Mini Project Report

Monte Carlo Simulation of Ising Model & Classical XY model

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1 Introduction

This project report explores the application of Monte Carlo simulation techniques to investigate the behavior of two fundamental models in statistical physics: the Ising model and the classical XY model. Through Monte Carlo simulations, we examine the phase transitions and critical phenomena exhibited by these models as a function of temperature and other parameters. By employing various algorithms, such as the Metropolis algorithm and the Wolff algorithm, we analyze the equilibrium properties, including magnetization,energy, heat capacity & susceptibility. The insights gained from this study contribute to a deeper understanding of phase transitions and critical phenomena in condensed matter systems, with potential applications in materials science, magnetism, and complex systems research.

2 Real Life Modelling

In many real-life scenarios, ranging from political elections to consumer behavior, understanding how individual opinions aggregate to form collective decisions is of paramount importance. Traditional models in social sciences often overlook the intricacies of interpersonal interactions and the dynamic nature of opinions.To capture the dynamics of opinion formation and voting behavior in a real-life setting, here is a thought experiment where we investigate the collective decision-making process in a classroom environment where students, initially unfamiliar with each other, vote to elect a class representative (CR). Being freshmen and unfamiliar with one another, they unanimously vote for

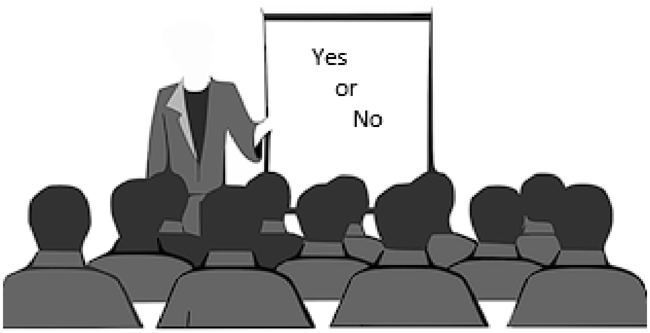


Figure 1: Voting in a Class

candidate A, who has engaged with everyone and organized a few class gatherings. However, as time progresses, the dynamics shift. Some students' opinions sway due to negative experiences with candidate A, leading to a fluctuating distribution of "Yes" and "No" votes over an extended period. These changes stem from personal encounters or are influenced by close friends, illustrating the complex and dynamic nature of opinion formation in real-world contexts. This scenario exemplifies how the Ising model, originally conceptualized in statistical mechanics, can be applied to understand and simulate the evolving dynamics of social decision-making.

In conclusion, the election process within a classroom setting exemplifies the intricate dynamics of real-life decision-making. Beginning with an initial consensus in favor of Candidate A, the evolving landscape of the election is characterized by shifting opinions, influenced by personal experiences and peer dynamics. This dynamic interplay underscores the complexity of decision-making processes and highlights the nuanced factors that shape voting behaviors in real-world scenarios.

3 Model Definitions

Few Terminologies

- **Lattice**: A lattice is a regular grid structure where each point (or site) in the grid represents a discrete location in space.
- **Spins**: Spins denote the orientation of magnetic moments within a lattice.

3.1 Ising Model [5] [2]

The Ising model is a mathematical model used in statistical mechanics to represent the behavior of magnetic materials

- **Spins:** For each lattice site $k \in \Lambda$, there is a discrete variable σ_k such that $\sigma_k \in \{-1, +1\}$, representing the site's spin.
- **Interaction Hamiltonian:** The energy of the system is described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

where $\mathbf{J}$: Interaction Constant & $\sigma_i = \pm 1$

3.2 Classical XY model [1]

The classical XY model describes a system of interacting spins on a lattice, where each spin represents a classical magnetic moment with a continuous.

- **Spins:** For each lattice site $k \in \Lambda$, there is a continuous variable s_k such that $\mathbf{s_k} = (\cos\theta_j, \sin\theta_j)$, representing the site's spin.

- **Interaction Hamiltonian:** The energy of the system is described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \tag{2}$$

where **J** : Interaction Constant & θ_i: Orientation of spin at site i

4 Monte Carlo Simulation [3] [6]

4.1 Markov Chains

A Markov chain or Markov process serves as a foundational stochastic model characterizing a sequence of potential events, where the likelihood of each event depends solely on the preceding state in the sequence. This process is characterized by a finite set of states, each possessing the Markovian property, and transition probabilities denoted as ρ_{ij}, representing the likelihood of transitioning from state i to state j.

