 'fork-like' shape.

III. RESULTS AND DISCUSSION

The fork-like shape of Figure 1 also known as the bifurcation diagram is a good representation of what we have discussed regarding fluctuations at the critical temperature. The solid lines indicate the branches of stable and unstable state emerge from zero magnetization and the only globally stable state is the zero magnetisation state. The figure implies that the system undergoes spontaneous symmetry breaking below the critical temperature.

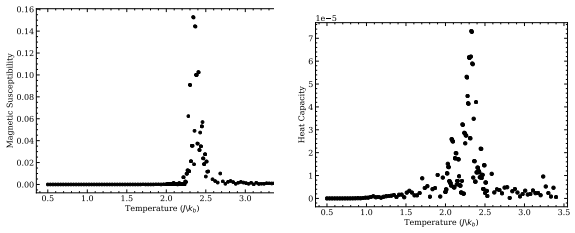
A sudden drop in average magnetization is found at T = 2.389 $\pm$ 0.1 J/k$_B$, which suggests the occurrence of phase transition. Thus we refer to this value of T as T_{crit}. Concurrently, the graphs of heat capacity (Fig. 2d) and magnetic susceptibility (Fig. 2c) show divergences that can be observed at the T_{crit}, which indicates a second-order phase transition. The energy is a continuous function of T and approaches ground state energy (-2J) as T goes towards 0, as expected.

The observations mentioned above can be seen in Figure 3, as the system undergoes a first-order phase transition at h=0.3.



(a) Reduced magnetisation

(b) Average Energy per Spin



(c) Magnetic Susceptibility

(d) Heat Capacity

FIG. 2: The measured observables for the 2D 50×50 square ferromagnetic lattice. Each point represents an average over 5 iterations of the Metropolis algorithm, for which 100 sweeps were made to reach the equilibrium and average over states was taken during 1000 sweeps.

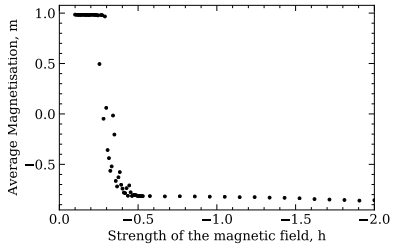


FIG. 3: Variation of the reduced magnetisation of 50 × 50 ferromagnetic lattice with strength of the external negative magnetic field h at a temperature of 1.5J/k_B

Function (6) with fitted parameters shows reasonable agreement with the exact solution for values close to T_{crit} (0.8 $T_{crit} < T < T_{crit}$) (Figure 4), as expected. The obtained value for β is 0.122, which is in good agreement with the exact value of 0.125.

Comparison of our graphs to exact solutions show great accuracy so far and support the idea that the Ising model estimates a valid approximations.

By conducting comparison of the results to actual ferromagnetic systems, our simulation data is shown to be in excellent agreement with the data for K_2CoF_4, K_2NiF_4, K_2MnF_4, MnF_2 from Ikeda et al.[5]

Finally, we would like to direct the viewer to Figure 6. A comparison between the characteristics of a model for

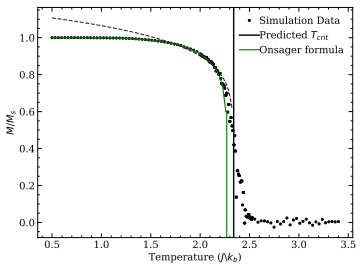


FIG. 4: Temperature variation of the reduced magnetisation along with Onsager's solution and fit for critical exponent. Predicted value for T_{crit} is displayed for comparison.

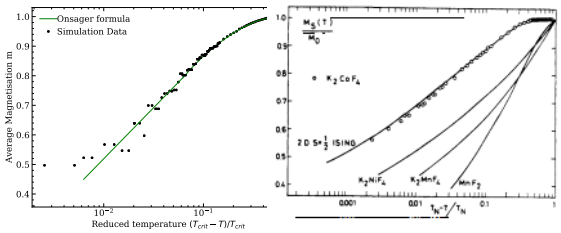


FIG. 5: Reduced magnetisation as a function of reduced temperature for simulated data (left), compared with data for several ferromagnetic compounds from [5] (right).

temperature around T_{crit} allows us to confirm theoretical deductions about critical phenomena. At the small scale matrices are virtually indistinguishable, but by scaling up and getting more general view of the system, we can observe that in (a) one state starts gaining dominance, whereas in (c) system becomes more and more symmetric (chaotic) with no apparent regions. In contrast, in (b) state is indifferent to scaling, which is a clear sign of infinite correlation length at T_{crit}. The limiting behaviour of the scaling is as follows: (a) would become a fully ordered state (either +1 or -1), (c) would be completely chaotic. In contrast, (b) would still preserve its self-similar nature.

Consequently, obtained value for $T_{crit} = 2.389 \pm 0.1$ J/k_B compares well with the theoretical value (4), which is 2,269 J/k_B.

IV. CONCLUSION

To conclude, the two-dimensional Ising model is an accurate way to describe the properties of a ferromagnetic system undergoing phase transitions. Despite computing approximations, the Metropolis Monte Carlo algorithm and equations allow us to consider the model to be similar to a ferromagnetic magnet and use it to understand

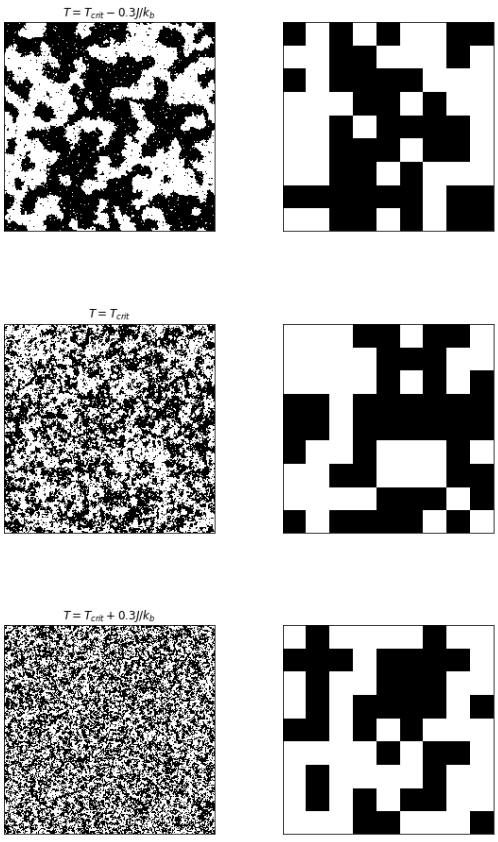


FIG. 6: States of 729 × 729 Ising model after 1000 sweeps of Metropolis algorithm (left) and after coarse-graining applied consequently 4 times (right) for (a) $T = Tcrit - 0.3J/k_B$; (b) $T = Tcrit$; (c) $T = Tricit + 0.3J/k_B$

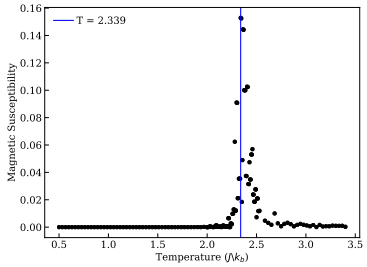


FIG. 7: T_{crit} corresponds to divergency in susceptibility

concepts too computer heavy to execute without inaccuracies. Further studies regarding the three-dimensional Ising model could be done with similar concepts used in this project wich lattices of greater sizes. This would probably require a supercomputer.

V. ACKNOWLEDGEMENTS

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