MINI PROJECT REPORT

TOPIC : MONTE CARLO SIMULATION OF ISING MODEL

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Introduction

Electrons possess a quantum mechanical property known as spin, where the value of spin measured along any axis is either $\hbar/2$ or $-\hbar/2$. Electrons, being negatively charged, repel each other electrostatically due to their like charges. Also, the Pauli exclusion principle dictates that no two electrons can occupy the same quantum state simultaneously. Thus, when considering a nearest-neighbour pair of electrons arranged on a regular grid, if they are anti-aligned, they can be close together since they occupy different quantum states, but they will repel each other electrostatically. Conversely, when aligned, they cannot approach each other closely without violating Pauli's exclusion principle, leading to weaker electrostatic repulsion between them. Hence arises the preference for alignment. Electrons on a regular lattice tend to align their spins in the same direction due to the energetically favourable parallel spin states. This alignment leads to the creation of a large net magnetic moment within the material.

Origin Of Ferromagnetism

Ferromagnetism arises from the collective alignment of electron spins in a material. When electron spins align in the same direction, the energy of the system decreases due to the exchange interaction, a quantum mechanical effect arising from the Pauli exclusion principle. As a result, neighboring electron spins in the material tend to align parallel to each other, leading to the formation of magnetic domains.

The energy difference between parallel and anti-parallel alignments of electron spins which is primarily electrostatic in nature drives the alignment of spins and results in the material exhibiting a spontaneous magnetization, even in the absence of an external magnetic field. Below a certain temperature called the Curie temperature, thermal fluctuations become insufficient to disrupt the alignment of spins, and the material retains its magnetization.

PROPERTIES OF FERROMAGNETIC MATERIALS:

- Permanent Magnetization: These materials retain significant magnetization even after the removal of an external magnetic field.

- Saturation Magnetization: At elevated magnetic fields, ferromagnetic materials reach maximum magnetization, termed saturation magnetization.
- Hysteresis: These materials display hysteresis, whereby their magnetization lags behind changes in the applied magnetic field. This characteristic is essential for various applications such as magnetic memory devices.
- Domain Structure: Ferromagnetic materials are comprised of multiple magnetic domains, each exhibiting uniform magnetization. Domain walls separate these domains, and their movement plays a pivotal role in the magnetization process.
- Soft and Hard Magnetic Materials: Ferromagnetic substances can be categorized into soft and hard magnetic materials based on their coercivity, which denotes resistance to demagnetization. Soft magnetic materials possess low coercivity and are easily magnetized and demagnetized, whereas hard magnetic materials have high coercivity and retain magnetization effectively.

Ising Model –A Brief Overview

Ising model is a mathematical tool to study how tiny magnets interact with each other in materials.

History: It was first proposed by Wilhelm Lenz and Ernst Ising in the 1920s to describe the magnetic properties of ferromagnetic materials.

Why we study Ising model: It is used to study phase transitions. It tells how some materials become magnets and others don't and how temperature affects this behaviour. It tells us about spin behaviour in materials.

Some Necessary Concepts and Formulas:

If a system is in thermal equilibrium with a temperature bath. Probability P_μ of being in state μ with energy E_μ is

$$P_\mu = \frac{1}{Z} e^{\beta E_\mu}$$

Where Z=$\sum_{\mu} e^{\beta E_{\mu}}$ is the partition function.

At equilibrium the following must be true :

$$\sum_{\mu} p_{\mu}\ P(\mu \ \rightarrow \mathrm{v}) = \sum_{v} p_{v}\ P(\mathrm{v}\ \rightarrow \mu\,)$$

Where $\boldsymbol{P}(\mu \ \rightarrow \mathbf{v})$ is probability of going from state μ to v. For our numerical methods. This is difficult to enforce but we can make it to be true by setting the

Detailed Balance Equation :

$$p_{\mu}\ P(\mu \ \rightarrow \mathrm{v}) = \ p_{v}\ P(\mathrm{v} \rightarrow \ \mu)$$

The Total energy(Hamiltonian) is :

$$\textbf{E}= -\boldsymbol{J}\sum_{<i,j>} \boldsymbol{\sigma_i \sigma_j}$$

Where σ_i is the spin of a single particle in the lattice(**either -1 or 1**) and the sum over $<\boldsymbol{i},\boldsymbol{j}>$ means summing over nearest neighbours for all points in the lattice.

Also *J* is the coupling constant representing the strength of interaction between adjacent spins.

