2D Ising Model

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Abstract

The goal of this exercise is to investigate the behavior of the 2D Ising model using the Metropolis-Hastings-based single-spin flip Monte Carlo method. The simulation is performed on a $L \times L$ square lattice with periodic boundary conditions.

Quantities such as absolute magnetization $\langle |M| \rangle$, energy $\langle E \rangle$, magnetic susceptibility χ, and heat capacity C_V are calculated at different temperatures and the critical temperature T_C is determined from the peaks of χ and C_V. The simulations revealed that the critical temperature lies between $2.045K$ and $3K$.

Simulations with different system sizes showed that as the lattice size increases, the phase transition at T_C becomes sharper, with the magnetization changes more abruptly between the ordered and disordered phases.

The evolution of magnetization M as a function of simulation time at a temperature $T < T_c$ exhibits sign flips. These flips result from thermal fluctuations and finite-size effects. Finite-size effects hinder spontaneous symmetry breaking and enable transitions between positive and negative magnetization states.

1 Introduction

We consider a 2D square lattice where each site i has a spin $s_i \in \{+1, -1\}$. The energy of a given spin configuration is given by the Hamiltonian:

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

where J is the interaction strength, and the sum runs over nearest-neighbor pairs $\langle i, j \rangle$.

The system exhibits different behaviors depending on temperature:

- At **high temperatures** ($T \gg T_c$), spins fluctuate randomly, leading to a **paramagnetic (disordered) phase**.
- At **low temperatures** ($T < T_c$), spins tend to align, resulting in a **ferromagnetic (ordered) phase**.
- The system undergoes a **second-order phase transition** at the critical temperature:

$$T_c \approx \frac{2.269J}{k_B} \tag{2}$$

To compute magnetic susceptibility and heat capacity, we use the fluctuation-dissipation theorem. In a finite system, we have [1]:

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

and

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

2 Results

2.1 Task 1, 2 and 3:

For each temperature T, 10^5 thermalization steps were carried out to ensure the system reached thermal equilibrium

The results for systems with different lattice sizes (L = 10, 15, 20) with parameters J = 1, $N_{\text{thermalization}} = 10^5$, $N_{\text{sample}} = 5000$ and $N_{\text{subsweeps}} = 10L^2$ are shown in Figures 1,2,3 respectively. The critical temperature is determined to be between $2.045K$ and $3K$ (or between $\beta = 0.333$ and $\beta = 0.489$) from the peaks of magnetic susceptibility and heat capacity. Moreover, the phase transitions in larger systems are sharper, causing higher peaks of magnetic susceptibility and heat capacity at T_C (see Fig. 4).

[1] In an infinite system, we use the spontaneous magnetization M_S instead of M.

