Two-Dimensional Ising model Monte Carlo simulation

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1 Introduction

The two-dimensional Ising model is a fundamental tool for understanding the behaviour of magnetic materials, particularly ferromagnets, at finite temperatures. It represents a square lattice of magnetic spins, each having a binary value of +1 or -1, arranged randomly in a two-dimensional grid. The system's energy arises from interactions between neighbouring spins and is governed by the Hamiltonian, which includes terms for spin interactions and the external magnetic field.

To simulate the two-dimensional Ising model, the code employs the Metropolis algorithm, which is a Monte Carlo method widely used in statistical physics. This algorithm iteratively updates the spin configuration based on the Boltzmann probability distribution, emulating thermal fluctuations to reach equilibrium. Physical quantities such as magnetization, specific heat capacity, and susceptibility are computed alongside energy to analyse the system's thermodynamic properties. The code begins with user-defined parameters such as magnetic field strength, lattice size, and the number of Monte Carlo sweeps. It then iterates over sweeps, updating the spin configuration and computing physical quantities to analyse the system's behaviour. By leveraging vectorized operations and using NumPy arrays, the simulation achieves a higher level of computational efficiency, allowing for the study of large lattice sizes and extended simulation times.

The simulation's accuracy and reliability are assessed by comparing its results to theoretical predictions and known properties of the two-dimensional Ising model. This involves testing the simulation across various parameter ranges, including different lattice sizes, temperature ranges, and magnetic field strengths. Additionally, the simulation's performance is evaluated by analysing its computational efficiency and ability to handle large-scale simulations. By comparing the simulated physical quantities to analytical solutions and experimental data from literature, the code's fidelity in capturing the behaviour of the two-dimensional Ising model can be effectively gauged.

2 Mathematical Modeling

The two-dimensional Ising model serves as a pivotal mathematical framework for understanding the complex dynamics of magnetic materials, particularly in the realm of ferromagnetism. At its core, the model represents a square lattice comprising discrete magnetic spins, each possessing binary values of either +1 or -1. These spins are distributed randomly across a two-dimensional grid, representing the spatial arrangement within the material.

2.1 Energy Hamiltonian

Central to the mathematical formulation of the Ising model is the concept of energy, which arises from the interactions between neighbouring spins within the lattice. This energy is encapsulated by the Hamiltonian, a fundamental operator describing the system's total energy. The Hamiltonian consists of two primary components: the interaction term representing the coupling between adjacent spins and an external magnetic field term influencing individual spins. The interaction term is characterized by the interaction strength parameter J, which quantifies the tendency for neighbouring spins to align or anti-align. Mathematically, this term involves summing over all pairs of adjacent spins ($\langle i, j \rangle$) and computing the product of their respective spin values ($s_i s_j$). Additionally, the Bohr magneton (μ) represents the magnetic moment associated with each spin, contributing to the overall energy of the system. Incorporating the external magnetic field (B) into the Hamiltonian allows for the modelling of magnetic materials under the influence of external stimuli. The presence of this field introduces an additional term involving the product of the external field strength and the individual spin orientations ($B \cdot s_i$), thus modulating the overall energy landscape of the system. Mathematically, the Hamiltonian H for the Two-Dimensional Ising Model is expressed as:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - \mu \sum_i B \cdot s_i \tag{1}$$

J represents the interaction strength between neighbouring spins,$\sum <i, j>$ denotes the summation over all pairs of adjacent spins, si and sj denote the spin values at lattice positions i and j respectively, (μ) represents the Bohr magneton, B denotes the external magnetic field strength. This comprehensive formulation of the Hamiltonian captures the intricate interplay between spin interactions and external influences, providing a robust mathematical foundation for studying the thermodynamic properties of magnetic materials within the Ising model framework.