Now satisfying the detailed balance

$$\frac{\boldsymbol{P}(\mu \rightarrow \mathbf{v})}{\boldsymbol{P}(\mathbf{v} \rightarrow \mu)} = \frac{\boldsymbol{p_v}}{\boldsymbol{p_\mu}} = \boldsymbol{e}^{\boldsymbol{\beta}(\,\boldsymbol{E_v}\ -\boldsymbol{E_\mu}\ )}$$

Phase Transitions:

In Simple words, phase transition is a change in the state of matter. In the context of the ising model, phase transitions are characterized by abrupt changes in system's behaviour. During the phase transition a paramagnetic material is becomes ferromagnetic as it is cooled below a critical temperature.

At high temperatures, thermal fluctuations dominate, and the spins of individual magnetic moments in the material are randomly oriented. This state is known as the paramagnetic phase. As the temperature decreases, the influence of thermal fluctuations weakens, and the spins begin to align with each other spontaneously, leading to the emergence of magnetic order. This transition from a disordered to an ordered magnetic state is the ferromagnetic phase transition. As the temperature is lowered below the critical temperature, the system undergoes a spontaneous symmetry breaking, and domains of aligned spins, known as magnetic domains, form within the material. These domains grow in size as the temperature decreases further, eventually leading to the establishment of long-range order in the system.

The Ising model captures this transition by considering a lattice of discrete spins, where each spin can take on two possible states: up or down. The interaction between neighbouring spins in the lattice is typically described by the Heisenberg exchange interaction, which favour parallel alignment of spins.

Critical Temperature: The critical temperature (Tc) in the Ising model represents the temperature at which the phase transition occurs. Below Tc, the system exhibits spontaneous magnetization, while above Tc, the magnetization vanishes. The critical temperature depends on various factors such as the dimensionality of the lattice, the strength of interactions, and the presence of external fields.

Universality of Critical Phenomenon : The critical behaviour of the Ising model exhibits universality, meaning that it is independent of microscopic details and depends only on certain macroscopic properties, such as dimensionality and symmetry. This universality allows researchers to classify different systems into universality classes based on shared critical behaviour.

Domain Theory : A Brief Overview

A domain is a Connected region of the lattice where all spins have the same value(all up or all down). Domains are separated by domain walls where neighbouring spins have different values

ENERGY AND DOMAIN WALLS

The energy of the ising model is lower when domains are formed because aligning neighbouring spins reduces the energy compared to random configurations. Domain walls increase the energy.

Metropolis Algorithm

THE IDEA: We want to find the equilibrium state μ in the magnet at a particular temperature $\beta. We$ will start with random lattice of spins, some pointing up and some pointing down and make it dance around using the equation above until it stabilizes itself into equilibrium

ALGORITHM:

- The current state is denoted as μ
- A random particle on the lattice is selected and it's spin is flipped, resulting in a new state, denoted as v.
  The objective is to determine the probability of accepting this new state.
- If $E_V > E_\mu$ then set **P(v->μ)=1** , thus
  P$(\mu \rightarrow \mathbf{v})$ = $\boldsymbol{e^{-\beta(E_v - E_\mu)}}$ **.** This satisfies the detailed balance equation.
  If $E_V < E_\mu$ then set **P**$(\mu \rightarrow \mathbf{v}) = \mathbf{1},$ ensuring that the detailed balance equation is maintained**.**
- The transition to state v is made based on the probabilities defined above. This process is repeated numerous times until an equilibrium state is reached.

  So The only thing that needs to be evaluated is
  -β($\boldsymbol{E_v - E_\mu}) = \sum_{k=1}^{4} \boldsymbol{\sigma_i \sigma_k}$
  where i represents the spin being flipped and σ_k are the four nearest neighbours to that spin.

  This evaluation is fundamental to Metropolis Algorithm.

Wolff Cluster Algorithm

1. A random selection is made of spin i.
2. The cluster is expanded by adding all nearest neighbours j of this spin, given that spins i and j are parallel and the bond between them has not been considered previously. The probability of adding a neighbour j to the cluster is determined by.

$$\boldsymbol{P_{ij} = 1 - exp(-2\beta J)}$$

3. Each spin j that is added to the cluster is also placed on a stack. Once all neighbours of spin i have been considered for inclusion in the cluster, a spin is retrieved from the stack, and the process is repeated for its neighbors.
4. Steps (2) and (3) are repeated iteratively until the stack is empty.
5. After the cluster is completed, all spins belonging to the cluster are inverted

Wolff Cluster Versus Metropolis Algorithm

Experimentally observed, The Wolff cluster algorithm is more efficient than the Metropolis algorithm for simulating the Ising model due to several reasons:

1. **Cluster Updates**: The Wolff algorithm updates spins in clusters rather than individually flipping each spin. This results in more significant changes to the configuration in a single update, leading to faster convergence to equilibrium configurations.
2. **Effective for Near-Critical Temperatures**: Near the critical temperature of the system, the Metropolis algorithm can become inefficient due to slow relaxation times and critical slowing down. In contrast, the Wolff algorithm

can efficiently update large clusters of spins, allowing for faster equilibration near critical points.

