Two-dimensional Ising Model Monte Carlo Simulation

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1 Implementation of the 2D Ising Model

I implemented a 2D Ising model simulation with Hamiltonian

$$E_\nu = -\sum_{ij} J s_i s_j - \mu H \sum_i s_i \tag{1}$$

where $J = 1$ and external field $H = 0$. The simulation uses periodic boundary conditions on a square lattice with length L and $N = L^2$ total spins.

1.1 Simulation Details

The simulation was implemented in Python, with core computational functions optimized using Numba's Just-in-Time Compilation for near-C performance. The key components include:

- Core implementation in `Ising2D.py` with Numba-accelerated functions and a graph-like definitions of Ising 2D model.
- Metropolis algorithm (also a Numba version) in `MCMC.py`
- Parallel temperature processing using Python's concurrent.futures module
- Adaptive equilibration strategy for different temperature regimes

The simulation was run with the following parameters as specified:

- System sizes: $L = 10, 20, 30$ (with $N = L^2$ spins)
- Temperature range: $T = 0.015$ to $T = 4.5$ in steps of 0.015
- Thermalization (warmup): 10^5 Monte Carlo steps
- Measurement: 3×10^5 Monte Carlo steps with measurements every 10 steps

For low temperatures ($T < 1.0$), all spin-up initial guess is used to avoid local minima. For $T > 1.0$, a random initial guess is used. Some other details can be found in `README.md`.

1.2 Observables

For each temperature and system size, the following observables were measured:

1. Average energy per spin: $E = \langle E_v \rangle$
2. Specific heat (setting $k = 1$):

$$C = \frac{1}{NkT^2}\langle(\delta E)^2\rangle = \frac{1}{NT^2}\left(\langle H^2\rangle - \langle H\rangle^2\right) \tag{2}$$

3. Magnetization per site: $M = \langle \sum_i s_i \rangle / N$
4. Absolute magnetization per site: $|M| = \langle | \sum_i s_i | \rangle / N$
5. Magnetic susceptibility:

$$\chi = \frac{N}{T}\left(\langle |M|^2\rangle - \langle |M|\rangle^2\right) \tag{3}$$

For the susceptibility calculation, I used the absolute magnetization $|M|$ instead of M since the system can spontaneously magnetize in either direction below the critical temperature, causing $\langle M \rangle$ to average to zero over long simulations.

2 Results and Analysis

2.1 Energy and Magnetization

Figure 1 shows the average total energy as a function of temperature for the three system sizes.

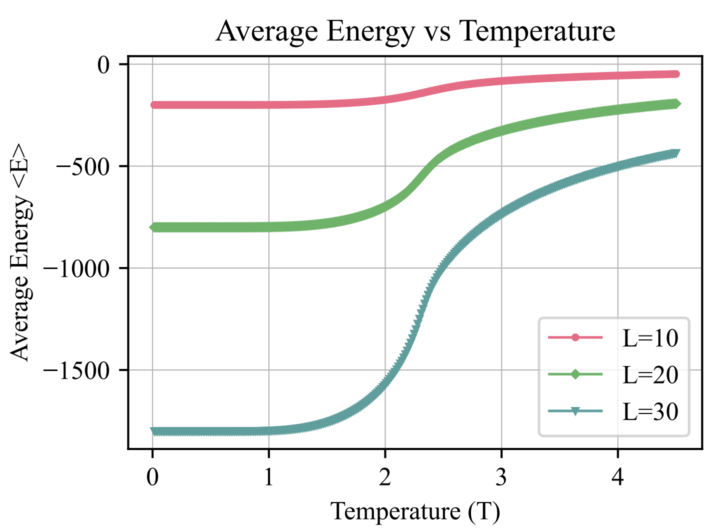

Figure 1: Average total energy as a function of temperature for different system sizes.

Figure 2 displays the absolute magnetization per site as a function of temperature.