2.2 Monte Carlo Probabilities

The Metropolis algorithm is used to perform Monte Carlo sweeps of the Ising model. It uses the Boltzmann factor to test the probability of each potential spin flip. The Boltzmann probability is pivotal in the Metropolis algorithm as it determines the acceptance or rejection of proposed spin flips, which is crucial for simulating the equilibrium state of a physical system. By quantifying the likelihood of accepting a spin flip based on the change in energy and the system's temperature, the Boltzmann factor (2) ensures that the simulation explores configuration space in a manner consistent with thermal equilibrium. At higher temperatures, the algorithm is more likely to accept spin flips that increase energy, reflecting increased thermal agitation, while at lower temperatures, the probability decreases, favouring lower energy configurations. This probabilistic approach enables the simulation to accurately sample configurations according to their relative probabilities, thereby capturing the equilibrium behaviour of the system governed by statistical mechanics.

$$P(e^{-\frac{\Delta E}{k_b T}}) \tag{2}$$

2.3 Physical Parameters

The physical quantities of the system, namely the magnetisation(3), specific heat capacity(4) and susceptibility (5) are calculated alongside the energy,

$$M = N_1 \sum_i s_i \tag{3}$$

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \tag{4}$$

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_b T} \tag{5}$$

3 Code Description

The simulation begins with a user input of determining parameters including magnetic field strength, lattice size and number of Monte Carlo sweeps per temperature. Additionally, the user can choose to run the simulation at a single temperature or multiple and produce plots of the calculated values. The Metropolis algorithm proceeds as follows: at each iteration (Monte Carlo sweep), a random spin on the lattice is chosen, and a trial change in its orientation is proposed. The change is accepted or rejected based on the Metropolis acceptance criterion, which depends on the change in energy (Δ E) and the temperature of the system. If the change decreases the energy of the system or is favoured by thermal fluctuations, the flip is accepted; otherwise, it is accepted with a probability determined by the Boltzmann factor.

3.1 Metropolis Algorithm

The core function metropolis_algorithm() implements this algorithm by iterating over the specified number of Monte Carlo sweeps. Within each sweep, it randomly selects lattice sites, calculates the energy change resulting from a spin flip, and updates the spin configuration accordingly. This process allows the system to explore different spin configurations and reach a state of thermal equilibrium.

3.2 Parameter Calculation

The calc_parameters() function computes various physical quantities of interest, including the energy, magnetization, specific heat, and susceptibility, by averaging over multiple Monte Carlo sweeps. These quantities provide insights into the thermodynamic properties of the system and how they evolve with temperature. Notably, the calculation of specific heat and susceptibility involves analysing fluctuations in energy and magnetization, respectively, which are indicative of the system's response to thermal and magnetic perturbations.

Throughout the simulation, the code tracks the evolution of these physical quantities as a function of temperature, allowing for the observation of phase transitions and critical phenomena. The results are then visualized using Matplotlib to generate plots depicting the temperature dependence of energy, magnetization, specific heat, and susceptibility, facilitating the analysis and interpretation of the simulation outcomes.

3.3 Computational Utility

To ensure computational efficiency, the code utilizes vectorized operations and Numpy arrays for fast computations. This optimization technique enables the simulation to handle large lattice sizes and long simulation times while maintaining reasonable execution times. Additionally, tqdm is employed to provide a progress bar during the simulation, enhancing user experience and providing feedback on the simulation's progress.