3. **Reduced Critical Slowing Down**: Critical slowing down refers to the phenomenon where the relaxation time of the system increases as it approaches criticality. The cluster-based updates of the Wolff algorithm can mitigate critical slowing down by effectively sampling configurations in the vicinity of critical points.
4. **Enhanced Ergodicity**: The cluster updates in the Wolff algorithm improve the ergodicity of the simulation by allowing for more extensive exploration of configuration space. This can lead to better sampling of phase space and more accurate estimation of thermodynamic properties.
5. **Fewer Rejections**: In the Metropolis algorithm, many proposed spin flips are rejected, especially at low temperatures when the energy barriers are high. The Wolff algorithm typically has a higher acceptance rate since it updates spins in clusters, leading to more efficient exploration of configuration space.

Overall, the Wolff cluster algorithm often outperforms the Metropolis algorithm for simulating the Ising model, particularly near critical points and at low temperatures, due to its ability to update spins in clusters and mitigate critical slowing down.

Lattice Behaviour At Different Temperatures

100 X 100 Lattice Temperature=1.25 and M=0.9986

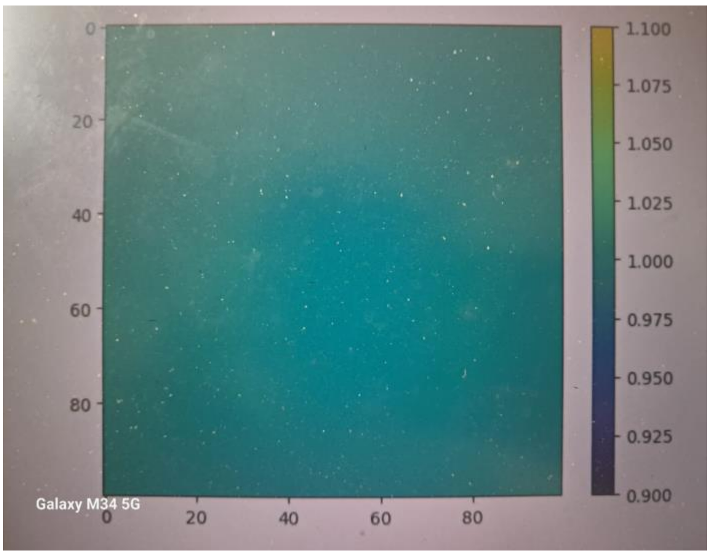


Fig 1

100X100 Lattice, Temperature=2.75 and M=0.0602

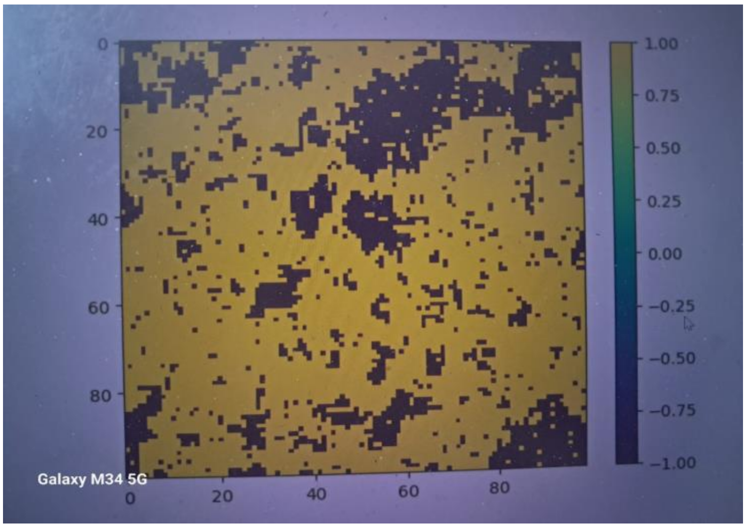


Fig 2

100X100 Lattice, Temperature=4 and M=0.0006

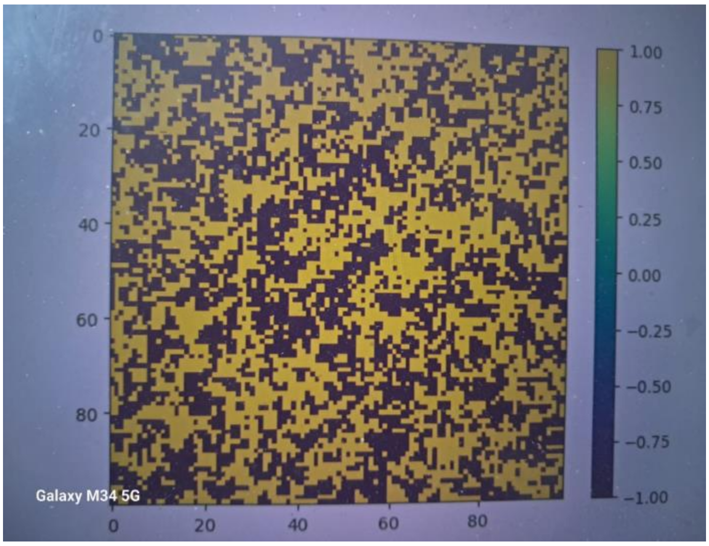
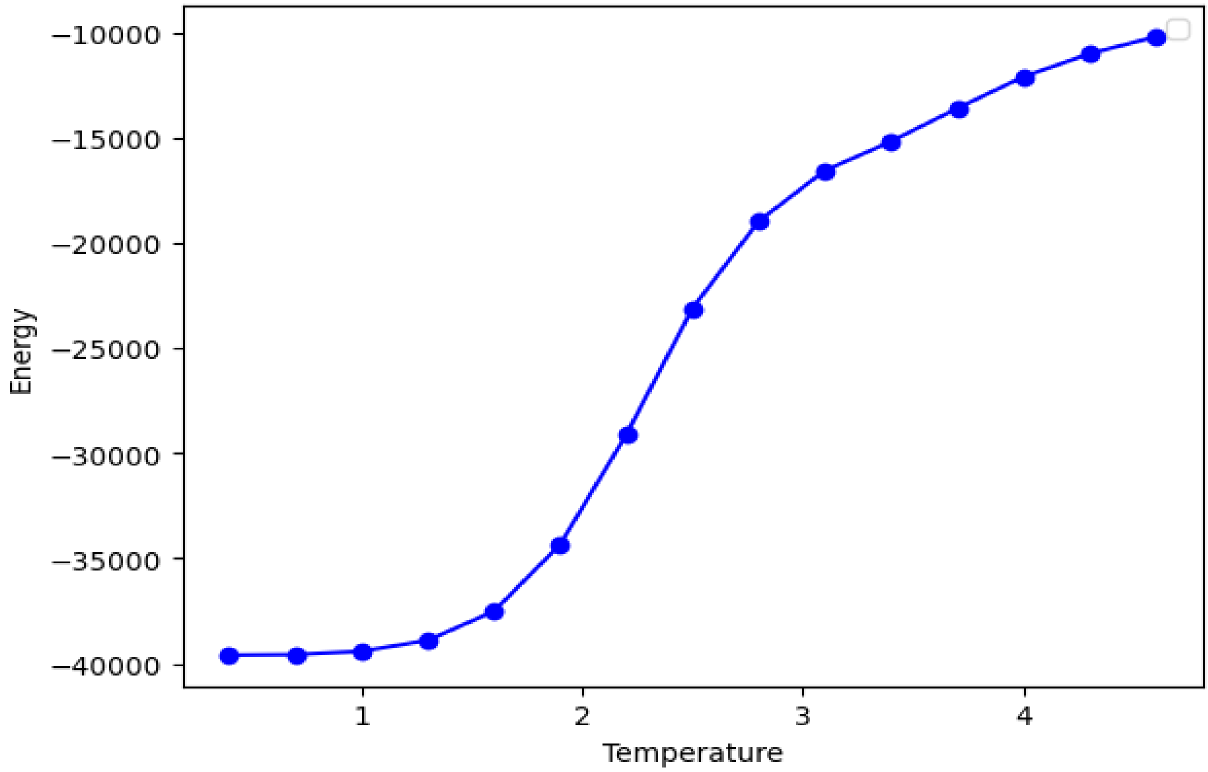


Fig 3

At low temperatures, the spins tend to align either all up or all down, resulting in a state of order known as ferromagnetism. As temperature increases towards the critical temperature, thermal fluctuations cause the spins to become less aligned, leading to a transition to a disordered state. Near the critical temperature, fluctuations become significant, and the system exhibits critical behaviour, characterized by the emergence of large-scale fluctuations. Above the critical temperature, the spins become highly disordered, resulting in a paramagnetic state where spins are randomly oriented. The behaviour of the lattice at different temperatures reflects these transitions from ordered to disordered states as thermal energy increases.