In the context of statistical processes, Markov chains play a pivotal role in generating **Importance Sampling—a technique designed to enhance the efficiency of simulations**. Importance sampling is based on the principle that specific arrangements of input random variables have a greater impact on the estimated parameter than others. As a result, by prioritizing these influential samples while de-emphasizing less impactful ones, the computational workload of the simulation can be reduced.Markov chains offer a powerful framework for simulating complex systems, importance Sampling utilizes these inherent properties to optimize computational processes and improve the precision of statistical estimations.

4.2 Principle of Detailed Balance

The principle of detailed balance is a fundamental concept and it asserts that in a system in equilibrium, the rate of transition between any two states must be balanced by the reverse transition, ensuring the system remains in a steady state.

Mathematically, this principle is expressed as:

$$\pi_i \rho_{ij} = \pi_j \rho_{ji} \tag{3}$$

where:

- π_i and π_j are the equilibrium probabilities of states i and j respectively.
- ρ_{ij} is the transition probability from state i to state j.

- ρ_{ji} is the transition probability from state j to state i.

This equation ensures that the flow of probability between states is balanced, maintaining equilibrium.

4.3 Metropolis Algorithm

The Metropolis algorithm is a Monte Carlo method used to generate samples from a probability distribution. It is particularly useful in statistical physics for simulating systems with many degrees of freedom.

The algorithm proceeds as follows:

1. **Initialize the System:** Start with an initial configuration of the system.
2. **Trial flip:** Randomly choose a spin and flip it.
3. **Calculate energy difference:** Compute the change in energy between the current and trial configurations.
4. **Accept or Reject:** Accept the trial configuration with a probability determined by the Metropolis acceptance criterion:

   $$\text{Acceptance Probability} = \min\left(1, e^{-\frac{P_{trial}}{P_{current}}}\right) = \min\left(1, e^{-\frac{\Delta E}{k_B T}}\right)$$

   where ΔE is the change in energy, k_B is the Boltzmann constant, and T is the temperature.
5. **Update configuration:** If the trial configuration is accepted, update the current configuration to the trial configuration. If it is rejected, keep the current configuration unchanged.
6. **Iterations:** Repeat steps 2-5 for a large number of iterations.

The expression $e^{-\frac{\Delta E}{k_B T}}$ represents the ratio of probabilities between the trial and current configurations, following the Boltzmann distribution. It serves as the basis for the Metropolis acceptance criterion, ensuring that the algorithm generates samples consistent with the desired probability distribution.

The Metropolis algorithm provides a powerful method for sampling from complex probability distributions, making it an essential tool in computational science and engineering.

4.4 Wolff Cluster Algorithm

The Wolff algorithm is a Monte Carlo method used for simulating spin systems, particularly in statistical physics and computational materials science. It is renowned for its efficiency in cluster updates, making it well-suited for studying phase transitions and critical phenomena in systems such as the Ising model.

The algorithm proceeds as follows:

1. **Initializing the Lattice** Begin with an initial configuration of the spin system.

2. **Cluster Growth:** Select a random spin from the lattice as a seed and grow a cluster of spins (using dfs) with the same orientation as the seed according to the acceptance probability .

$$\text{Acceptance Probability} = \min\left(1, 1 - e^{-2\beta}\right)$$

   where $\beta = \frac{1}{k_B T}$ and k_B is the Boltzmann constant.

3. **Flipping whole cluster:** After there is no more lattice site to add in the cluster, flip the cluster.

4. **Update quantities:** Update the measured quantites, according to the updated configuration.

5. **Iteration:** Repeat steps 2-4 for a large number of iterations.

5 Fundamental Concepts in Phase Transitions and Boundary Conditions

5.1 Second order phase transitions

Second-order phase transitions, occurring at a critical point, involve a gradual and continuous change in a material's properties without any latent heat being absorbed or released. These transitions are characterized by the breaking of a continuous symmetry, leading to the emergence of long-range order in the system. Near the critical point, critical phenomena such as power-law behavior and diverging fluctuations become prominent, governed by scaling laws and described by theoretical frameworks like renormalization group theory. Examples include the liquid-gas transition, ferromagnetic-paramagnetic transition, and superconducting-normal transition, highlighting their significance in various fields for understanding complex systems near critical points.[4]

5.2 Periodic Boundary Conditions

Periodic boundary conditions are constraints applied to simulate an infinite system within a finite space. At the edges of the simulation box, particles wrap around, maintaining continuity as if the system repeats indefinitely. Periodic boundary conditions are constraints applied to simulate an infinite system within a finite space. At the edges of the simulation box, particles wrap around, maintaining continuity as if the system repeats indefinitely.

