Monte Carlo Simulations of the 2D Ising model

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1 Background of Study

The Ising model is a mathematical construct in statistical mechanics that describes ferromagnetism in statistical physics. In the 2D Ising model, discrete variables known as spins can occupy one of two states (+1 or -1). These spins are arranged on a lattice, with interactions occurring between neighboring spins. The 2D Ising model, a frequently studied system in statistical physics, demonstrates intriguing phase transitions. This report details the results and observations from Monte Carlo simulations of the 2D Ising model. Using the Metropolis algorithm, the simulations aimed to explore the dynamics and properties of the model across various temperatures. Given that the energy of a configuration in the Ising model is described by the Hamiltonian:

$$H(\sigma) = -J \sum_{(i,j)} \sigma_i \sigma_j$$

Where $\sigma = (\sigma_i)_{i\in\Lambda}$ denotes a configuration of spins on Λ, with $\sigma_i \in \{1, +1\}$, and where the sum is taken over pairs of adjacent spins. where J is the interaction energy between neighboring spin; in the case of the study J is assumed to be 1. Lastly, σ_i is the spin at site i.

2 Numerical Simulations and Results

In our simulations, we considered a square lattice with a linear size of $L = 100$ and interaction energy $J = 1$, and the critical phase transition becomes:

$$T_c = \beta_c^{-1} = \frac{2}{ln(1+\sqrt{2})} \approx 2.269$$

$L = 100$ and Time is measured in number of sweeps $N = L^2$. The initial Configurations on the spins considered are for all $i \in \Lambda$ σ_i as:
1. $\sigma_i = +1$
2. $\sigma_i = 1$
3. $\sigma_i = +1$ with probability 1/2 this is the random case

2.1 Thermalization Time

To ensure accurate results, we first determined the thermalization time of the system. The thermalization time refers to the time required for the system to reach equilibrium. The thermalization time was measured in terms of the number of sweeps, where each sweep corresponds to updating all spins in the lattice once. This process is crucial as it allows us to distinguish between the initial non-equilibrium transient behavior and the equilibrium properties of the system. The Thermalization time is observed from the simulations of the following observables:

1. Magnetization (m): The magnetization per site as a function of time. It is given by

$$m(\sigma) = \frac{1}{N} \sum_{i \in \Lambda} \sigma_i$$

and is simulated for when $T = 2 < T_c = 2.269$ and $T = 2.5 > T_c = 2.269$ using the initial configuration above.

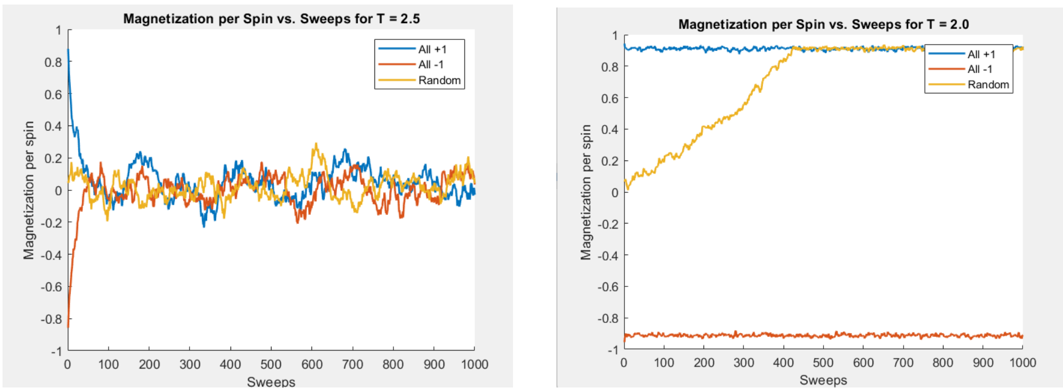

Figure 1: Magnetization per site vs time. above are the results for $T = 2.5$ (left panel) and $T = 2$ (right panel). The different colours of the curves refer to different initial configuration.

Figure 1 shows the magnetization per site as a function of time for temperatures 2 and 2.5. In the right panel, corresponding to $T < T_c$, we observe that the magnetization reaches a steady state after an initial transient period. Different initial configurations, including spin=+1, spin=-1, and random configurations, lead to slightly different magnetization curves. In the right panel, corresponding to $T > T_c$ the magnetization remains close to zero, indicating a lack of spontaneous magnetization.

2. Energy (e): The energy per site as a function of time. It is calculated using the Hamiltonian of the Ising model and averaging over all pairs of adjacent spins. It is given by

$$e(\sigma) = \frac{H(\sigma)}{N}$$

and is simulated for when $T = 2 < T_c = 2.269$ and $T = 2.5 > T_c = 2.269$ and using the initial configuration above.