4 Results

4.1 Validation

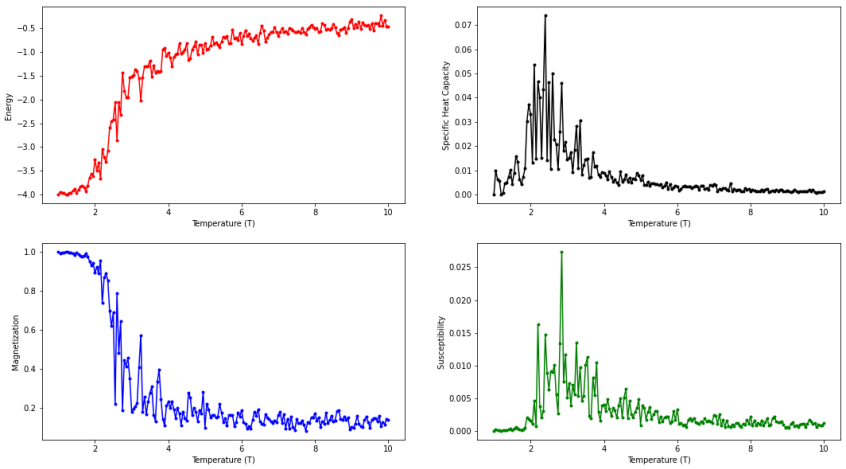

Figure 1: Simulation data results ran at 16x16 lattice size at 1000 at a temperature range 1K to 10K and step of 0.1k (a) energy (b) Specific Heat Capacity (c) Magnetism (d) Susceptibility

The simulation effectively captured the critical behaviour of the two-dimensional Ising model, as evidenced by the replication of scaling laws derived from theoretical predictions. Figure 1 presents the results of the simulation conducted on a 16×16 lattice with 1000 Monte Carlo steps and zero magnetic field strength. This choice ensures minimal interference with spin configurations outside the Metropolis algorithm, allowing for a clear observation of critical phenomena.

The specific heat capacity exhibits a pronounced spike at approximately 2.2 Kelvin (figure 1b), corresponding to the calculated critical temperature of the two-dimensional Ising model [**?**]. Beyond this critical point, the specific heat capacity remains close to zero, aligning with the expected behaviour described by the scaling law $C \propto |T - T_c|^0$. This observation supports the model's fidelity in capturing critical transitions. Similarly, the magnetization plot displays a prominent peak followed by a rapid decline post-critical temperature (figure 1c), consistent with theoretical expectations. The shape of the curve closely resembles the predicted behaviour governed by the scaling law $M \propto |T - T_c|^{1/8}$, indicating a successful simulation of magnetization dynamics. The energy graph confirms theoretical predictions,

with the average energy plateauing around zero as temperature increases (figure 1a). This behaviour reflects the system's tendency to approach equilibrium configurations at higher temperatures. Notably, the susceptibility plot exhibits a sharp increase near the critical temperature, just as it represents the drastic drop off in magnetism to near zero at the critical temperature (figure 1d). This correspondence with the scaling law $\chi \propto |T - T_c|^{-7/4}$ further corroborates the simulation's accuracy in capturing critical phenomena.

4.2 Limitations

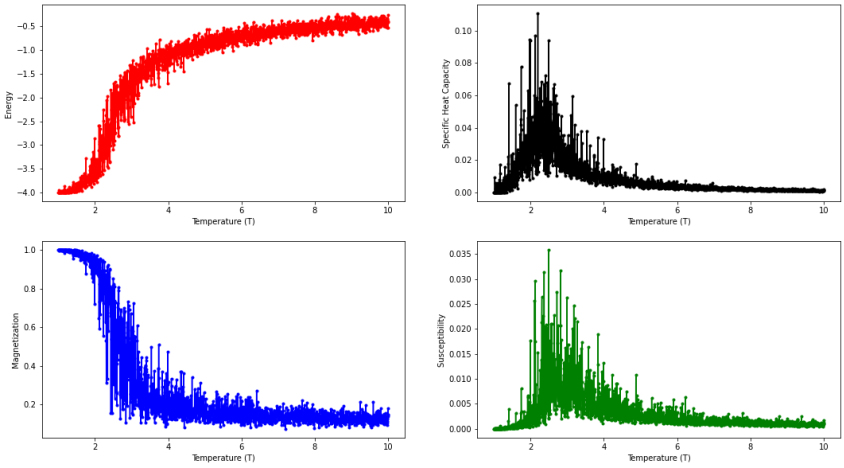

Figure 2: Simulation data results ran at 16x16 lattice size at 1000 algorithm steps at a temperature range 1K to 10K and step of 0.005 (a) energy (b) Specific Heat Capacity (c) Magnetism (d) Susceptibility

