Ising Model: Metropolis Algorithm

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Background

The Ising model is a mathematical model used in statistical physics to study phase transitions and critical phenomena in ferromagnetic systems. This model consists of a lattice where each site hosts a spin that can be in one of two states: up +1 or down -1 (shown in figure 1).

The interactions between sites are limited to nearest neighbors. The fact that the state of the system depends only on the local interaction makes it a simple but very useful model.

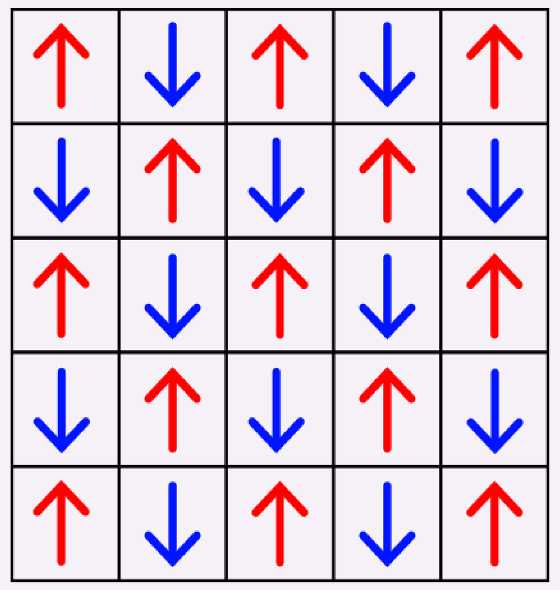

Figure 1: 5X5 2D Ising Model

The Ising lattice exhibits an ordered phase at low temperature, where spins are predominantly aligned. By contrast, a disordered phase characterized by random spin orientations is prevalent at high temperature.

The transformation between the ordered and the unordered phases, known as a phase transition, occurs near a characteristic point called the critical temperature (T_c). For the two-dimensional square lattice Ising model, the theoretical critical temperature is given by $Tc \approx 0.269$. Near this temperature, the system exhibits large-scale fluctuations, forming extended clusters of aligned spins.

Research Question

How do key physical quantities of the 2D Ising model—such as energy, magnetization, specific heat, susceptibility, and Binder cumulant—behave near the critical temperature, and what insights can be gained about critical phenomena through finite-size scaling using the Metropolis algorithm?

Method

We begin with a randomly initialized L x L spin lattice. The system evolves via the Metropolis algorithm, where each Metropolis sweep involves iterating over all lattice sites and probabilistically flipping spins based on the energy change ΔH:

$$P_{flip} = \begin{cases} e^{-\Delta H/k_B T}, & \Delta H > 0 \\ 1, & \Delta H \leq 0 \end{cases}$$

where,

$$\Delta H = 2 s_i J \sum_{nn} s_j$$

Here:

- s_i is the spin at site i,
- s_j nearest neighbors of s_i (with periodic boundary conditions),
- K_B Boltzmann Constant,
- J is the coupling constant (J > 0 for ferromagnetic interactions),
- T is the system temperature.

For each site, a random number r between 0 and 1 is generated; the spin is flipped if $r < P_{flip}$.

To ensure thermal equilibrium before taking measurements, we perform 200–1000 initial Metropolis sweeps, depending on the temperature. To reduce autocorrelation, measurements are taken at intervals of 10 sweeps.