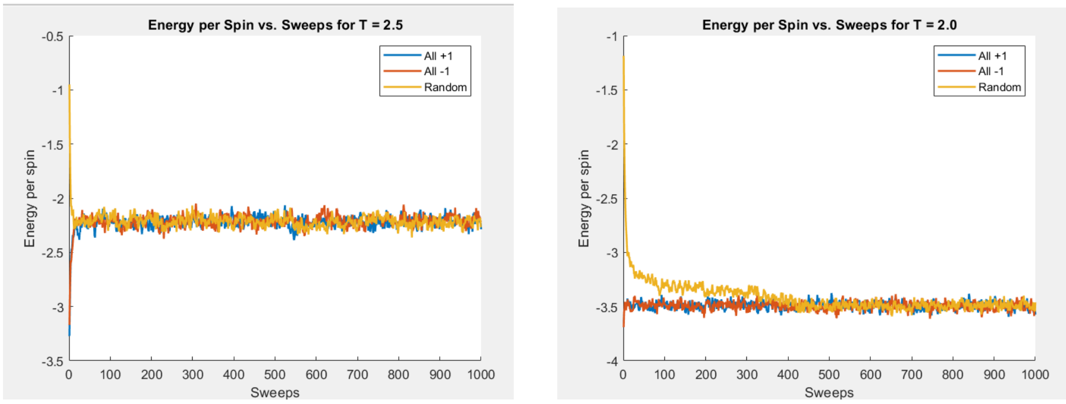

Figure 2: Energy per site of a two-dimensional Ising model on a square lattice with L = 100 and $T = 2.5$ (left panel) and $T = 2$ (right panel). The different colours of the curves refer to different initial data.

Figure 2 presents the energy per site as a function of time for the same temperatures. In the right panel (T < Tc), the energy reaches a steady state after the initial transient period. Different initial configurations lead to slightly different energy curves. In the left panel (T > Tc), the energy fluctuates around a higher value, indicating a higher energy state compared to the case below the critical temperature.

2.2 Phase Transition

Mean Magnetization and Mean Energy: Simulating the mean magnetization and mean energy which is a functions of temperature, the following phase transitions were observed:

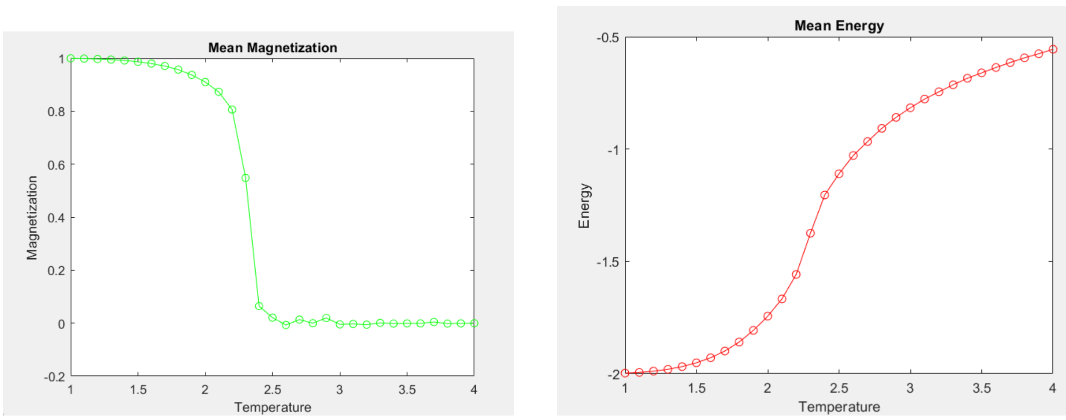

Figure 3: Left panel: Magnetization per site vs temperature T. Right panel: Energy per site as a function of T

Figure 3 shows the left panel represents the magnetization per site as a function of temperature. The green circles represent the results obtained from the Monte Carlo simulations, while the solid line represents the exact result obtained by Yang (1952). We observe a clear transition from a non-zero magnetization below the critical temperature to zero magnetization above the critical temperature. Figure 3 also presents the energy per site as a function of temperature in the right panel. The energy exhibits a smooth variation with temperature, without any sharp transition.

