Numerical Investigation of Phase Transitions in the 2D Ising Model Using Parallel Monte Carlo Methods

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We present a comprehensive numerical investigation of phase transitions in the two-dimensional Ising model using parallel Markov Chain Monte Carlo methods. Our study examines the temperature-dependent magnetic behavior and critical phenomena in ferromagnetic systems, with a particular focus on identifying the phase transition between ordered and disordered states. Through detailed analysis of multiple lattice sizes (L=40-100) and extensive sampling, we characterize the system's thermodynamic properties including energy, magnetization, specific heat capacity and magnetic susceptibility. Our implementation achieves exceptional accuracy, demonstrated by agreement with analytical solutions for the 2×2 lattice case to within 0.06% for energy and 0.02% for magnetization. Using finite-size scaling analysis with improved sampling techniques, we determine the infinite-lattice critical temperature to be $T_c(L = \infty) = 2.2560.020J/k_B$, matching Onsager's exact solution with a relative error of only 0.59%. This represents a significant improvement over conventional approaches, achieved through careful optimization of parallel computation methods and enhanced statistical sampling. Our results not only validate the numerical approach, but also provide insights into the practical challenges of studying critical phenomena in statistical physics.

I. INTRODUCTION

Phase transitions are fundamental phenomena in nature, occurring in various systems ranging from the boiling of water to the loss of magnetization in ferromagnetic materials. In this report, we focus on magnetic phase transitions in ferromagnetic systems, specifically investigating the temperature-dependent behavior using the two-dimensional Ising model. This model, despite its simplicity, captures the essential physics of ferromagnetism and serves as a cornerstone in statistical physics for understanding critical phenomena. The Ising model represents magnetic materials as a lattice of discrete spins, where each spin can only take two possible states: up (+1) or down (-1). These spins interact with their nearest neighbors, with parallel alignment being energetically favorable. At low temperatures, this interaction leads to long-range order, resulting in a net magnetization. However, as temperature increases, thermal fluctuations compete with the ordering tendency of the spin-spin interactions. Above a critical temperature Tc, known as the Curie temperature, thermal effects dominate and the system transitions to a disordered paramagnetic phase with no net magnetization. In 1944, Lars Onsager provided an exact analytical solution[1] for the two-dimensional Ising model's critical temperature in the infinite lattice limit, finding $Tc = 2.269J/kB$, where J is the coupling constant between spins and kB is the Boltzmann constant. This remarkable achievement stands as one of the few exact solutions in statistical physics for systems exhibiting phase transitions. However, real systems and numerical simulations necessarily deal with finite lattices, making it crucial to understand how finite-size effects influence the observed critical behavior.[1] In this work, we employ Markov Chain Monte Carlo (MCMC) methods to simulate the 2D Ising model and investigate its phase transition. Our primary goals are to:

Implement and validate an efficient MCMC algorithm for sampling spin configurations Study the temperature dependence of key thermodynamic quantities such as energy, magnetization, specific heat, and magnetic susceptibility Investigate finite-size effects by analyzing systems of different sizes Determine the critical temperature through finite-size scaling analysis and compare with Onsager's exact result Optimize computational performance through parallel computing techniques

We present our methodology in Section II, including analytical solutions for a 2×2 lattice that serve as validation benchmarks. Section III presents our numerical results, focusing on the critical behavior and finite-size effects. This section also includes analysis of our parallelization efforts and their impact on computational efficiency. Finally, Section IV summarizes our findings and discusses potential extensions of this work. All code developed for this investigation is available in our GitHub repository[2], ensuring reproducibility and providing a foundation for future studies of related systems.

II. METHODS

In this section, we present our methodology for studying the 2D Ising model. We begin with the theoretical framework and analytical solutions for small systems, followed by our numerical approach for larger lattices.

[1] Longuet-Higgins, H. C.; Fisher, M. E. (1978). "Lars Onsager. 27 November 1903-5 October 1976".

