Energy and Magnetization in 1D & 2D Ising Models —— Xuanlin Zhu

Abstract
This report investigates the thermodynamic behavior of the 1D and 2D Ising models using Monte Carlo simulations based on the Metropolis-Hastings algorithm. Energy and magnetization were recorded under various inverse temperatures ($\beta \in [0.1, 1.0]$). The results show that the 2D model exhibits a clear phase transition near $\beta \approx 0.5$, while the 1D model remains disordered at all temperatures. These findings align well with theoretical predictions.

1, Introduction

One of the most important and fundamental models in statistical physics is the Ising model. It was one of the earliest steps to understand the magnetism of objects such as ferromagnetism.

Each particle, i.e. a spin in the structure of this model, has only two options: -1 or +1. Each bit interacts only with its neighbors. However, we are currently able to understand the emergence of behaviors present in more complex models based on very simple assumptions.

Simulation methods help us discover features caused by random fluctuations far from a stable equilibrium point. The smallest of these model simulation methods can be called Monte Carlo (MC) methods. They can give us insights into thermodynamics if they lack information about the energy of interactions between particles.

After that, scientists often use another group of tools called Markov chain MC methods - named after the Russian mathematician Andrey Markov. The simplest application of such chains may involve simulating the so-called Metropolis-Hastings process. The principle behind it is not difficult if I know it - generate some randomness to test each choice, observe what happens after a sufficiently long time has passed; and wait for things to develop a trend given certain initial condition.

Our task is now simple: using a Monte Carlo method based on the above ideas, find different values of conventional power and their corresponding average magnetization simultaneously when decreasing/increasing the temperature of the 1D and 2D Ising lattice arrays. Our goal is still simple - try to qualitatively describe the obvious differences between the two sets of outputs, especially around significant signs that a phase transition has occurred between the different temperatures being studied (i.e., the hotter/colder scenario).

2， Methods

2.1 Model Description

The primitive model featured in this project is the Ising model, which takes discrete spin variables ***si=±1*** that arrange in either a one-dimensional chain or a two-dimensional square lattice. Each spin only interacts with its nearest neighboring spins, and the total energy of the system is defined as:

$$E = -J \sum_{\{\langle i,j \rangle\} s_i} s_j$$

where ***J*** is the coupling constant (fixed to 1 for this work), and the sum is over all pairs of nearest neighbors. To reduce the edge effects, 1D and 2D models apply periodic boundary conditions.

2.2 Simulation Algorithm

Monte Carlo simulations were conducted using the **Metropolis-Hastings algorithm**, a widely used method for sampling from the Boltzmann distribution. The algorithm proceeds as follows:

1. **Initialization**: The spin configuration is initialized randomly with each spin set to either +1 or −1 with equal probability.
2. **Update Step**: A spin is selected at random and flipped. The energy change ΔE caused by this flip is computed.
3. **Acceptance Criterion**: The new configuration is accepted with probability

$$P = min\left(1, e^{\{-\beta\Delta E\}}\right)$$

Where $\beta = \frac{1}{k_B T}$ is the inverse temperature (with $k_B = 1$).

4. **Repeat**: Steps 2–3 are repeated for a sufficiently large number of iterations.

One full **sweep** is defined as NN update attempts, where NN is the total number of spins in the system (100 for 1D, 10,000 for 2D).

2.3 Parameter Settings

Simulations were conducted over a range of inverse

temperatures β∈[0.1,1.0] with increments of 0.1. For each β value:

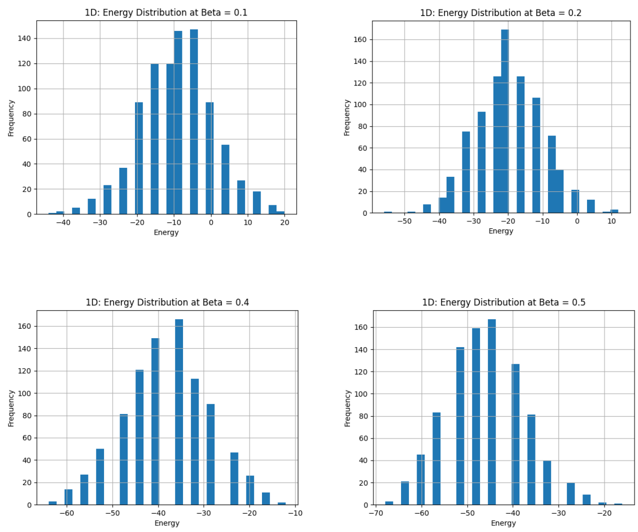
- **Total sweeps**: 10,000
- **Burn-in steps**: First 1,000 steps discarded to allow for thermal equilibration
- **Sampling interval**: Every 10 sweeps after burn-in
- **Measurements**: Energy and magnetization were recorded at each sampling point

This procedure was performed independently for both 1D and 2D models. To assess convergence, energy vs. step plots were generated for selected β values.

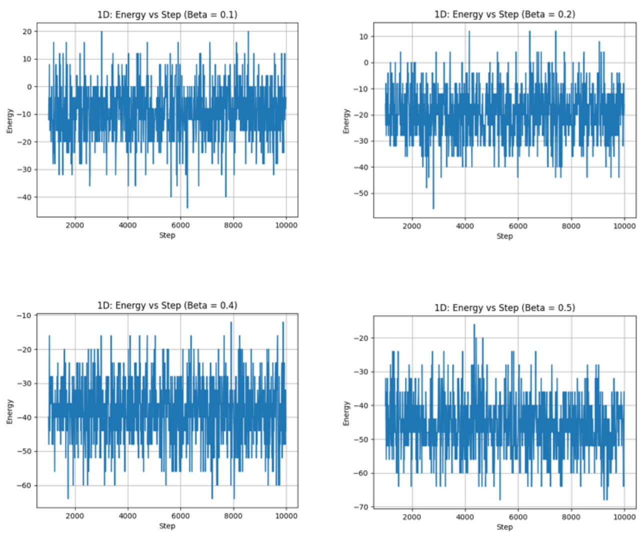
3， Results Analysis of simulation results

3.1 Convergence & stability of energy (1D)

To check whether the system has achieved thermal equilibrium, for each value of β, we monitored how the energy of the system varies with the number of steps in the simulation. From the figure (Figure: 1D Energy Vs Step at $\beta = 0.1 \sim 0.5$) we also can see that as the number of steps increases, the energy gradually tends to a steady-state fluctuation, which indicates that the system has reached thermal equilibrium, and the sampling process can begin.