5.2.1 Why do we use PBCs:

Periodic boundary conditions are employed to mimic an infinite lattice within the simulation's finite computational domain. This approach ensures that the behavior of spins near the lattice edges is representative of spins in the bulk of the system. Without PBCs, edge effects could distort the results, leading to inaccurate representations of the system's thermodynamic properties.

The periodic boundary conditions are mathematically expressed as:

For $x, y \in [1, N]$, where N is the lattice size:

$$\begin{aligned}
&\text{For right neighbor:} && x_{\text{right}} = (x+1) \mod N \\
&\text{For left neighbor:} && x_{\text{left}} = (x-1) \mod N \\
&\text{For bottom neighbor:} && y_{\text{bottom}} = (y+1) \mod N \\
&\text{For top neighbor:} && y_{\text{top}} = (y-1) \mod N
\end{aligned}$$

By applying periodic boundary conditions, the simulation accurately captures the behavior of the spin system, allowing for meaningful analyses and insights into its thermodynamic properties.[4]

5.3 Critical Phenomenons & Universality

Critical phenomena refer to the behaviors observed near critical points in physical systems, where small changes in external conditions lead to dramatic changes in the system's behavior. Two well-known models that exhibit critical phenomena are the Ising model and the classical XY model. Both models belong to the broader class of statistical mechanics models used to study phase transitions. The universality of critical phenomena suggests that the behavior near critical points is governed by universal properties that are insensitive to the microscopic details of the system. This universality allows researchers to classify different physical systems into universality classes based on their critical behavior, providing valuable insights into the underlying physics of phase transitions and critical phenomena.

5.4 Critical Exponents

Critical exponents are mathematical parameters that quantify how physical properties of a system change near its critical point. They describe the power-law behavior of observables such as correlation lengths, specific heat, magnetization, and susceptibility as the system approaches criticality. These exponents provide valuable information about the universality class of a phase transition, indicating the underlying symmetries and interactions governing the system's behavior.[1] [4] [2]

1. **Correlation Length Exponent** (ν): Describes how the correlation length diverges near the critical point, indicating the spatial extent of correlations in the system.

2. **Critical Temperature Exponent** (α): Governs how the specific heat diverges as the system approaches criticality, providing insights into the thermodynamic properties of the phase transition.

3. **Order Parameter Exponent** (β): Quantifies the strength of spontaneous symmetry breaking near the critical point, characterizing the behavior of the order parameter.

4. **Susceptibility Exponent** (γ): Determines how the susceptibility diverges near criticality, reflecting the system's response to external fields and fluctuations in the order parameter.

5. **Dynamic Exponent** (z): Characterizes the time scale divergence near the critical point, governing the relaxation dynamics of the system and critical slowing down phenomenon.

6 Data Analysis

6.1 Physical Quantities

Throughout the simulation, several key physical quantities were observed and calculated to characterize the behavior of the spin system. These quantities provide valuable insights into the system's dynamics and its response to changes in temperature.

6.1.1 Average Magnetization

The average magnetization per spin was calculated to understand the overall alignment of spins in the system. It quantifies the net magnetic moment and

reveals the presence of magnetic ordering or disordering.
The average magnetization per spin was calculated using the formula:

$$M = \frac{1}{N} \sum_{i=1}^{N} s_i$$

where N is the total number of spins and s_i represents the spin value at site i.

6.1.2 Energy

The average energy per spin was computed to evaluate the system's total energy under different configurations. It indicates the stability of the system and reflects the balance between ferromagnetic and thermal energies.
The average energy per spin was computed using the expression:

$$E = -\frac{1}{N} \sum_{<ij>} J s_i s_j$$

where J is the coupling constant, and the sum is taken over nearest neighbor spins.

6.1.3 Heat Capacity

The heat capacity per spin was determined to assess the system's response to changes in temperature. It measures the amount of heat required to change the system's temperature and is indicative of phase transitions and critical phenomena. It is the measure of fluctuations in the energy
The heat capacity per spin was determined as:

$$C_V = \frac{1}{N} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \cdot \frac{1}{k_B T^2}$$

where $\langle E \rangle$ and $\langle E^2 \rangle$ represent the average energy and its square, respectively.

6.1.4 Susceptibility

The susceptibility per spin was analyzed to study the system's susceptibility to external magnetic fields. It quantifies the system's response to small changes in the applied magnetic field and helps identify magnetic phase transitions. It is the measure of fluctuations in the average magnetization of the system.
The susceptibility per spin was analyzed using the formula:

$$\chi = \frac{1}{N} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \cdot \frac{1}{k_B T}$$

where $\langle M \rangle$ and $\langle M^2 \rangle$ denote the average magnetization and its square, respectively.