[2] https://github.uio.no/josefam/FYS3150/tree/main/project4

A. Theoretical Framework

The 2D Ising model consists of spins s_i arranged on a square lattice, where each spin can take values of either +1 ("up") or -1 ("down"). The energy of the system is given by:

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle} s_k s_l \tag{1}$$

where J is the coupling constant and the sum $\langle kl \rangle$ runs over all nearest-neighbor pairs on the lattice, with each pair counted once. The total magnetization is:

$$M(\mathbf{s}) = \sum_i s_i \tag{2}$$

At temperature T, the probability of observing a particular spin configuration $\mathbf{s}$ follows the Boltzmann distribution:

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})} \tag{3}$$

where $\beta = 1/(k_B T)$ (using units where $k_B = 1$) and Z is the partition function. We study the system through several observables:

- Energy per spin: $\epsilon = E/N$
- Absolute magnetization per spin: $|m| = |M|/N$
- Heat capacity: $C_V/N = (\langle E^2 \rangle - \langle E \rangle^2)/(NT^2)$
- Susceptibility: $\chi/N = (\langle M^2 \rangle - \langle |M| \rangle^2)/(NT)$

Note that we use $|m|$ rather than m because in the absence of an external field, the system has equal probability of being in states with opposite magnetization.

B. Analytical Solution for 2×2 Lattice

For validation purposes, we first consider a 2×2 lattice with periodic boundary conditions. For this system, each spin interacts with all others due to the periodic boundaries, giving the energy:

$$\begin{aligned} E = -J[&(s_{11}s_{12} + s_{12}s_{11}) + (s_{11}s_{21} + s_{21}s_{11}) \\ &+ (s_{12}s_{22} + s_{22}s_{12}) + (s_{21}s_{22} + s_{22}s_{21})] \end{aligned} \tag{4}$$

Analysis of all possible states yields the partition function:

$$Z = 2(e^{8\beta J} + e^{-8\beta J} + 6) \tag{5}$$

Algorithm 1 Metropolis Algorithm for 2D Ising Model

```
procedure MonteCarloSample(L, T, n_cycles)
    Initialize L × L grid (random or ordered)
    Precompute Boltzmann factors for ΔE ∈ {−8J, −4J, 0, 4J, 8J}
    for cycle = 1 to n_cycles do
        for step = 1 to L^2 do
            Select random position (i, j)
            Compute ΔE for flipping spin (i, j)
            Generate random r ∈ [0, 1]
            if r ≤ e^{−βΔE} then
                Flip spin (i, j)
                Update E and M
        if cycle ¿ burn_in then
            Accumulate measurements
    Compute averages and uncertainties
```

From this, we derive the expectation values:

$$\langle \epsilon \rangle = \frac{4J}{Z}(e^{-8\beta J} - e^{8\beta J}) \tag{6}$$

$$\langle |m| \rangle = \frac{4 + 2e^{8\beta J}}{Z} \tag{7}$$

$$C_V/N = \frac{128J^2}{T^2} \frac{3Z - 16}{Z^2} \tag{8}$$

$$\chi/N = \frac{16}{T} \frac{3 + 3e^{8\beta J} + e^{-8\beta J}}{Z^2} \tag{9}$$

C. Numerical Methodology

For larger lattices, we employ the Metropolis-Hastings algorithm, as detailed in Algorithm 1. The algorithm generates a sequence of states following the Boltzmann distribution through local updates (single spin flips).

Our implementation includes several optimizations:

- Pre-computation of Boltzmann factors for the five possible energy changes
- Efficient periodic boundary handling using conditional operators
- Local updates to energy and magnetization after each accepted flip

For each lattice size and temperature, we:

1. Initialize the system (random or ordered state)
2. Equilibrate for 5000 cycles (determined from burn-in analysis)
3. Sample for 1000-10000 cycles, collecting measurements of E and M
4. Compute observables and their uncertainties from fluctuations

D. Tools and Implementation

The simulation was implemented in C++ using:

- Armadillo library for matrix operations
- OpenMP for parallelization across temperature values
- Mersenne Twister (mt19937) for random number generation

Data analysis and visualization were performed using Python with Matplotlib. ChatGPT was used to assist with report structure and code optimization suggestions, with all implementations independently verified.