Magnetic Susceptibility and Specific Heat

Also, we could observe the phase transition in the simulation of:

Magnetic Susceptibility: The magnetic susceptibility as a function of temperature and it is given by:

$$\chi = \beta N(\langle m^2\rangle - \langle m\rangle^2)$$

Specific heat: The specific heat is a function of temperature and it is given by:

$$c = \beta^2 N(\langle e^2\rangle - \langle e\rangle^2)$$

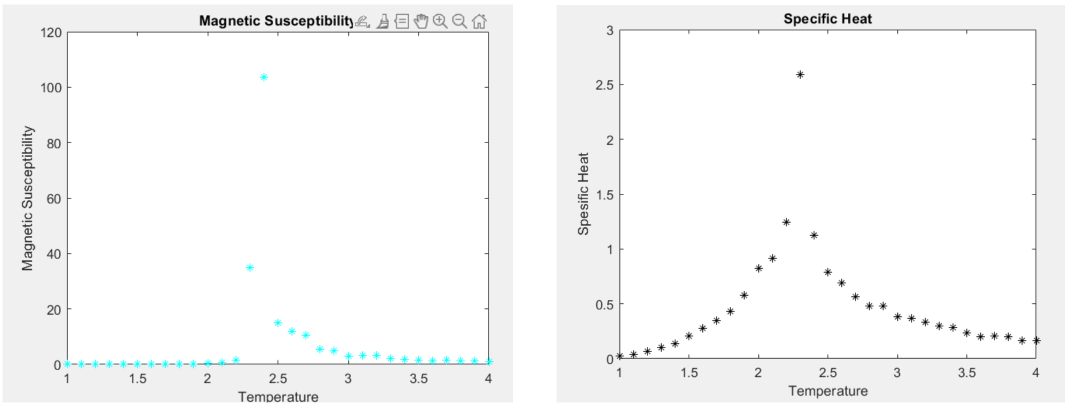

Figure 4: Left panel: Magnetic susceptibility (left panel) and specific heat (right panel) as functions of T

Figure 4 shows the magnetic susceptibility and specific heat as functions of temperature. The magnetic susceptibility increases sharply near the critical temperature, indicating the susceptibility of the system to external magnetic fields. The specific heat also exhibits a peak near the critical temperature, indicating the presence of a phase transition.

2.3 Microscopic Configurations

We examined the microscopic configurations of the Ising model at different times for temperatures below and above the critical temperature. Figure 5 displays the configurations for T = 2 < Tc, while Figure 6 shows the configurations for T = 2.5 > Tc. In both cases, we observe the evolution of the system from a fully disordered initial configuration to the formation of ordered domains. At each time, the Magnetization and Energy is computed and can be seen in the plot.