6.2 Results of Ising Model

6.2.1 Lattice behaviour with temperature

100x100 Lattice at different temperatures

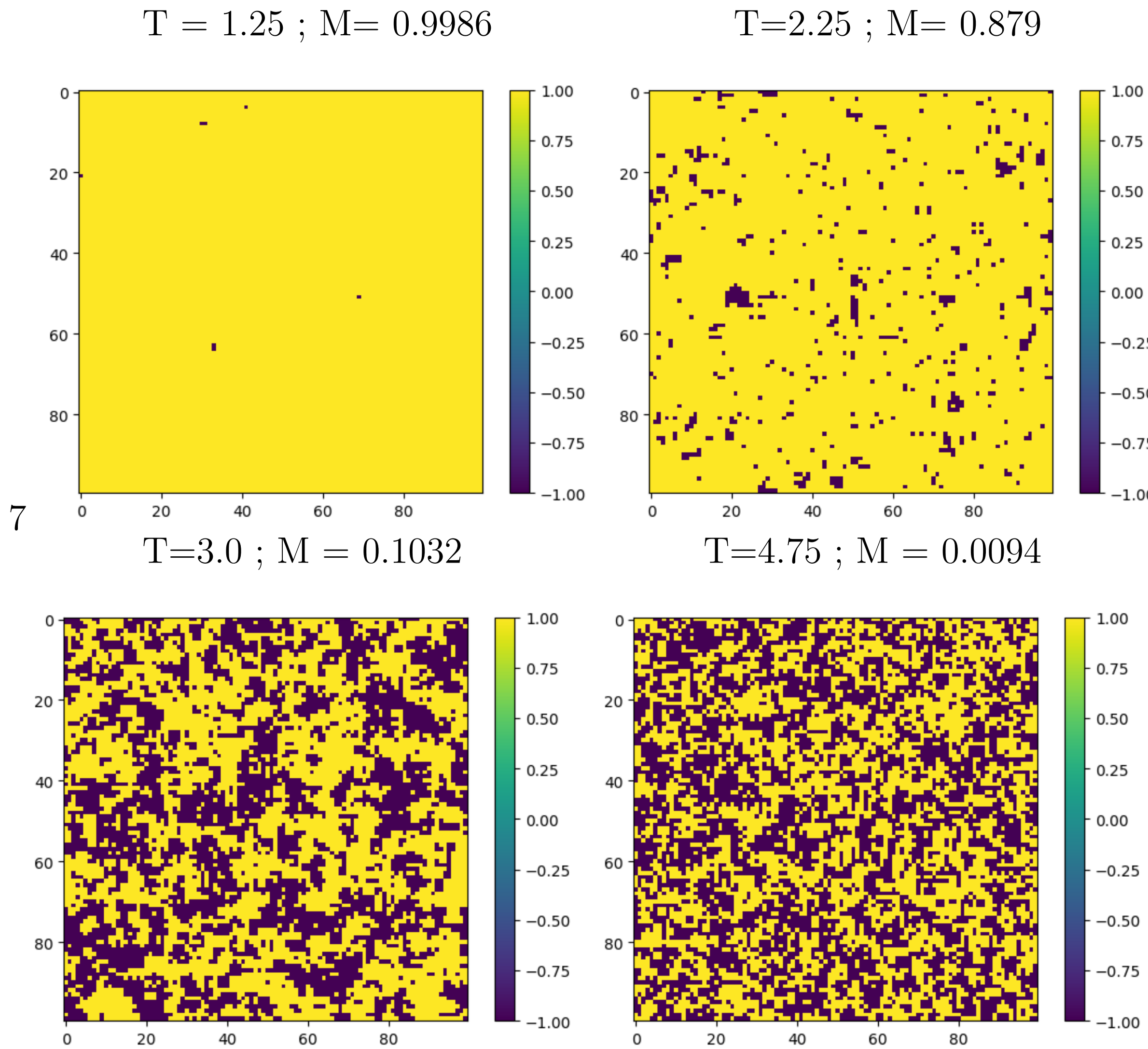


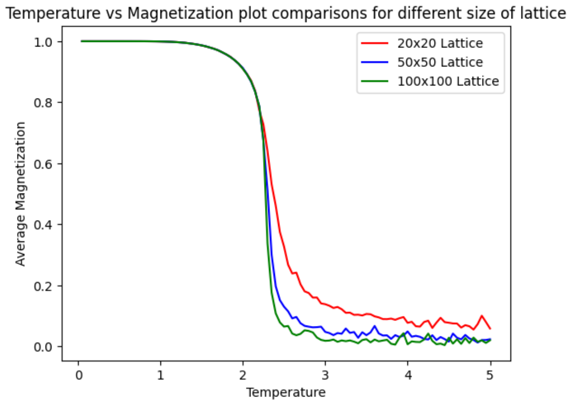
Figure 2: Lattice at different temperatures

We initiated the system with all spins oriented upwards, represented by the yellow color. This initial alignment reflects a state of ordered magnetization, characteristic of low-temperature regimes. However, as the temperature increases, thermal fluctuations become more pronounced, disrupting the ordered arrangement of spins. Consequently, the spins gradually lose their alignment and transition into a more random orientation.