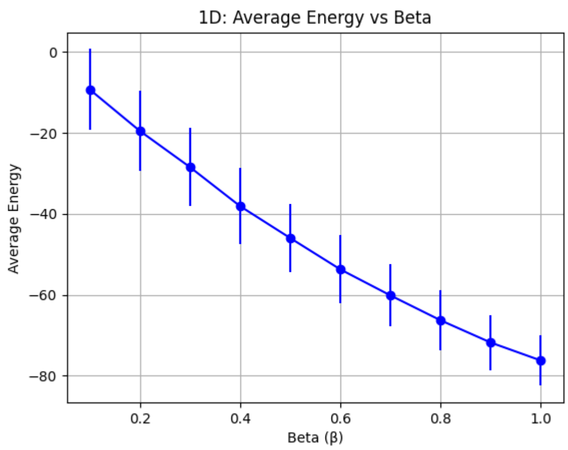
Graphics: 1D distribution vs beta



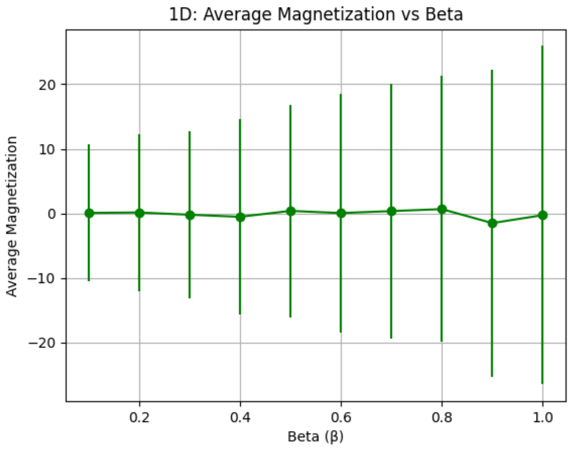
Additionally, when comparing the energy curves of different β, it can be observed that with the increase of β (the temperature decreases), the average energy of the whole system decreases, and the fluctuation amplitude gradually decreases, reflecting the trend of a more ordered system and lower energy at low temperatures.

3.2 Relationship between average energy and average magnetization and β (1D)

The average energy is shown in the figure "1D: Average Energy vs. β". As β increases, the average energy increases. From the results, as β changes from 0.1 to 1.0, the average energy decreases significantly, and the error becomes smaller and smaller, which is consistent with the physical behavior of spontaneous order and the trend of energy decrease.



The figure "1D: Average Magnetization vs. β" shows that the overall magnetization generally remains near 0 but also oscillates greatly around 0. This shows that the 1D Ising model does not show obvious phase transition or spontaneous magnetization at non-zero T, which is consistent with theoretical expectations.

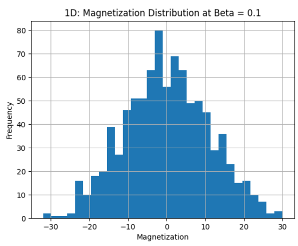


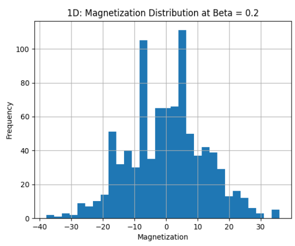
3.3 Energy and magnetization intensity distribution behavior (1D)

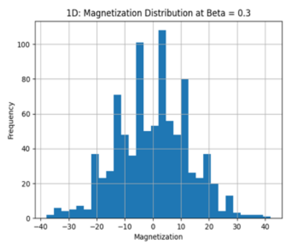
Then, we quantified the energy and magnetization intensity distribution at different temperatures in the range of β=0.1 to 0.5 (Figure: 1D energy distribution/magnetization intensity distribution when β=0.1-0.5):

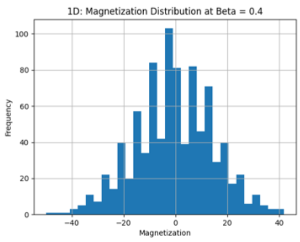
The energy distribution gradually tends to the low region, while the distribution width becomes smaller, indicating that the system is more inclined to the low energy state.

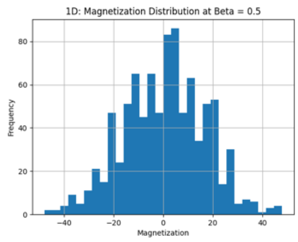
The magnetization intensity distribution is always approximately symmetrical with 0 as the center, without obvious offset or double peak structure, which better indicates that the 1D system does not have spontaneous symmetry breaking behavior.