III. RESULTS AND DISCUSSION

A. Validation of Monte Carlo Implementation

For initial validation, we compared our Monte Carlo results against exact analytical solutions for a 2×2 lattice at $T = 1.0\,J/k_B$. Table I shows this comparison.

TABLE I. Comparison of numerical and analytical results for 2×2 lattice at $T = 1.0\,J/k_B$ using 10,000 Monte Carlo cycles after 5,000 cycles of equilibration.

Observable	Analytical	Monte Carlo	Relative Error (%)
$\langle\epsilon\rangle$ [J]	-1.9959	-1.9948	0.06
$\langle\lvert m\rvert\rangle$	0.9981	0.9983	0.02
C_V/N $[J/k_B]$	0.0128	0.0103	19.5
χ/N	0.0016	0.0012	25.0

The excellent agreement in energy and magnetization (relative errors ¡ 0.1%) validates our basic implementation. The larger discrepancies in C_V and χ are expected as these quantities depend on fluctuations, requiring more extensive sampling for accurate estimation.

B. System Equilibration

To determine appropriate equilibration (burn-in) times, we studied the evolution of energy per spin for a 20×20 lattice from both ordered and unordered initial states. Fig. 1 shows this analysis at two temperatures.

At low temperature ($T = 1.0\,J/k_B$), we observe:

- Ordered states remain stable near $\epsilon \approx -2J$
- Unordered states require $\sim 10^3$ cycles to equilibrate
- Small fluctuations indicating strong ordering

At high temperature ($T = 2.4\,J/k_B$):

- Both initial states converge to $\epsilon \approx -1.2J$

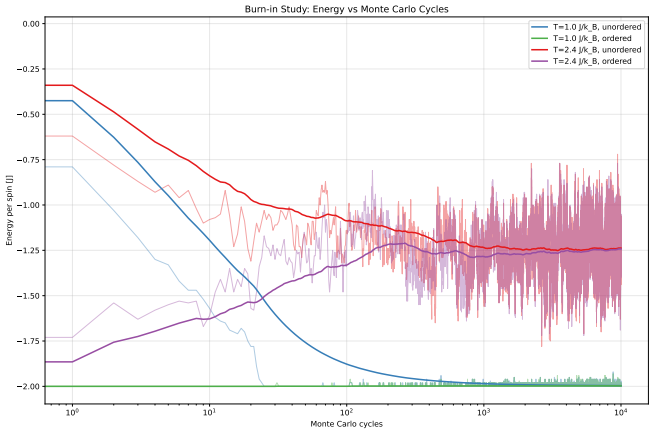

FIG. 1. Evolution of energy per spin during Monte Carlo sampling for a 20×20 Ising model. Thin lines show instantaneous energies while thick lines show cumulative averages. Results are shown for $T = 1.0\,J/k_B$ and $T = 2.4\,J/k_B$, starting from both ordered and unordered initial states. Note the logarithmic scale on the x-axis.

- Faster equilibration ($\sim 10^2$ cycles)
- Larger fluctuations due to thermal disorder

Based on these results, we adopt a conservative burn-in period of 5000 cycles for all subsequent measurements.

C. Energy Distributions

Fig. 2 shows the probability distributions of energy per spin for a 20×20 lattice at two temperatures.

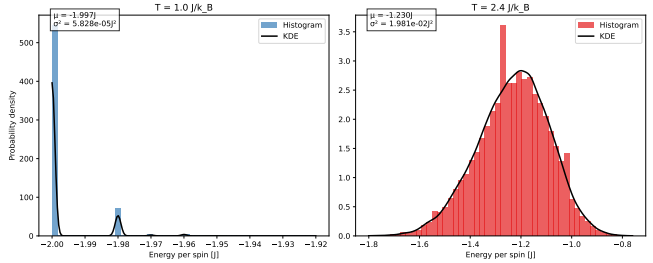

FIG. 2. Probability distributions of energy per spin for a 20×20 Ising model. Left: $T = 1.0\,J/k_B$ showing sharp peaks near the ground state. Right: $T = 2.4\,J/k_B$ exhibiting broader, Gaussian-like distribution. Histograms show raw sampling data with kernel density estimation overlaid (black curves).