The simulations were run at a higher resolution to test their limitations and the results are shown in Figure 2. Similar results were found at this higher resolution however the accuracy of the results started to deteriorate as the margin of error increased. The number of outlying data increased as the resolution of temperature increased. Any higher resolution and the critical temperature would be hard to distinguish from the plots. However, the general curve of each of the plots do match the scaling laws proposed [2].

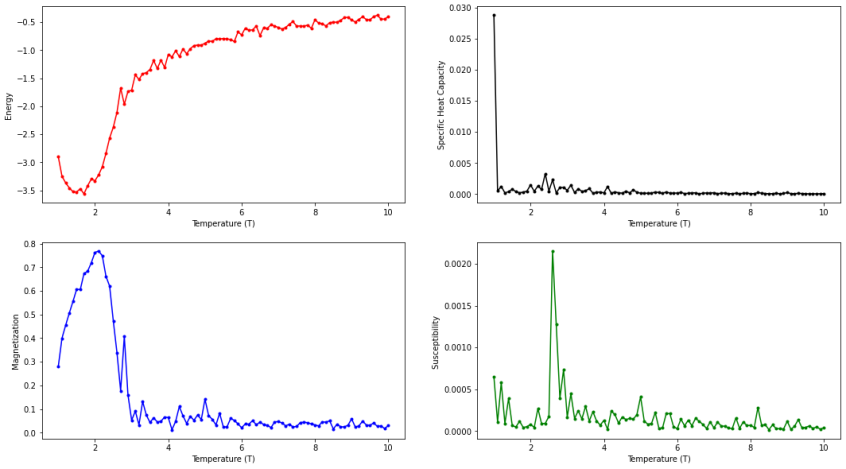

Figure 3: Simulation data results ran at 30x30 lattice size at 1000 algorithm steps at temperature range 1K to 10K and step of 0.1K (a) energy (b) Specific Heat Capacity (c) Magnetism (d) Susceptibility

Higher lattice size simulations were run up to 30x30 (figure 3). Which significantly increased the run time for the simulation. The specific heat capacity plot does still show a small peak at 2.2 but it is not as clear as the other simulations as the initial specific heat capacity is still relatively hight in comparison to the plateauing data due to the increased lattice size. The other plots show no outlining data and keep to showing the expected scaling law proportionalities. Which solidifies the consistency of the program and simulation.

5 Conclusion

In conclusion, the Monte Carlo simulation of the two-dimensional Ising model successfully replicated critical phenomena and scaling laws predicted by theoretical frameworks. By employing the Metropolis algorithm, the code effectively emulated thermal fluctuations to achieve equilibrium spin configurations, providing valuable insights into the thermodynamic properties of magnetic materials. The mathematical model, encapsulated by the Hamiltonian formulation, accurately captured the complex dynamics of spin interactions and external influences within the system. Through rigorous testing across various parameter ranges and resolution levels, the simulation demonstrated robustness and consistency, further validating its fidelity in capturing critical behaviour. Overall, the results obtained from the simulation exhibited excellent agreement with theoretical expectations, highlighting the model's efficacy in studying the intricate behaviour of the two-dimensional Ising model near critical points. This comprehensive analysis contributes to a deeper understanding of magnetic materials' behaviour and lays the groundwork for future research in this field.

References

[1] H. Gould, J. Tobochnik, and W. Christian An Introduction to Computer Simulation Methods: Applications to Physical Systems Chapter 17 – Monte Carlo Simulation of the Canonical Ensemble Addison-Wesley (2006)

[2] L. Onsager, Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition Phys. Rev. 65 117 (1944)