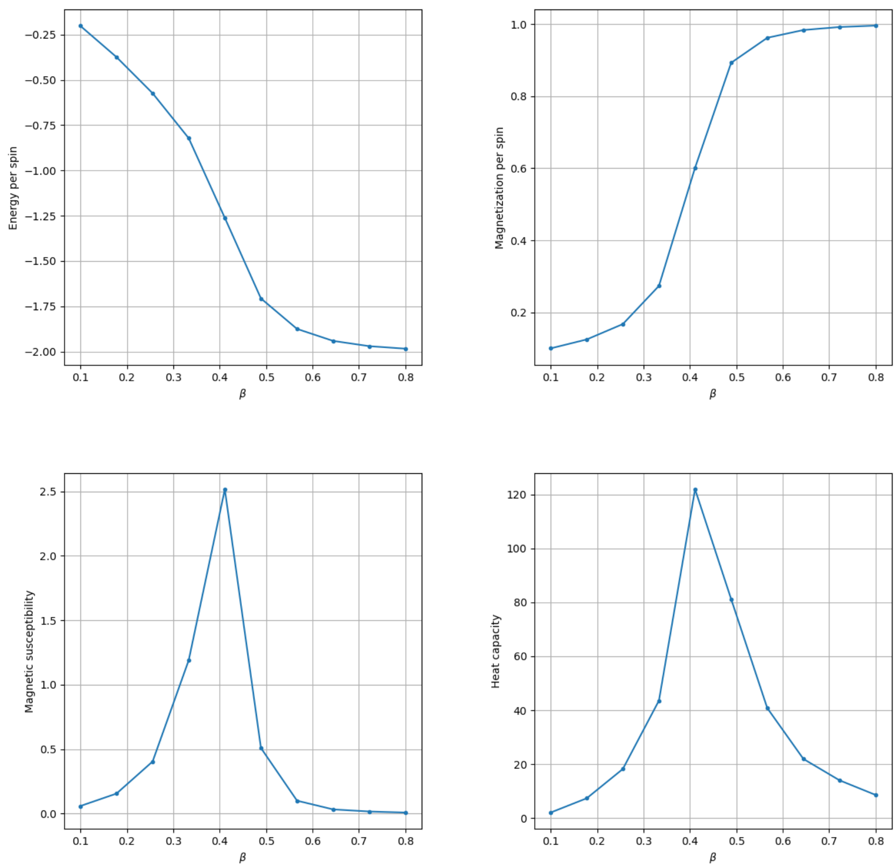

Figure 1: Energy, magnetization, magnetic susceptibility and heat capacity for $L = 10$ at different temperatures. Error bars are present but too small to be clearly visible.

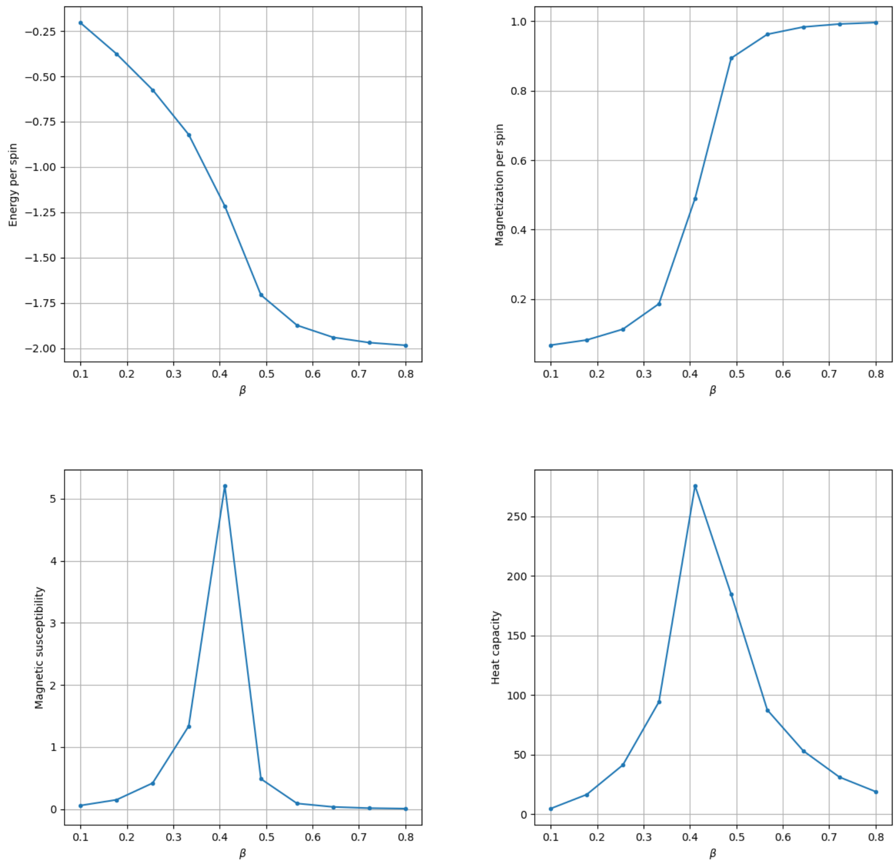

Figure 2: Energy, magnetization, magnetic susceptibility and heat capacity for $L = 15$ at different temperatures. Error bars are present but too small to be clearly visible.