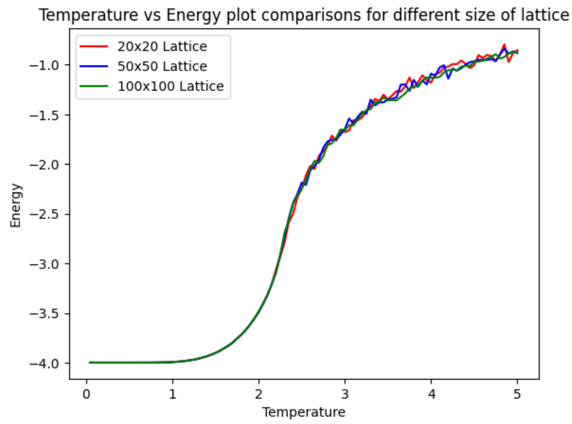
In these visuals, the yellow color signifies an upward spin, indicating a positive magnetization, while purple indicates a downward spin, corresponding to a negative magnetization. The transition from predominantly yellow to a mix of yellow and purple hues reflects the gradual breakdown of magnetic order as the system approaches its critical temperature.

6.2.2 Plots

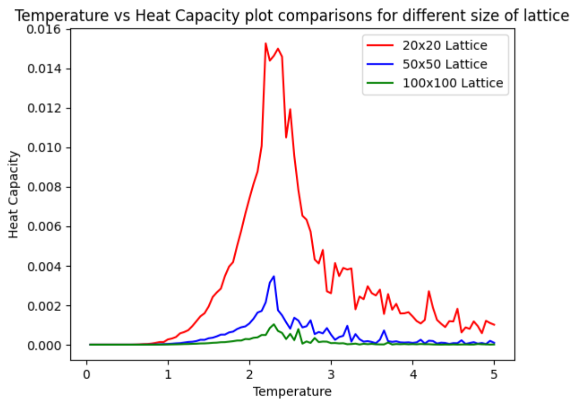
Plots of different quantities such as average magnetization, energy, heat capacity and susceptibility with the variation of temperature:



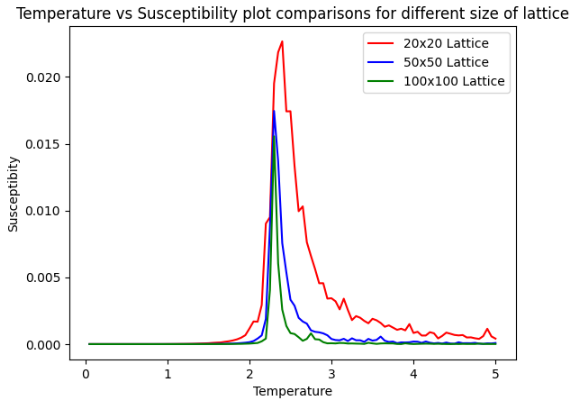
(a)



(b)



(c)



(d)

Figure 3: Variation of different quantities with temperature
(a): Temperature vs Average magnetization (b): Temperature vs Energy (c): Temperature vs Heat Capacity (d): Temperature vs Susceptibility

The analysis of the presented graphs reveals notable shifts in the behaviors of average magnetization, energy, heat capacity, and susceptibility as the system approaches its critical temperature. Thus by analyzing the corresponding temperature **the critical temperature is determined to be approximately 2.25, with a margin of error of ±0.05**. It's imperative to note that due to the discrete nature of our simulation, continuous iteration through temperature values was not feasible.

Moreover, it's essential to underscore that the derived results stem from simulating the Ising model across three distinct lattice sizes: 20x20, 50x50, and 100x100. This approach allows for a comprehensive exploration of the system's behavior across varying scales.