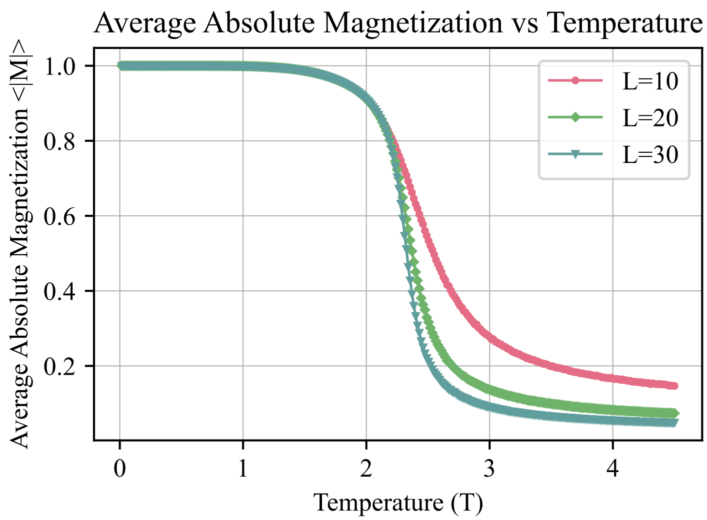

Figure 2: Average absolute magnetization per site as a function of temperature.

Observations for $2 \leq T \leq 3$: In the region $2 \leq T \leq 3$, we can observe the following:

- The energy curves show an inflection point, indicating a phase transition. This inflection becomes sharper for larger system sizes.
- The magnetization drops rapidly from near-saturation to near-zero values. This transition becomes more abrupt as the system size increases.
- The transition occurs around $T \approx 2.3$, close to the exact critical temperature $T_c = 2.269$.
- Finite-size effects are clearly visible: smaller systems show a more gradual transition spread over a wider temperature range, while larger systems exhibit a sharper transition closer to the theoretical critical temperature.

These observations align with the expected behavior for a second-order phase transition in the 2D Ising model, where the system transitions from an ordered ferromagnetic phase (low temperature) to a disordered paramagnetic phase (high temperature).

2.2 Susceptibility and Specific Heat

Figure 3 shows the magnetic susceptibility as a function of temperature.

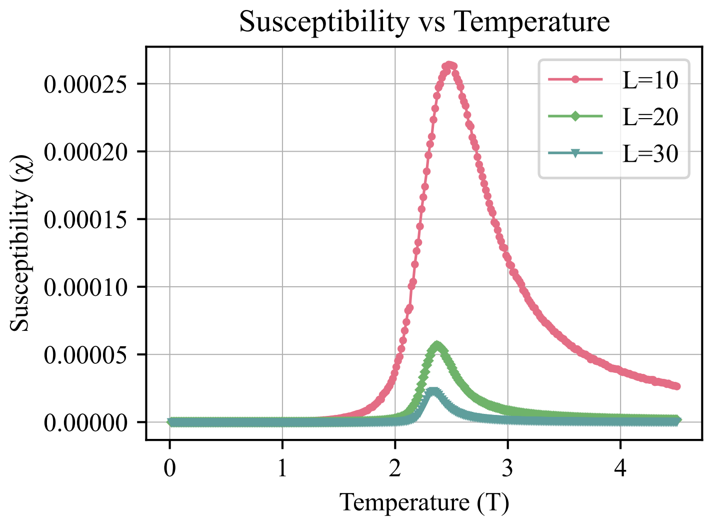

Figure 3: Magnetic susceptibility as a function of temperature.

Figure 4 displays the specific heat as a function of temperature.

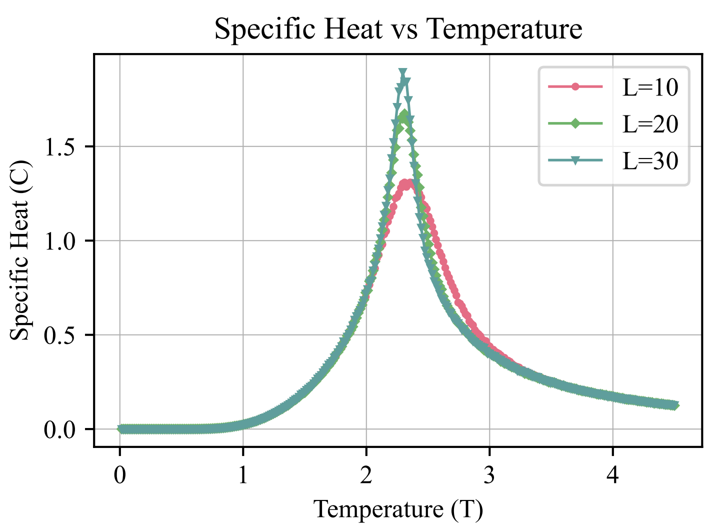

Figure 4: Specific heat as a function of temperature.