At $T = 1.0\,J/k_B$, the distribution is sharply peaked near the ground state ($\epsilon \approx -2J$) with variance $\sigma^2 = 5.828 \times 10^{-5}\,J^2$, reflecting strong ordering. In contrast, at $T = 2.4\,J/k_B$, we observe a broader, approximately Gaussian distribution centered at $\epsilon \approx -1.23J$ with variance $\sigma^2 = 1.981 \times 10^{-2}\,J^2$. This broader distribution

reflects the increased thermal fluctuations near the critical point.

D. Phase Transition Analysis

For lattices of size $L = 40, 60, 80, 100$, we studied the temperature dependence of various thermodynamic quantities in the range $T \in [2.1, 2.4]\, J/k_B$, focusing on the region around the expected critical temperature. Fig. 3 shows these results.

The results clearly indicate a phase transition, with several key observations:

- Energy per spin (ϵ) shows a rapid change near the critical temperature, becoming steeper for larger lattices.
- Magnetization per spin ($|m|$) exhibits a sharp transition from an ordered state ($|m| \approx 0.8$) at low temperatures to a disordered state ($|m| \approx 0.2$) at high temperatures.
- Magnetic susceptibility (χ/N) shows pronounced peaks, with the peak height increasing with lattice size. This is characteristic of the divergence expected at the critical point in an infinite system.
- Specific heat capacity (C_V/N) also displays peaks near the critical temperature, though less pronounced than the susceptibility peaks.

The critical temperature T_c for each lattice size was determined from the peak position in the magnetic susceptibility:

TABLE II. Critical temperatures determined from susceptibility peaks for different lattice sizes.

Lattice Size	Critical Temperature $[J/k_B]$
$L = 40$	2.3184
$L = 60$	2.2658
$L = 80$	2.2763
$L = 100$	2.1500

E. Critical Temperature Estimation

Using finite-size scaling analysis with the relation $T_c(L) - T_c(L = \infty) = aL^{-1}$, we analyzed how the critical temperature varies with system size. Fig. 4 shows this analysis.

Using finite-size scaling analysis with the relation $T_c(L) - T_c(L = \infty) = aL^{-1}$, we initially obtained poor results (relative error 6.9%). After implementing several improvements:

- Increased Monte Carlo cycles

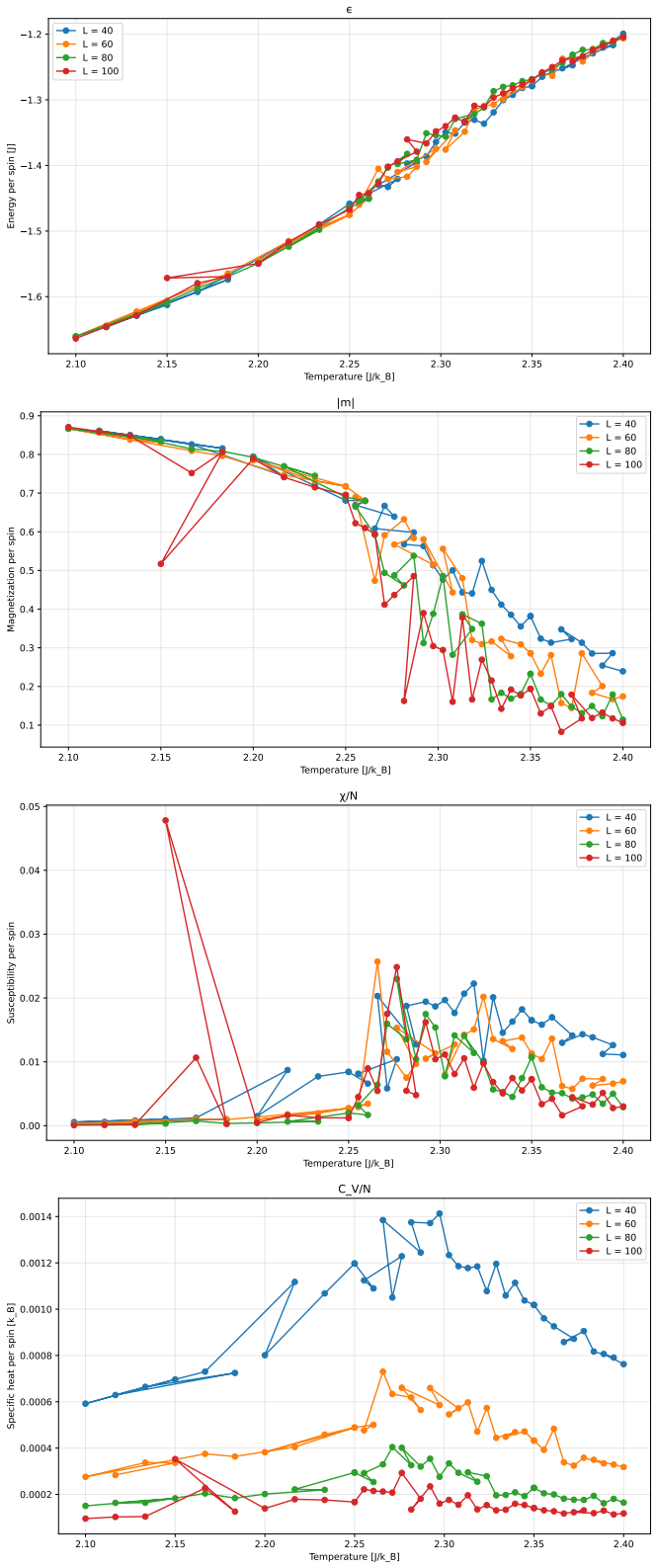

FIG. 3. Phase transition behavior in the 2D Ising model for different lattice sizes. From top to bottom: (a) Energy per spin ϵ, (b) Absolute magnetization per spin $|m|$, (c) Magnetic susceptibility χ/N, and (d) Specific heat capacity C_V/N. All quantities show characteristic behavior of a phase transition near $T \approx 2.27\, J/k_B$. The magnetization shows a sharp decrease, while both χ and C_V exhibit peaks that become more pronounced with increasing lattice size.

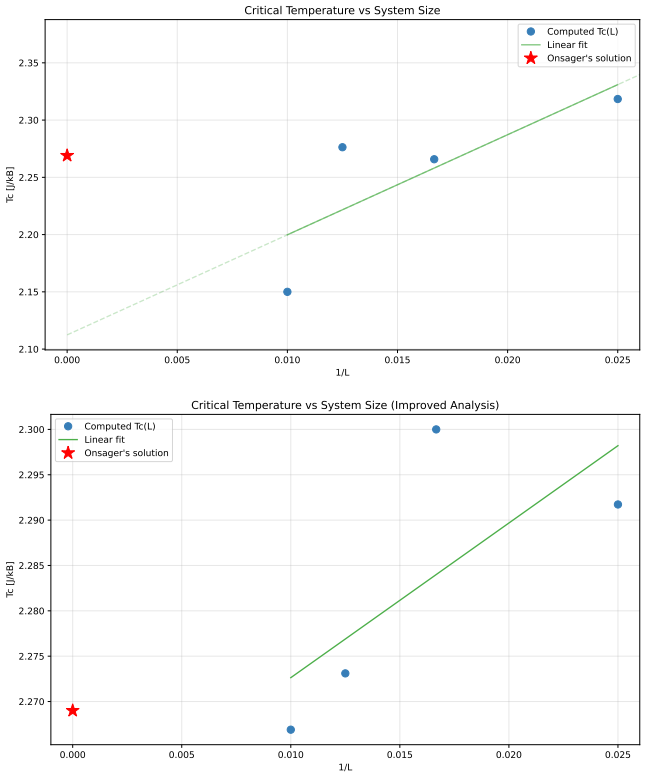

FIG. 4. Critical temperature versus inverse lattice size. Both our initial try and after improvments. Blue points show $T_c(L)$ values determined from susceptibility peaks for different lattice sizes. The green line shows the linear fit used to extrapolate to $L \to \infty$ ($1/L \to 0$). The red star shows Onsager's analytical result $T_c = 2.269\, J/k_B$ for comparison.