6.3 Results of Classical XY model

6.3.1 Lattice behaviour with temperature

20x20 Lattice at different temperatures

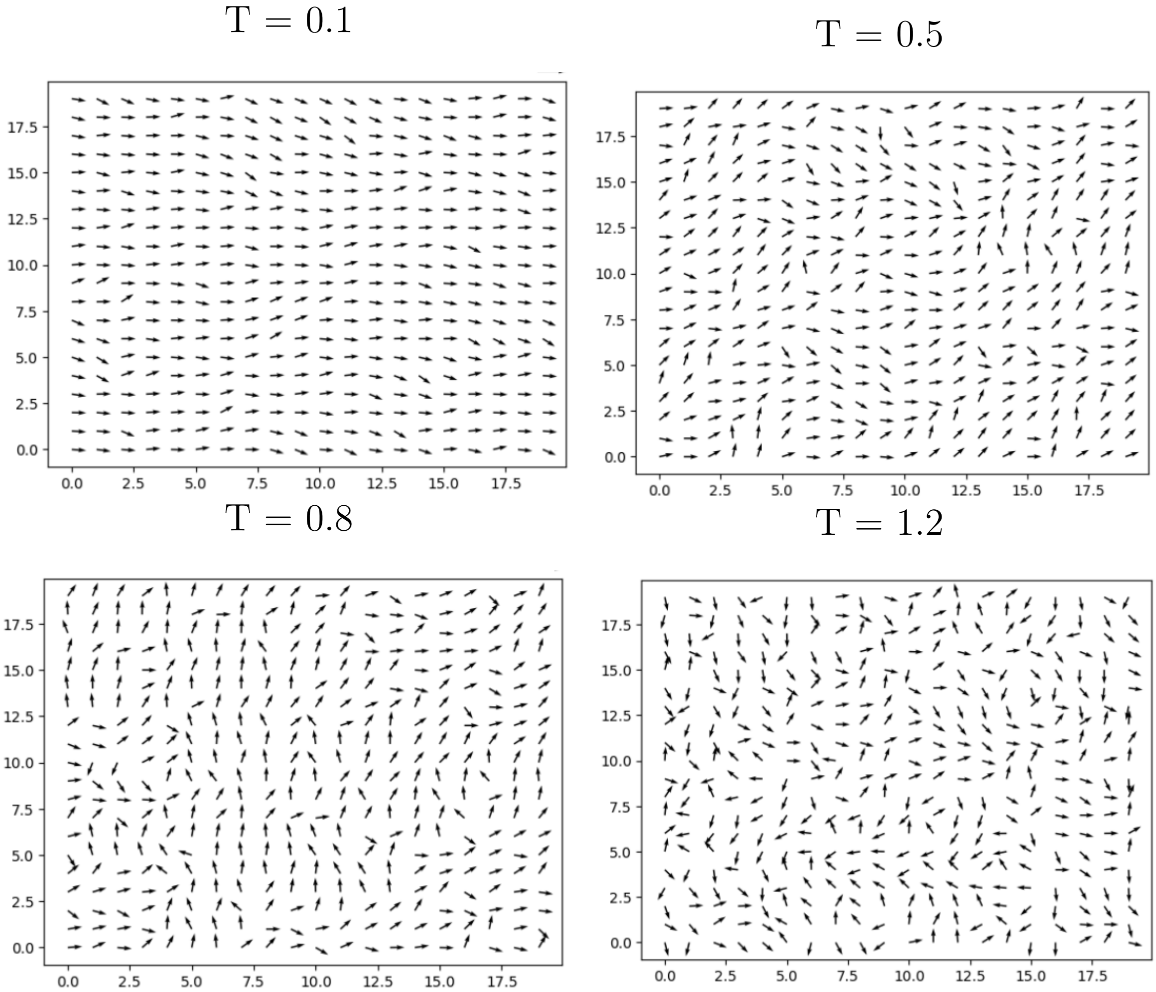


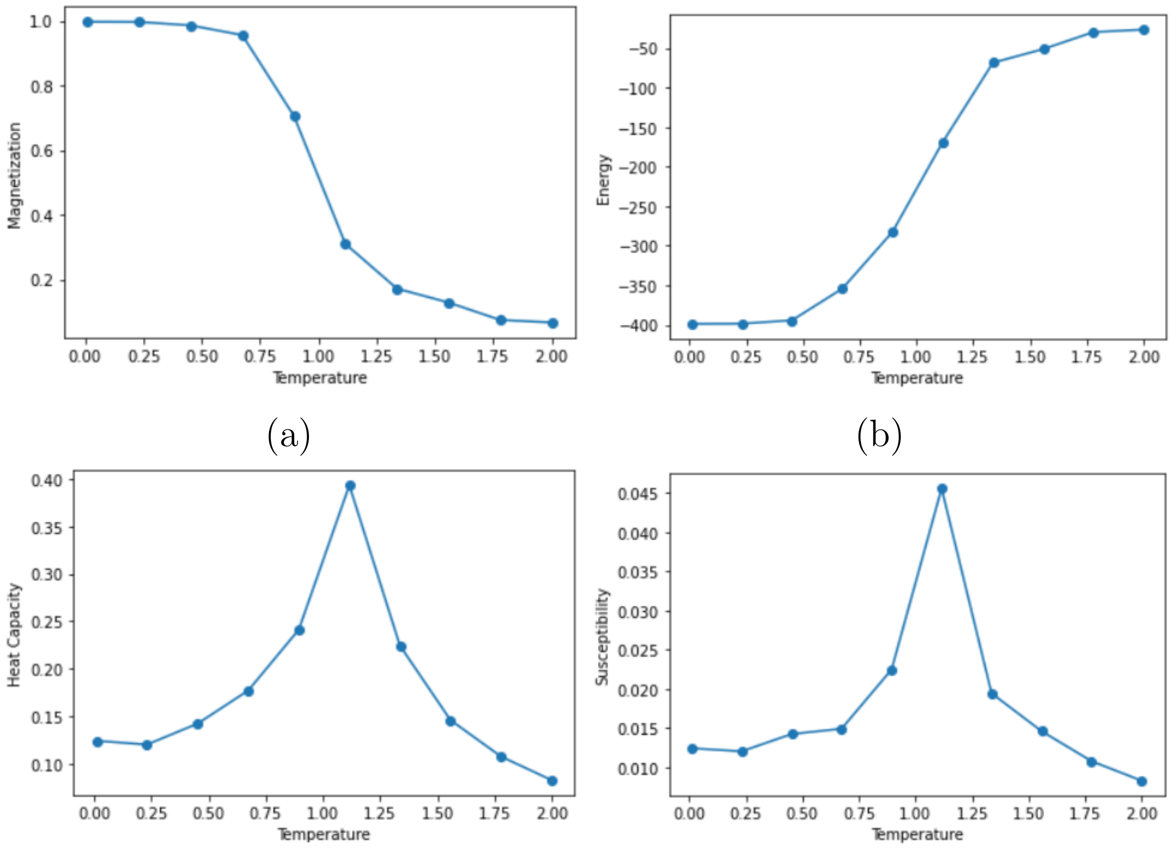
Figure 4: Lattice at different temperatures

The images above depict a 20x20 lattice at various temperatures, captured during Monte Carlo simulations of the classical XY model. Initially, all spins on the lattice were aligned in one direction. However, as the temperature increases, a noticeable transition occurs, leading the spins to gradually orient themselves randomly.

Each arrow corresponds to the spin orientation at a lattice site, with its direction indicating the orientation of the spin. Initially all the spins were oriented in positive x-direction according to rectangular coordinate system. As the temperature rises, the arrangement of arrows becomes increasingly disordered, reflecting the system's transition from an ordered to a disordered state. This dynamic interplay between spin orientations and temperature underscores the complex behavior exhibited by the classical XY model near its critical point.

6.3.2 Plots

Plots of different quantities such as average magnetization, energy, heat capacity and susceptibility with the variation of temperature:



(a) (b) (c) (d)

Figure 5: Variation of different quantities with temperature
(a): Temperature vs Average magnetization (b): Temperature vs Energy (c): Temperature vs Heat Capacity (d): Temperature vs Susceptibility