Energy Versus Temperature(100X100) (Fig 4)



As temperature increases in the Ising model, the energy typically increases due to the increasing thermal disorder, with more pronounced changes occurring near the critical temperature where phase transitions occur.

For T<Tc

> At low temperatures, spins tend to align to minimize the interaction energy, leading to a low-energy state. As temperature increases, thermal fluctuations become more pronounced, causing spins to flip and the energy to increase slightly due to the increased disorder.

For T=Tc

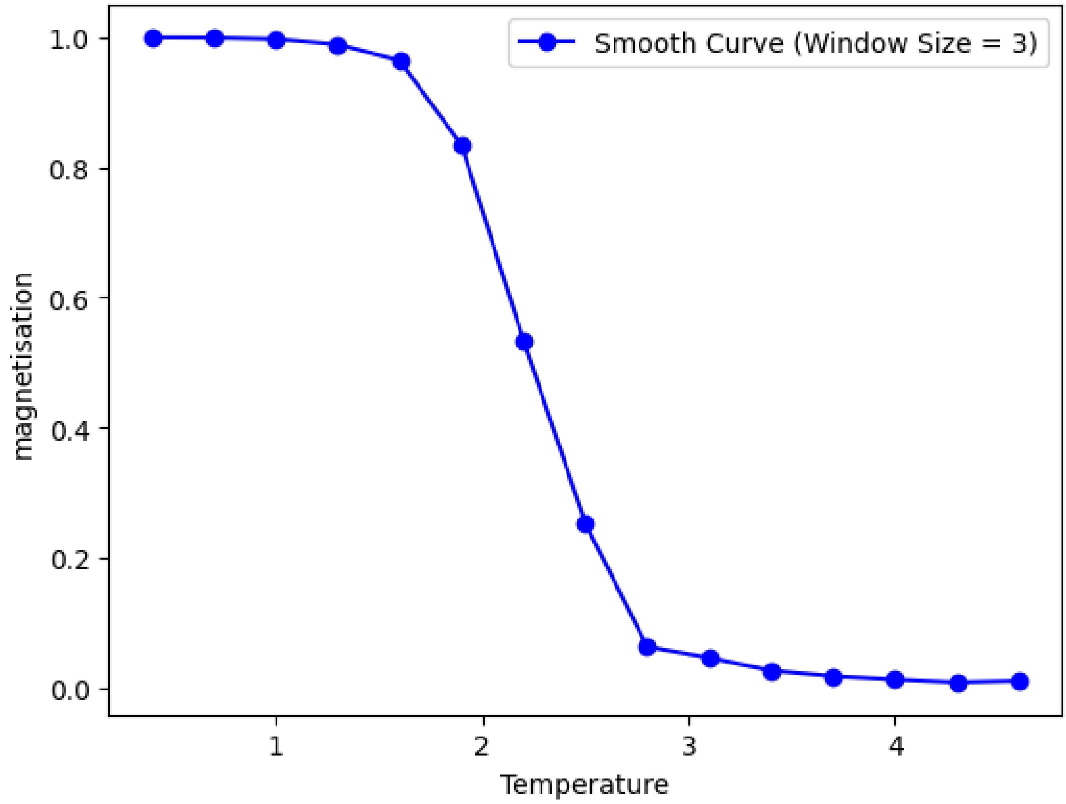
> Close to the critical temperature, the behavior of energy becomes more complex. The energy may exhibit abrupt changes, such as a discontinuity

or a peak, indicating the presence of critical phenomena associated with the phase transition.

For T>Tc

Thermal fluctuations dominate, causing spins to become increasingly disordered, leading to a further increase in energy as temperature increases.

Magnetization versus Temperature(100x100) (Fig 5)



Magnetization(m)= $\frac{\mathbf{1}}{\boldsymbol{N}}\sum_{\boldsymbol{i}=\mathbf{1}}^{\boldsymbol{N}}\boldsymbol{S_i}$

where S_i is the spin value at site i and N is the total number of spins in the lattice.

For T<Tc

At low temperatures, spins tend to align in the same direction, resulting in a net magnetic moment and non-zero magnetization.As temperature increases, thermal fluctuations become more pronounced, leading to spin disorder and a decrease in magnetization.