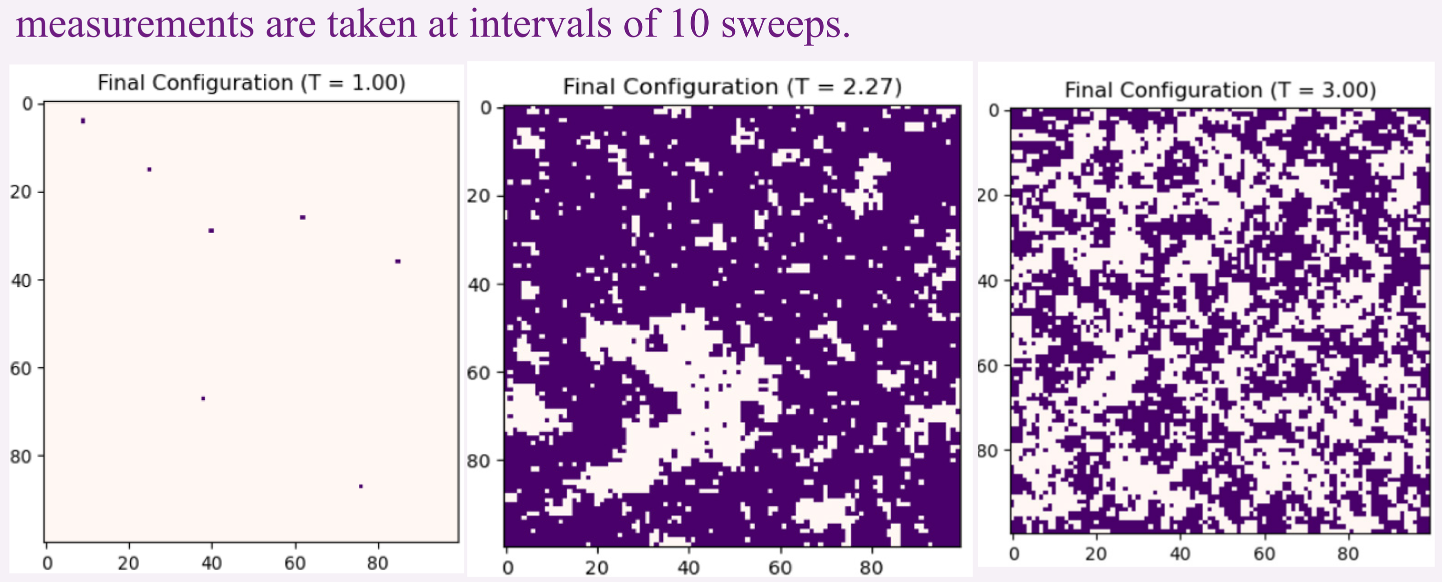

Figure 2: Final state of 100x100 lattice after running 1000 Metropolis sweeps on the initial random lattice at (a) low, (b) critical, and (c) high temperature. The purple and white sites represent up and down spins respectively.

Results

Energy:

The average energy per site is computed by summing the interaction energy at each site, based on Equation 2. The resulting expression is:

$$\langle \mathcal{H} \rangle = \frac{1}{2L^2} \sum_i^{L^2} (-J \sum_{\langle i,j \rangle} s_i s_j)$$

The factor of 1/2 avoids double-counting spin interactions between neighboring sites.

As shown in Figure 3, the energy exhibits a sharp raise near the critical temperature, indicating a phase transition. This behavior reflects the system's shift from an ordered (low-temperature) to a disordered (high-temperature) state.

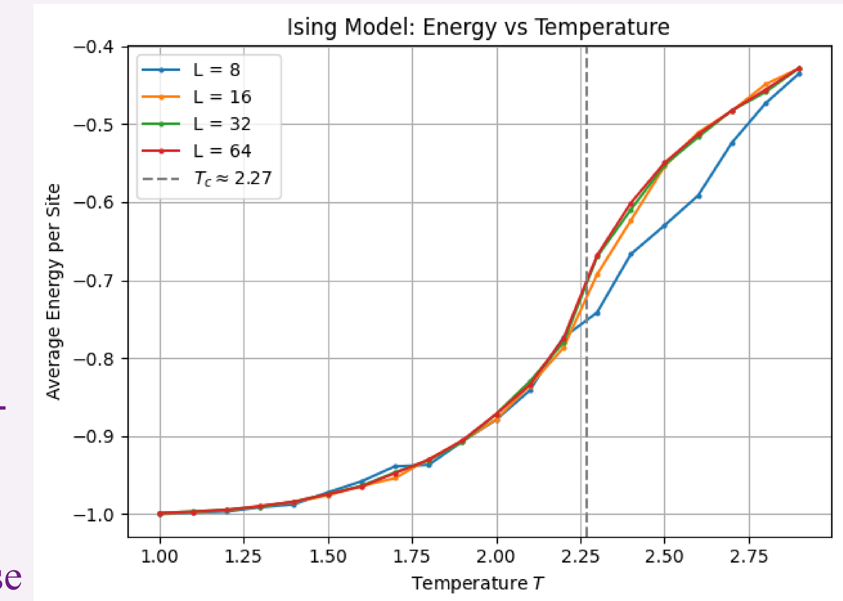

Figure 3: Average energy per site vs temperature for L = 8, 16, 32, 64

Magnetization:

In the two-dimensional Ising Model, magnetization describes the overall alignment of spins the the system. The average magnetization per spin is given by:

$$\langle m \rangle = \frac{1}{L^2} \langle |M| \rangle = \frac{1}{L^2} \langle |\sum_{i=1}^{N} s_i| \rangle$$

As shown in figure 4, the system goes from highly aligned state at low temperature (<m> ~ 1) to disaligned state at high temperature (<m> ~ 0).

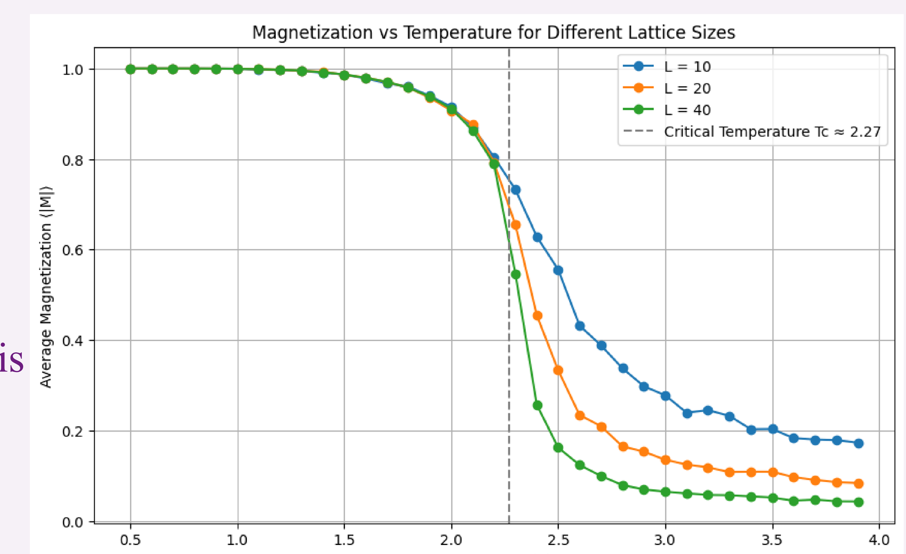

Figure 4: Average absolute magnetization per site vs temperature for L = 10, 20, 30

Binder's Cumulant:

Binder's Cumulant (U_L) is dimensionless quantity that provides a reliable indicator of critical behavior. It is defined is:

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3 \langle m^2 \rangle_L^2}$$

U_L as a function of T is shown in figure 5. The curves cross each other at critical temperature as the U_L for larger lattices drops more drastically.