Based on the data depicted in the graphs, it's apparent that the average magnetization, energy, heat capacity, and susceptibility display pronounced fluctuations around the critical temperature. Analysis indicates that the critical temperature lies at approximately 0.9, with a margin of error of ± 0.1.

Our observations reveal distinct trends near the critical temperature. Specifically, we noted a rapid decrease in the average magnetization, accompanied by a sharp increase in energy. Moreover, both the heat capacity and susceptibility exhibit pronounced peaks precisely at the critical temperature.

7 Applications

Ising Model:

1. **Magnetic Materials and Ferromagnetism**: The Ising model originated in understanding ferromagnetic materials, where spins of neighboring atoms tend to align. It's crucial in designing and understanding magnetic materials used in data storage (like hard drives) and magnetic sensors.

2. **Phase Transitions in Materials Science**: Ising model variants are employed to study phase transitions in materials. For instance, in understanding the behavior of liquid crystals undergoing phase transitions, where the orientation of molecules changes in response to temperature or other factors.

3. **Neuroscience**: Ising models are used to model the behavior of neurons in the brain. By considering neurons as spins, researchers can study phenomena like synchronization, information processing, and the emergence of patterns in neural networks.

4. **Social Dynamics and Opinion Formation**: In sociology and political science, Ising-like models are used to simulate opinion dynamics within populations. This helps understand how opinions spread, consensus forms, and how external factors influence collective behavior.