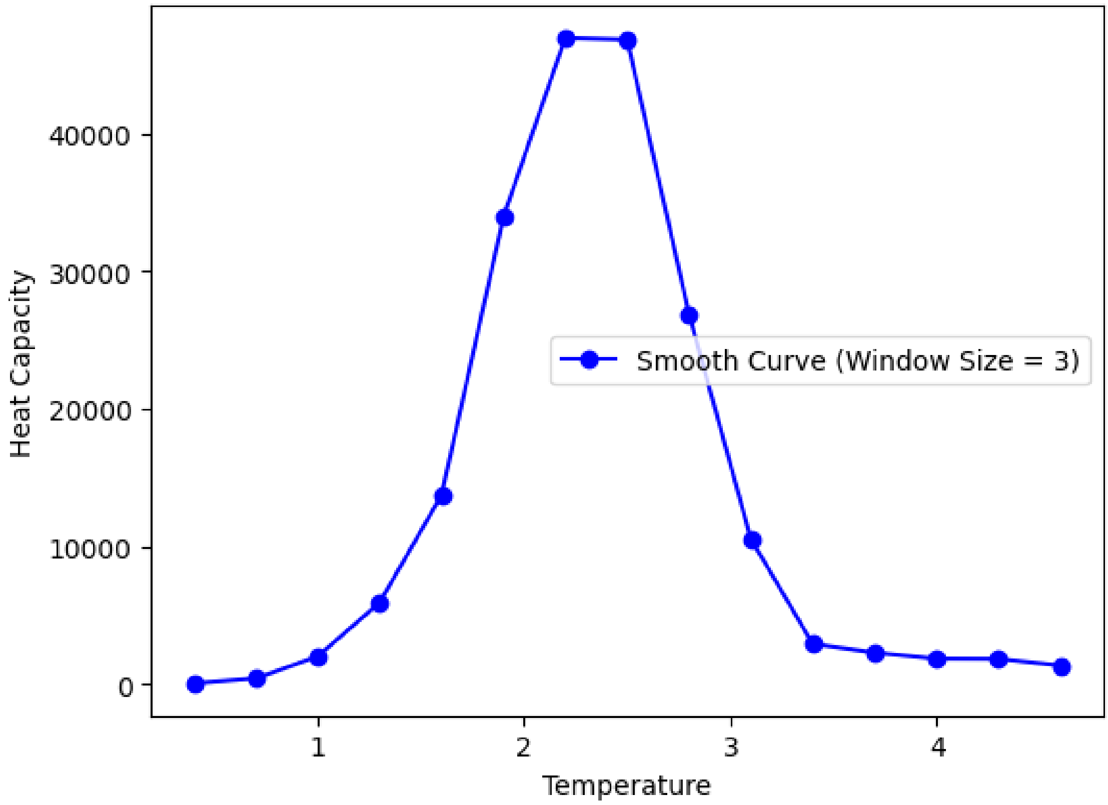
For T=Tc

The system undergoes a phase transition, where the magnetization may exhibit abrupt changes, such as a discontinuity or a peak, indicating the onset of order or disorder.

For T>Tc

Beyond the critical temperature, the system transitions to a disordered phase.Thermal fluctuations dominate, causing spins to become increasingly disordered, resulting in a decrease in magnetization towards zero.

Heat Capacity versus Temperature(100x100)(Fig 6)



The heat capacity (C) of a system can be related to the variance of energy (σ_E) through the following formula:

$$C=k_B\beta^2\sigma_E^2$$

For T<Tc

At low temperatures, the heat capacity tends to be relatively low as thermal fluctuations are minimal, and the system is typically in an ordered state. As temperature increases, thermal fluctuations become more pronounced, leading to a gradual increase in heat capacity as the system gains thermal energy.