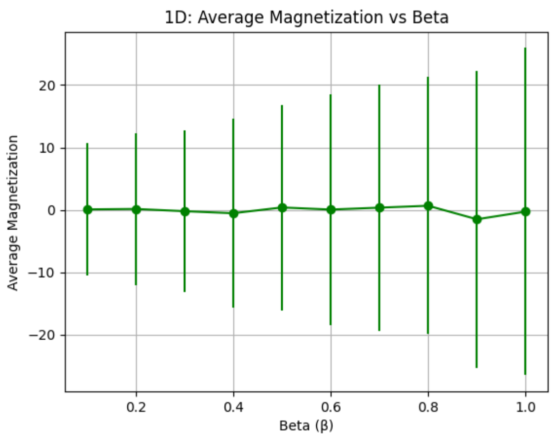






3.4 Convergence analysis of energy and magnetization (1D)

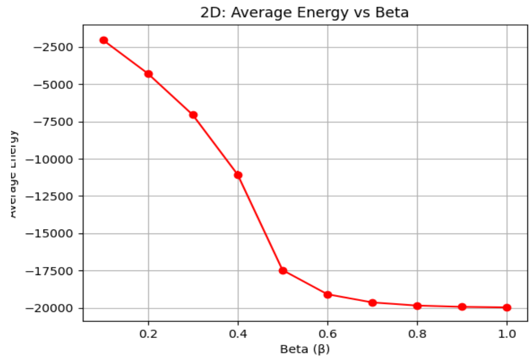
Figure “Magnetization vs Step” shows the fluctuation of magnetization with the number of simulation steps under different β values. It can be observed that the magnetization always fluctuates around 0, and with the increase of β value, the fluctuation amplitude increases slightly, but no stable offset occurs. This shows that the system does not have spontaneous magnetization phenomenon at different temperatures.

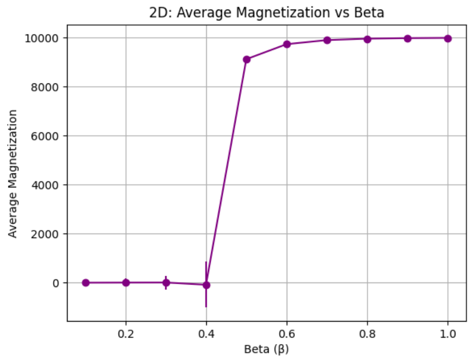


3.5 Variation of average energy and average magnetization with β (2D)

In the two-dimensional Ising model, the figure “2D: Average Energy vs β” shows that as β increases, the system energy decreases rapidly and tends to be flat near β ≈ 0.5, indicating that the system gradually enters a low-energy stable state.

More characteristic is the mutation phenomenon in the figure “2D: Average Magnetization vs β” - when β increases from 0.4 to 0.5, the average magnetization suddenly jumps from close to 0 to close to the system saturation value (about 10,000). This mutation clearly reveals the existence of phase transition in the two-dimensional system.



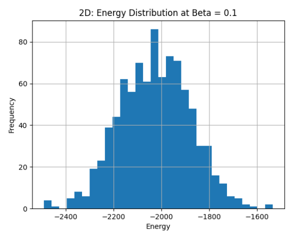


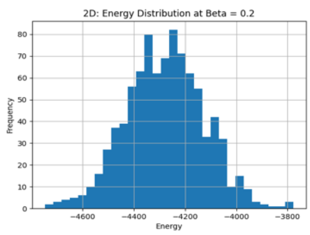
Average Energy vs Beta

Average Magnetization vs Beta

3.6 Energy and magnetization distribution behavior (2D)

Figure “2D Energy Distribution at β = 0.1–0.3” shows that the energy distribution of the system at high temperature is relatively symmetrical and wide.