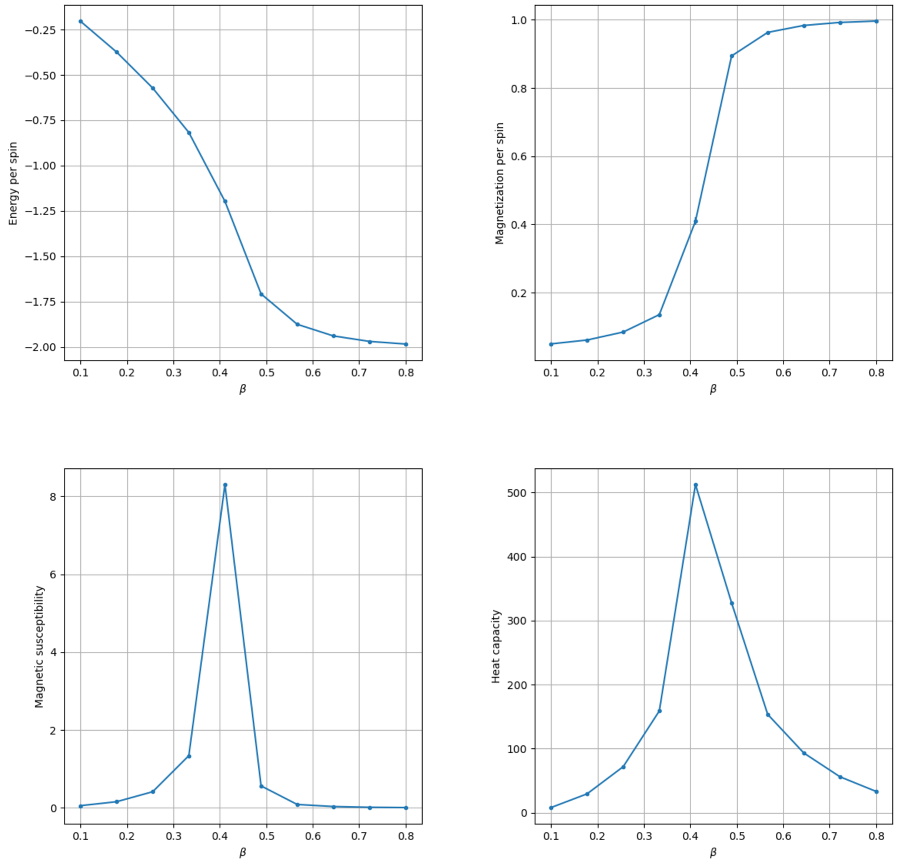

Figure 3: Energy, magnetization, magnetic susceptibility and heat capacity for $L = 20$ at different temperatures. Error bars are present but too small to be clearly visible.