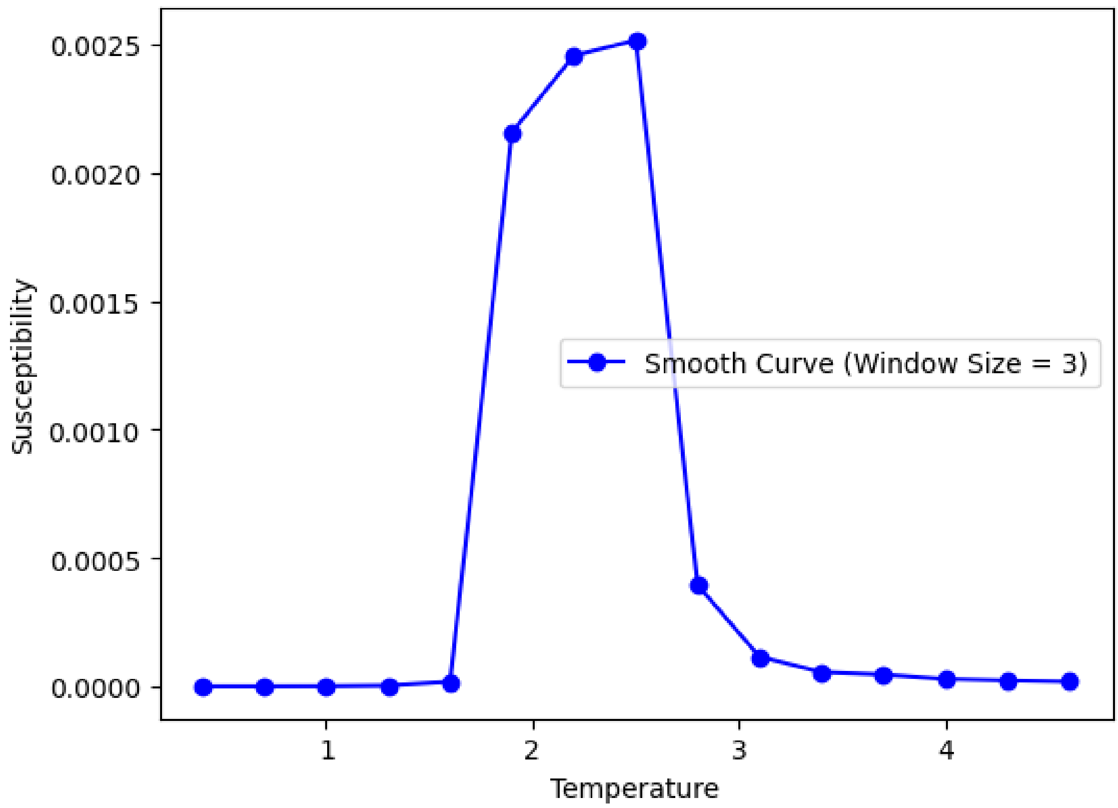
For T=Tc

The system undergoes a phase transition, characterized by the sudden onset of order or disorder. The heat capacity exhibits a peak or divergence near the critical temperature, indicating the presence of critical phenomena associated with the phase transition.

For T>Tc

Beyond the critical temperature, the system transitions to a disordered phase. Thermal fluctuations dominate, leading to a decrease in heat capacity as temperature increases. This decrease occurs because the system becomes more disordered, and additional thermal energy does not contribute significantly to increasing the disorder further. Instead, it primarily serves to increase the kinetic energy of particles, leading to a decrease in the heat capacity.

Susceptibility versus Temperature(100X100) (Fig 7)



Susceptibility is a measure of how much the magnetization of the system changes with the applied magnetic field.

$\boldsymbol{\chi = \sigma_M^2 / k_B}$**T** where σ_M is the Variance of Magnetization and χ is the susceptibility.

For T<Tc

At low temperatures, the system tends to be in an ordered phase with spins aligned. The susceptibility is typically low because the spins respond strongly to an external magnetic field due to their alignment.

For T=Tc

Near the critical temperature (Tc), the behaviour of the system undergoes significant changes as it approaches the phase transition. Thermal fluctuations become more significant, causing fluctuations in the alignment of spins. These fluctuations lead to an increase in the susceptibility as the system becomes more responsive to changes in the external magnetic field.

For T>Tc

Beyond the critical temperature, the system transitions to a disordered phase. Thermal fluctuations dominate, causing spins to become increasingly disordered, leading to a decrease in susceptibility. The decrease in susceptibility occurs because the spins lose their collective alignment and become less responsive to changes in the external magnetic field.

Critical Temperature

The critical temperature is the temperature at which a phase transition occurs in the Ising model. Below Tc, the system exhibits long-range order, with spins aligning in a particular direction. Above Tc, the system transitions to a disordered phase, where spins are randomly oriented.

Critical Exponents

In the Ising model, critical exponents and critical temperature play crucial roles in characterizing the behaviour of the system near a critical point, where a phase transition occurs. Critical exponents are scaling factors that describe the behaviour of physical quantities near the critical point. They govern how various properties of the system, such as correlation length, susceptibility, and specific heat, diverge as the system approaches the critical temperature.

Alpha (α): Alpha represents the behavior of the specific heat capacity near the critical point. It is defined as the rate of change of the specific heat with respect to temperature at the critical point. In the Ising model, α is typically positive.

$$\mathbf{C} \sim |\boldsymbol{T} - \boldsymbol{T_c}|^{-\boldsymbol{\alpha}}$$

Where α is the specific Heat Critical Exponent and C is the Heat Capacity

Beta (β): Beta describes the behavior of the order parameter (such as magnetization) near the critical point. It quantifies how the order parameter changes as the temperature approaches the critical point. In the Ising model, β is usually positive, indicating a non-zero order parameter at the critical point.