5. **Econophysics**: Ising models have been applied to study financial markets. By modeling traders as spins and their interactions as interactions between spins, researchers can simulate market behaviors, bubbles, and crashes, helping in risk assessment and market regulation.

6. **Protein Folding and Biomolecular Interactions**: Ising-like models are used to understand the folding of proteins and the interactions between biomolecules. By considering the energy landscape of different configurations, researchers can predict protein structures and study molecular recognition processes.

7. **Materials Design and Optimization**: Ising models are employed in material science and engineering for optimizing material properties. By simulating different configurations and interactions, researchers can predict material behavior, optimize properties like strength or conductivity, and design new materials.

8. **Machine Learning and Optimization Algorithms**: Ising models serve as the foundation for certain machine learning algorithms, particularly in optimization tasks. For example, simulated annealing, a technique

inspired by the Ising model, is used to find approximate solutions to optimization problems.

Classical XY Model

1. **Phase Transitions in Two-Dimensional Systems**: The classical XY model is to study 2^{nd} order phase transitions and critical phenomena in two-dimensional systems that we just saw the report. By analyzing the model using numerical simulations and analytical techniques, researchers gain insights into universal properties of phase transitions, such as critical exponents and scaling laws.

2. **Superfluidity and Supersolidity**: The classical XY model is used to describe the behavior of two-dimensional superfluids, where particles exhibit coherent motion with no viscosity. It helps in understanding phenomena like superfluid helium and the onset of supersolidity, where solid materials exhibit superfluid-like behavior.

3. **Vortex Dynamics in Superconductors**: In condensed matter physics, the classical XY model is employed to study the dynamics of vortices in superconducting materials. By treating vortices as two-dimensional spins with continuous orientations, researchers can investigate the properties of superconductors, including critical currents and flux pinning.

4. **Magnetic Domain Walls**: The classical XY model is used to study the behavior of magnetic domain walls in ferromagnetic materials. By considering the spins as continuous vectors representing magnetic moments, researchers can model the formation, motion, and interactions of domain walls, which are crucial in magnetic storage devices and spintronics.

5. **Liquid Crystals**: The classical XY model serves as a theoretical framework for understanding the behavior of liquid crystals, which are materials with properties between those of conventional liquids and solids. It helps in studying phase transitions, defect formation, and optical properties of liquid crystal materials used in displays, sensors, and electro-optical devices.

6. **Biological Systems**: The classical XY model has been applied to model biological systems such as cell membranes and lipid bilayers. By considering the orientation of lipid molecules as continuous spins, researchers can study phase transitions and structural properties of biological membranes, which are essential in understanding cell function and organization.

7. **Cosmology**: The classical XY model has connections to cosmology, particularly in the study of cosmic strings and defects in the early universe.

By modeling the evolution of field configurations using the XY model, researchers can investigate the formation of cosmic strings and their implications for cosmological phenomena such as galaxy formation and cosmic microwave background radiation.

8. **Quantum Spin Systems**: The classical XY model serves as a semiclassical approximation to describe quantum spin systems, such as the Heisenberg model and the XY model in quantum magnetism. It provides insights into the behavior of quantum spins, phase transitions, and quantum criticality in condensed matter systems.

8 Conclusion

In conclusion, the Monte Carlo simulations of the Ising model and classical XY model have provided valuable insights into the critical behavior and phase transitions of these systems. Through meticulous analysis of various thermodynamic quantities such as magnetization, energy, heat capacity, and susceptibility, we have gained a comprehensive understanding of the behavior of these models near their critical points.

In the case of the Ising model, we observed a clear phase transition from a magnetically ordered state to a disordered state as the temperature approached the critical point. The critical temperature, determined to be approximately $\mathbf{2.25 \pm 0.05}$, was characterized by significant changes in magnetization and energy, indicative of the system undergoing a phase transition. Additionally, the heat capacity and susceptibility exhibited sharp peaks at the critical temperature, further confirming the presence of critical phenomena.

Similarly, in the classical XY model, we observed analogous behavior near the critical temperature. The system transitioned from an ordered phase to a disordered phase as temperature increased, with notable changes in magnetization, energy, heat capacity, and susceptibility. The critical temperature, determined to be approximately $\mathbf{0.9 \pm 0.1}$, marked the point at which these thermodynamic quantities exhibited pronounced fluctuations and peaks, signifying the onset of critical behavior.

Overall, our Monte Carlo simulations have provided valuable insights into the critical phenomena and universality observed in the Ising model and classical XY model. By studying these models, we have deepened our understanding of phase transitions and critical behavior in condensed matter systems, contributing to the broader body of knowledge in statistical mechanics and theoretical physics.

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