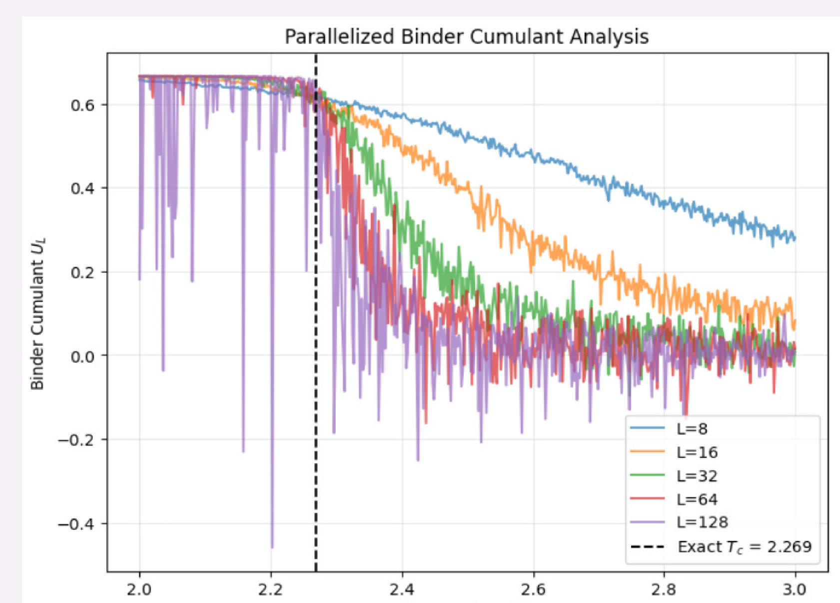

Figure 5: Binder's Cumulant vs temperature for L = 8, 16, 32, 64, 128

Two Point Correlation:

The two-point correlation function (C(r)) shows how spin at two distinct sites s_i and s_j at distance r are statistically related. It is defined as:

$$C(r) = \langle s_i \cdot s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

C(r) as a function of r = $|s_i - s_j|$ for different T is shown in figure-6 (upper panel), which resembles exponential decay:

$$C(r) = A \cdot e^{-r/\xi}$$

ξ represents correlation length – a measure of distance between the sites after with the correlation decreases significantly. ξ as a function of T is shown in figure-6 (lower panel). ξ peaks near T_c indicating highly correlated system at critical temperature.

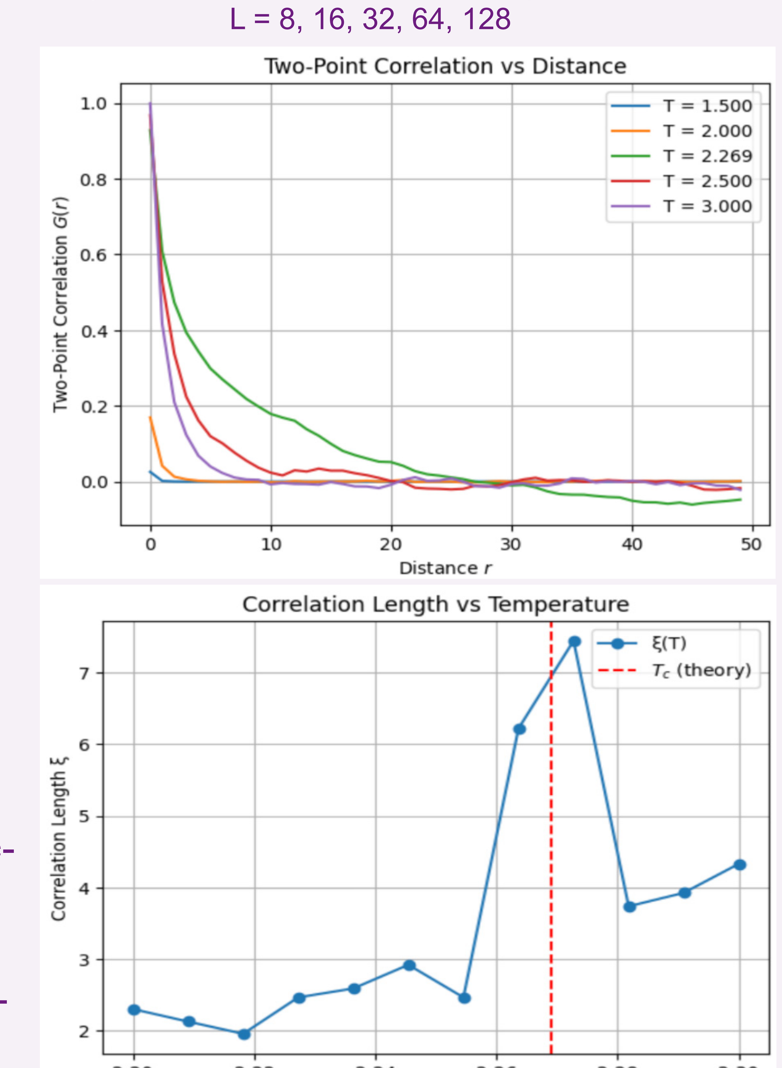

Figure 6: (Upper) C(r) vs r for a 100x100 lattice, (lower) Correlation length vs temperature for L = 65

Results

Specific Heat:

Specific heat (C_V) is a measure of system's energy fluctuation with temperature. We define specific heat as follows:

$$C_V = \frac{1}{k_B T^2} [\langle E^2 \rangle - \langle E \rangle^2]$$

C_V as a function of T is shown in figure-7.