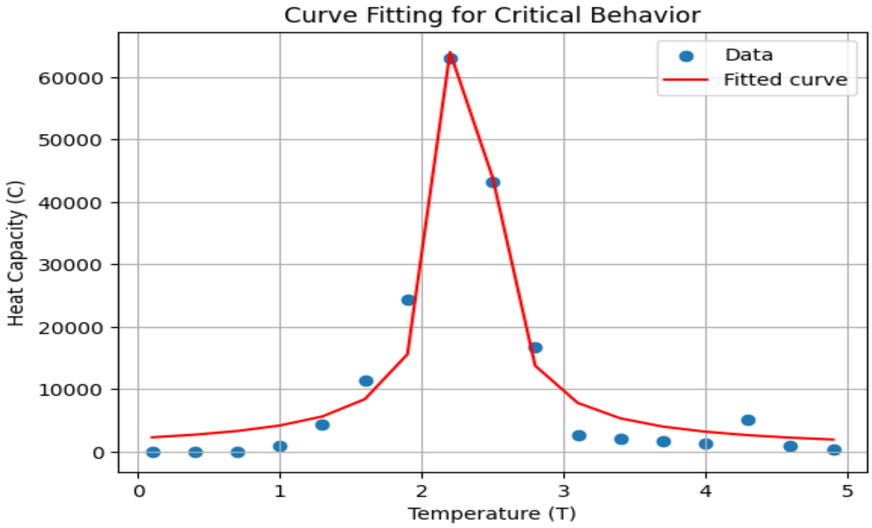
Gamma (γ): Gamma characterizes the divergence of the susceptibility near the critical point. It measures how the susceptibility (a measure of the material's response to an external magnetic field) increases as the temperature approaches the critical point. In the Ising model, γ is typically positive, indicating a divergence in susceptibility at the critical point.

$$\boldsymbol{\chi} \sim |\boldsymbol{T} - \boldsymbol{T_c}|^{-\boldsymbol{\gamma}}$$

Where γ is the Susceptibility Critical Exponent and χ *is the Susceptibility*.

These relations between critical exponents and the divergence of physical quantities near the critical temperature provide valuable insights into the universal behaviour of the Ising model and other systems undergoing phase transition.

EXPERIMENTAL RESULTS FOR Tc and α (Fig 8)



Estimated Critical Temperature (Tc): 2.325839165522601

Formulae : C $\sim |T - T_c|^{-\alpha}$

Estimated Critical Exponent (alpha): 1.1574506564307157

Applications in Different Sectors

1. **FINANCE:**

Market Dynamics: Monte Carlo simulations of the Ising model can also be used to study market dynamics and the emergence of patterns in financial markets. By modeling traders as spins in the Ising model and interactions between traders as interactions between spins, researchers can study phenomena such as herding behavior, market crashes, and the formation of market bubbles.

Portfolio Optimization : Monte Carlo simulations of the Ising model can be used for portfolio optimization. The Ising model can represent interactions between financial assets, and the energy of the model can correspond to the risk or volatility associated with different portfolio allocations. By simulating the Ising model, one can find optimal portfolio allocations that maximize returns while minimizing risk.

2. **STUDYING CRITICAL PHENOMENA :**

The Ising model is a paradigmatic example for understanding critical phenomena in statistical physics. It helps in studying universal behaviour near critical points and the scaling properties of physical systems undergoing phase transitions.

3. **BIOLOGICAL SYSTEMS:**

Biological Pattern Formation: The Ising model has been used to study pattern formation in biological systems, such as the development of animal coats and the organization of cells in tissues. By simulating the Ising model, researchers can explore how interactions between cells or molecules give rise to complex spatial patterns observed in biological systems.

Neural Networks : The Ising model has been applied to model neural networks in the brain. In this context, neurons are represented as spins, and interactions between neurons are modeled by pairwise coupling strengths. By simulating the Ising model, researchers can study collective phenomena in neural networks, such as synchronization, pattern formation, and information processing.

Conclusion

In summary, employing Monte Carlo simulations to analyse the Ising model yields valuable insights into the dynamic behaviour of magnetic systems across temperature gradients. This computational approach enables the observation of phase transitions, including critical phenomena near the critical temperature threshold. Such simulations serve as a robust methodology for investigating the intricate interplay of spins within a lattice, shedding light on phase transitions and critical phenomena. Furthermore, they contribute significantly to our comprehension of complex systems and aid in the design of innovative materials boasting tailored magnetic characteristics.

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