2.3.1 Case $T < T_c$

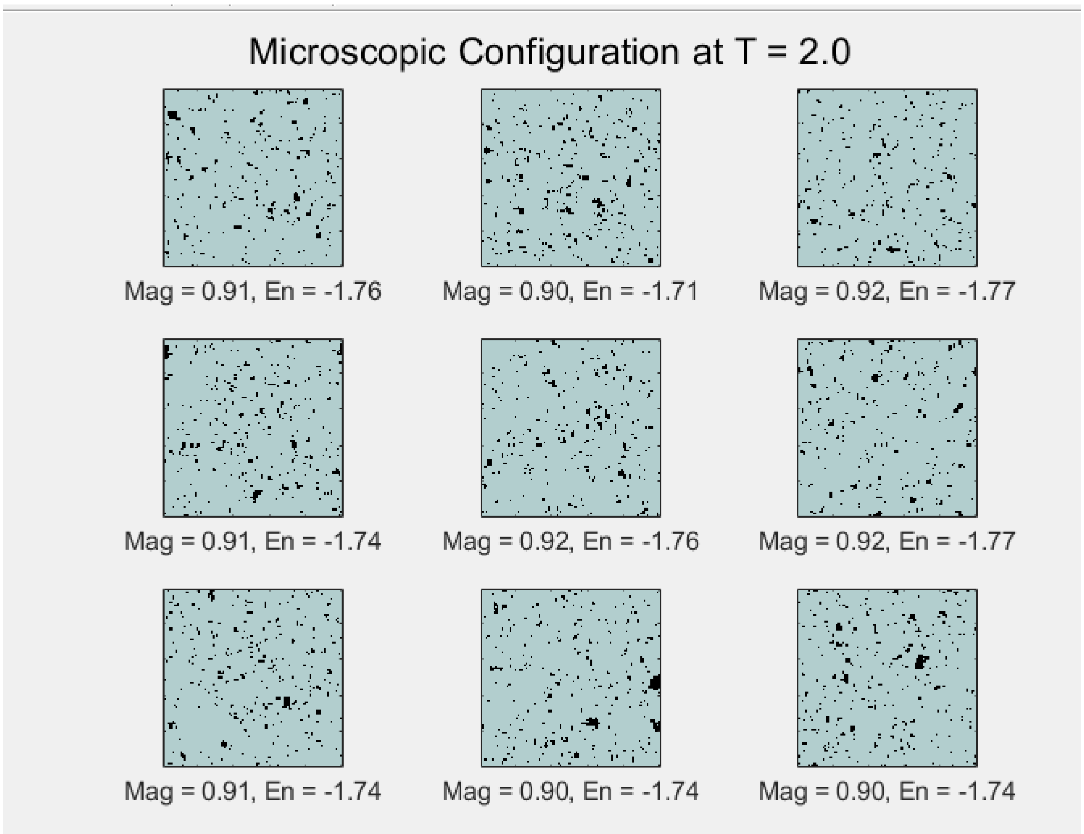

Figure 5: Microscopic configurations corresponding to $T = 2$ at times (left to right, top to bottom) 2×10^3, 4×10^3, 6×10^3, 8×10^3, 10^4, 1.2×10^4, 1.4×10^4, 1.6×10^4 and 1.8×10^4.

2.3.2 Case $T > T_c$

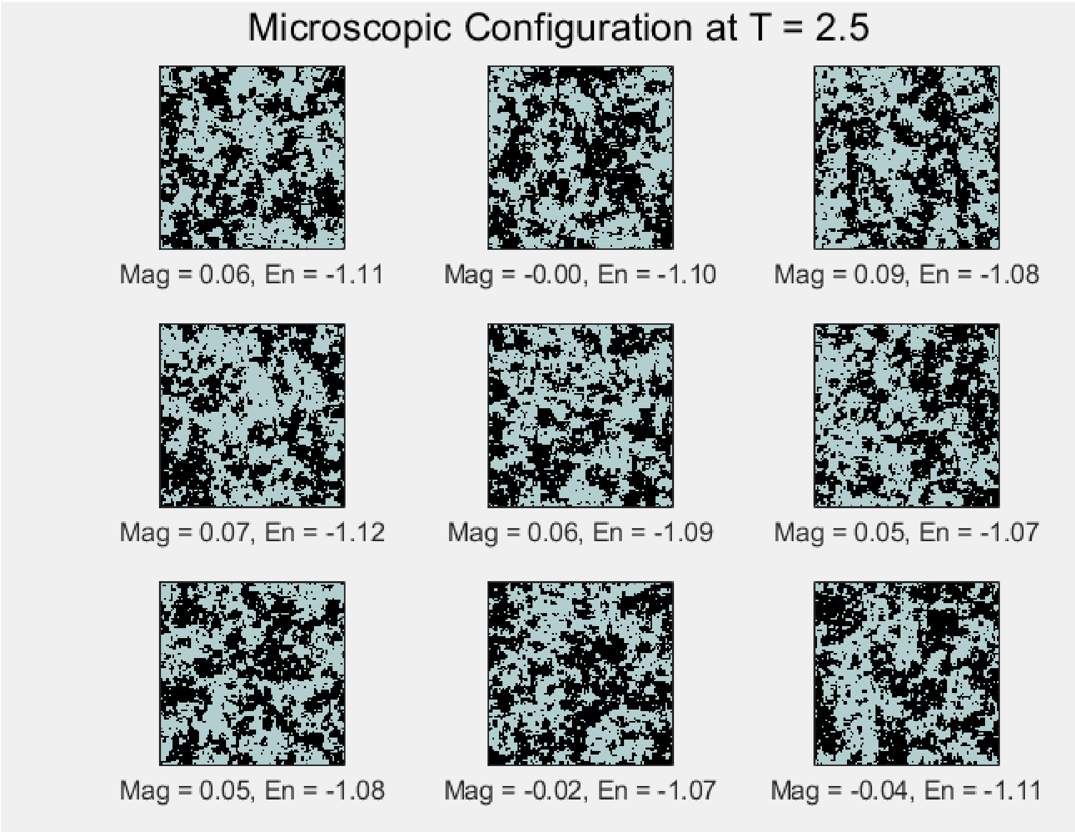

Figure 6: Microscopic configurations corresponding to $T = 2.5$ at times (left to right, top to bottom) 2×10^3, 4×10^3, 6×10^3, 8×10^3, 10^4, 1.2×10^4, 1.4×10^4, 1.6×10^4 and 1.8×10^4.

Conclussion

The Monte Carlo simulations of the 2D Ising model provided valuable insights into the dynamics and properties of the system. The results confirmed the presence of a phase transition at the critical temperature, characterized by a transition from non-zero to zero magnetization. The energy and magnetization dynamics revealed the behavior of the system at different temperatures. The microscopic configurations demonstrated the evolution of the system from disorder to order. Overall, these simulations contribute to our understanding of the 2D Ising model and its phase transition phenomena.