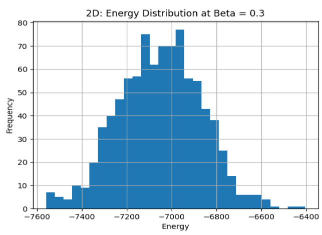


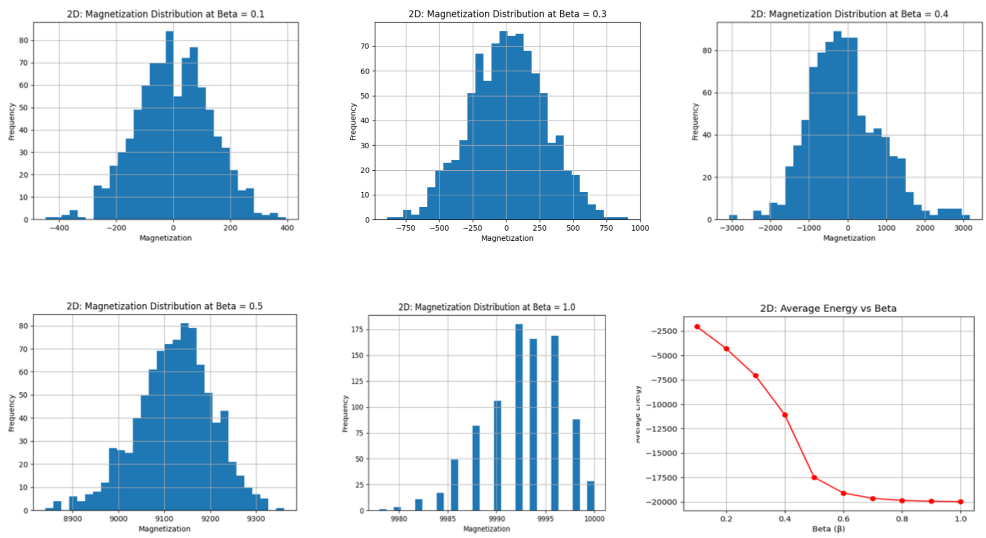
Figure “2D Magnetization Distribution”: When β = 0.1 ~ 0.3, the magnetization distribution is approximately centered at 0 and symmetrically expanded, indicating that the system is in a high-temperature disordered phase, the spin orientation is random, and no overall magnetization direction is formed.

At β = 0.4, the distribution begins to stretch significantly, the variance increases, and there is a trend of expanding from the center to both ends, indicating that the system begins to tend toward magnetization, but is still not completely oriented.

From β = 0.5, the magnetization distribution shifts significantly, and the overall peak value concentrates close to the saturation value (about 10,000), indicating that the system has spontaneously broken symmetry and entered a low temperature ordered phase.

When β = 0.6 ~ 1.0, the distribution gradually becomes concentrated and biased towards the extreme point, and the peak shape gradually becomes sharp, indicating that the system magnetization tends to be stable and most of the spins in the system are aligned.

This series of changes is highly consistent with the mutation points in the "2D: Average Magnetization vs β" figure, indicating that the two-dimensional Ising system undergoes a second-order phase transition near β ≈ 0.45–0.5.



4. Discussion

By comparing the simulation results of the one-dimensional and two-dimensional Ising models, the following rules can be observed:

Energy distribution: As the β value increases, the system energy tends to a lower value and the distribution gradually concentrates. This is consistent with physical expectations, that is, the system tends to a stable low-energy state at low temperatures.

Magnetization intensity distribution:

In the one-dimensional model, the average magnetization intensity is always close to 0, indicating that the system is difficult to maintain a spontaneous magnetization state at all temperatures, which is consistent with the theoretical prediction that the one-dimensional system does not undergo phase transition.

In the two-dimensional model, the average magnetization intensity suddenly changes near $\beta \approx 0.4$, jumping sharply from close to 0 to close to the maximum value, indicating that the system undergoes a phase transition here and enters an ordered state with spontaneous magnetization.

Convergence analysis: The convergence diagram shows that after a certain number of thermalization steps, the energy and magnetization intensity values tend to be stable, indicating that the sampling process is sufficient, and the simulation results have high reliability.

5. Conclusion

This experiment used the Metropolis Monte Carlo method to simulate the one-dimensional and two-dimensional Ising models and investigated the change law of system energy and magnetization intensity under different temperature (β) conditions.

The results show that:

The one-dimensional system does not undergo phase transition at any temperature, and spontaneous magnetization cannot be maintained.

The two-dimensional system exhibits critical behavior near $\beta \approx 0.4$, showing obvious phase transition characteristics.

The simulation results are highly consistent with the theoretical expectations of the Ising model, verifying the accuracy and effectiveness of the implemented algorithm.