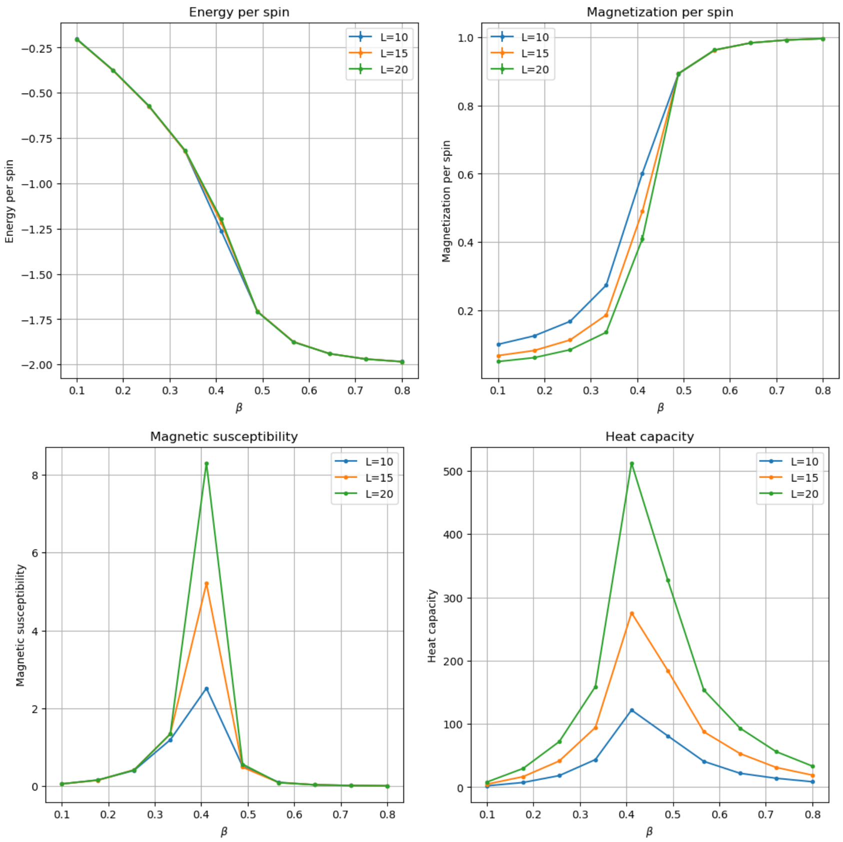

Figure 4: Energy, magnetization, magnetic susceptibility and heat capacity for $L = 10, 15, 20$ at different temperatures. Error bars are present but too small to be clearly visible.

2.2 Task 4:

The possible energy changes from flipping a spin are given by the formula $\Delta E = 2Js_ih_i$, where $h_i = \sum_{\langle i,j \rangle} s_j$. In our case, $J = 1$, $s_i \in \{+1, -1\}$ and the sum h_i can take values in $\{-4, -2, 0, 2, 4\}$. This gives us the possible energy changes as $\Delta E \in \{-8, -4, 0, 4, 8\}$. We can compute exponentials for these ΔE's and store them in a dictionary as shown in the code below:

```
J = 1 # coupling constant
beta = np.linspace(0.1, 0.8, 10) # inverse temperatures

# lookup table for acceptance probabilities
dE_values = np.array([-8, -4, 0, 4, 8]) # possible energy changes
lookup_table = {dE: np.exp(-dE * beta) for dE in dE_values}
```

2.3 Task 5:

The plot for the dependence of M on the simulation time at a temperature $T < T_C$ is given in Fig. 5. We observe sign flips of the magnetization. This is a result of the finite-size of the lattice. Finite-size effects hinder spontaneous symmetry breaking and enable transitions between positive and negative magnetization states. The effect is more prominent in smaller lattices.

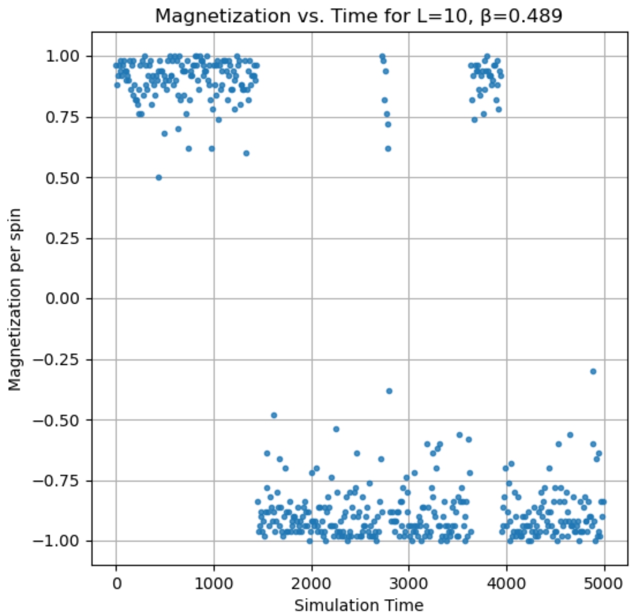

Figure 5: 2D Ising model Monte Carlo magnetization time evolution

3 Conclusion

This project investigated the behavior of the 2D Ising model through Monte Carlo simulations with the Metropolis algorithm. By plotting susceptibility and heat capacity, the critical temperature was estimated to lie within the range $2.045K \leq T_C \leq 3K$.

Larger systems exhibited sharper phase transitions, whereas sign flips of magnetization were observed in smaller systems due to finite-size effects.

The results align with the theory. In the future, more efficient algorithms could be implemented, such as cluster updates to improve critical slowdown.