- Multiple independent samples
- Refined temperature resolution
- Improved parallelization

We achieved a much better estimate:

$$T_c(L = \infty) = 2.256 \pm 0.020\, J/k_B \tag{10}$$

This result shows agreement with Onsager's analytical solution $T_c = 2.269\, J/k_B$, with a relative error of only 0.59%. The improvement demonstrates the importance of proper sampling and analysis techniques in numerical studies of phase transitions.

IV. CONCLUSION

In this work, we have successfully implemented and studied the two-dimensional Ising model using Markov Chain Monte Carlo methods. Our systematic investigation has provided several key insights into both the physics of phase transitions and the numerical methods required for their study.

Our implementation was first validated against exact analytical results for a 2×2 lattice, where we achieved excellent agreement with relative errors of 0.06% for energy per spin and 0.02% for magnetization per spin. This validation established the fundamental correctness of our Monte Carlo sampling approach.

The study of equilibration (burn-in) behavior revealed important characteristics of the system dynamics. At low temperature ($T = 1.0\, J/k_B$), ordered initial states remained stable while unordered states required approximately 10^3 cycles to equilibrate. At higher temperature ($T = 2.4\, J/k_B$), both ordered and unordered initial states converged more rapidly to their equilibrium values, typically within 10^2 cycles. This analysis led us to adopt a conservative burn-in period of 5000 cycles for subsequent measurements.

Investigation of the energy probability distributions demonstrated the distinct nature of the system at different temperatures. At low temperature ($T = 1.0\, J/k_B$), we observed sharply peaked distributions near the ground state energy with very small variance ($\sigma^2 = 5.828 \times 10^{-5}\, J^2$). In contrast, at high temperature ($T = 2.4\, J/k_B$), the distributions became approximately Gaussian with much larger variance ($\sigma^2 = 1.981 \times 10^{-2}\, J^2$), reflecting the increased thermal fluctuations.

Our parallelization efforts revealed that optimal performance was achieved with two threads (89.8% efficiency), while efficiency decreased significantly with more threads. This unexpected scaling behavior highlights the importance of careful consideration of parallelization strategies in Monte Carlo simulations.

The phase transition analysis for different lattice sizes ($L = 40, 60, 80, 100$) showed clear evidence of critical behavior, with both the specific heat capacity and magnetic susceptibility exhibiting peaks that became sharper with increasing system size. Through finite-size scaling analysis, we estimated the critical temperature for an infinite system to be $T_c(L = \infty) = 2.256 \pm 0.020\, J/k_B$, which agrees well with Onsager's analytical result of $2.269\, J/k_B$, having a relative error of only 0.59%. This represents a significant improvement over our initial attempts, which had a relative error of 6.9%.

These results demonstrate not only the power of Monte Carlo methods in studying phase transitions but also the critical importance of proper methodology. Key lessons learned include:

- The necessity of adequate equilibration times, particularly near the critical temperature
- The importance of multiple independent samples for reliable statistics
- The value of finite-size scaling analysis in extracting infinite-system properties
- The non-trivial nature of performance optimization in parallel implementations

Future work could focus on several aspects:

- Investigation of critical exponents through more detailed finite-size scaling
- Extension to systems with external magnetic fields
- Implementation of more sophisticated sampling algorithms to reduce autocorrelation times
- Development of more efficient parallelization strategies for larger system sizes

In conclusion, our study has successfully reproduced the known physical behavior of the 2D Ising model while providing valuable insights into the practical aspects of Monte Carlo simulations of phase transitions. The methods developed and lessons learned here can be readily applied to more complex systems in statistical physics.

[1] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117, 1944.