- The curves exhibit a prominent peak near the T_c.
- The height and sharpness of the peak increase with system size.
- The peak position converges toward T_c as L increases.

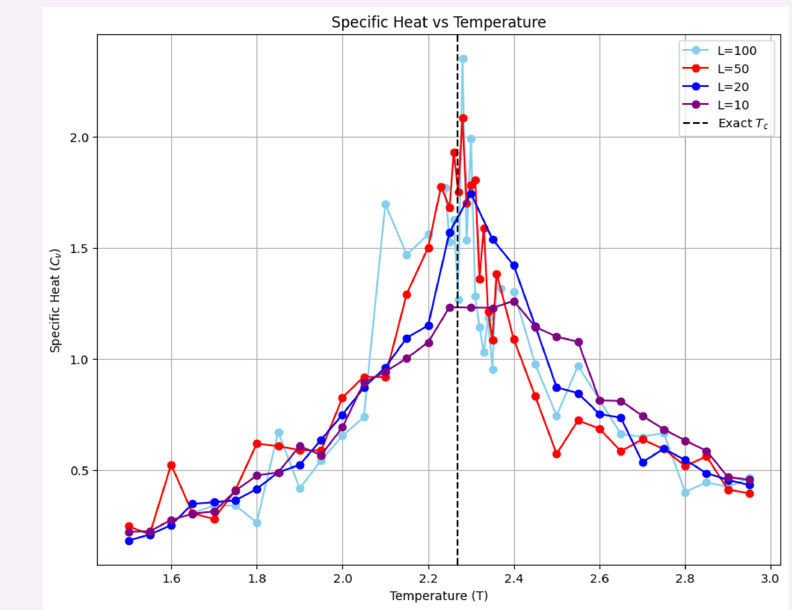

Figure 7: Specific heat (C_V) vs temperature (T) for L = 10, 20, 50, 100

Susceptibility:

Susceptibility (χ) is a measure of system's magnetization fluctuation. We define susceptibility as follows:

$$\chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle |M| \rangle^2)$$

Susceptibility as a function of T is shown in figure-8.

- The peaks of the susceptibility curves lie just to the right of the theoretical T_c.
- As the lattice size increases, the peaks shift leftward toward the T_c, consistent with the expected finite-size scaling behavior

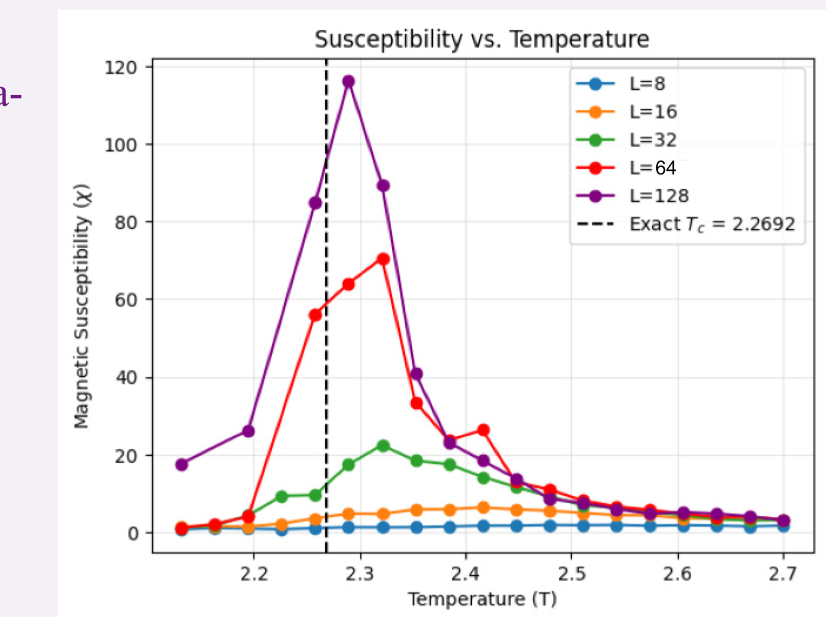

Figure 8: Suscpetibility (χ) vs temperature (T) for L = 8, 16, 32, 64, 128

Finite Size Scaling:

The parameters obtained for finite lattices can be extrapolated to an infinite lattice using finite-size scaling. For this analysis, we focused on magnetic susceptibility (χ).