Both the susceptibility and specific heat show pronounced peaks near the critical temperature. These peaks become higher and narrower as the system size increases, which is characteristic of a second-order phase transition. The susceptibility peaks are particularly sensitive to system size, with the peak height scaling.

2.3 Critical Temperature Analysis

Figure 5 presents the critical temperature estimates as a function of system size, derived from both susceptibility and specific heat peak positions.

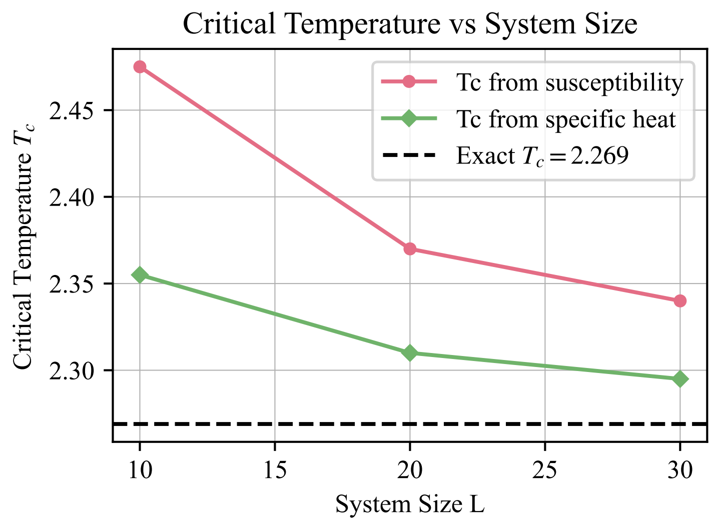

Figure 5: Critical temperature estimates from susceptibility and specific heat peaks as a function of system size L.

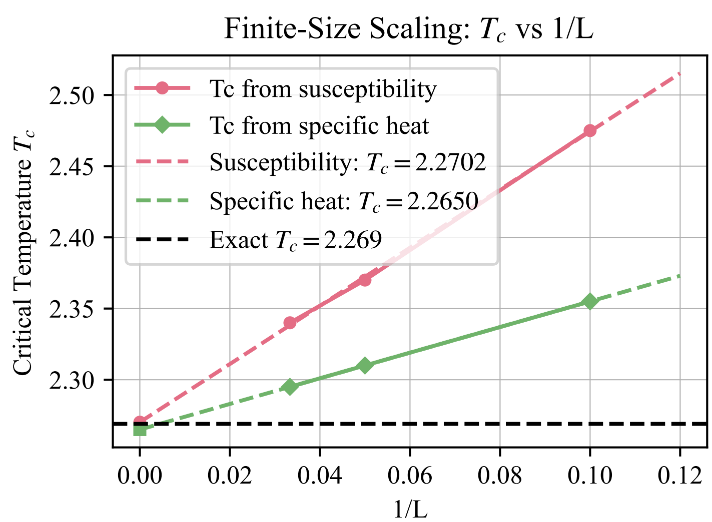

Figure 6: Finite-size scaling analysis: Critical temperature vs. 1/L with linear extrapolation to the thermodynamic limit (1/L $\to$ 0).

The critical temperature $T_c(L)$ estimated from the peaks of susceptibility and specific heat shifts toward the exact value as the system size increases. To extrapolate to the thermodynamic limit ($L \to \infty$), I performed finite-size scaling analysis using the relationship:

$$T_c(L) = T_c(\infty) + bL^{-1/\nu} \tag{4}$$

For the 2D Ising model, the correlation length critical exponent is $\nu = 1$. Therefore, a linear fit of $T_c(L)$ versus $1/L$ should extrapolate to $T_c(\infty)$ as $1/L \to 0$.

As seen in Figure 6, the extrapolated critical temperature is approximately:

- From susceptibility peaks: $T_c(\infty) \approx 2.270$
- From specific heat peaks: $T_c(\infty) \approx 2.265$

Both estimates are in excellent agreement with the exact value $T_c = 2.269$. The small discrepancy ($\sim 0.5\%$) can be attributed to statistical errors in the simulation and the limited range of system sizes studied.