Figure 9 shows how χ varies with T for different lattice sizes. The temperatures at which the susceptibility peaks—representing the effective critical temperatures T_c (L) – are plotted against 1/L in Figure 10. The relationship is approximately linear, and fit suggests that at 1/L→0, T_c (L→∞) = 2.28 ± 0.03.

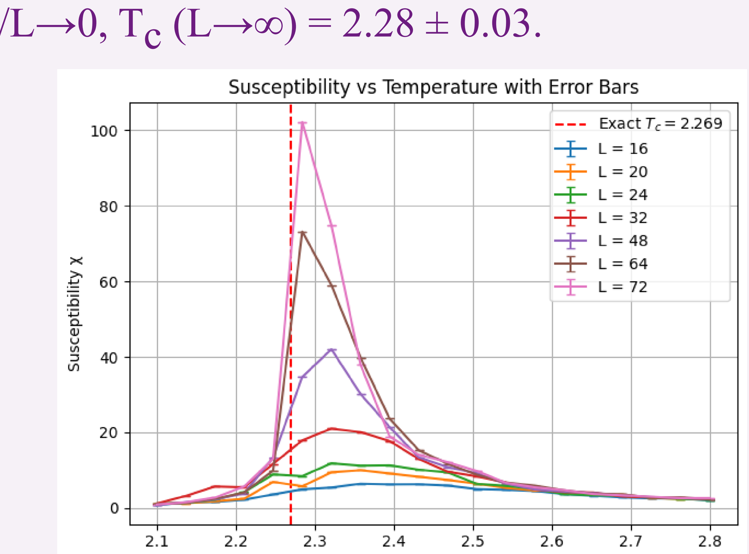

Figure 9: Suscpetibility (χ) vs temperature (T)

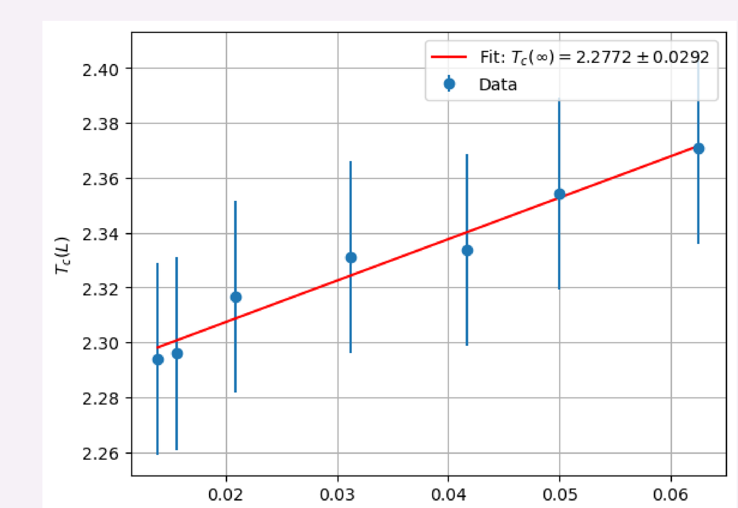

Figure 10: Extrapolated peak temperature vs 1/L

Conclusion

- Using the Metropolis algorithm, we investigated key physical properties of the 2D Ising model and estimated T_c (L→∞) = 2.28 ± 0.03. Theoretical value T_c = 2.269 [2] falls within the uncertianty limit.
- The observables we studied (e.g., energy, magnetization, susceptibility) are consistent with the theoretical expectations[2].
- These physical observables remain consistent for other algorithms, allowing our findings to serve as a benchmark for validating alternative simulation methods.