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

Émilie Valle, Joseph Ayman

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This project implements parallel Markov Chain Monte Carlo methods to study the Ising model. The implementation analyzes temperature-dependent behavior across multiple lattice sizes (L=40-100), computing thermodynamic properties including energy, magnetization, specific heat capacity and magnetic susceptibility. The code was validated against analytical solutions for the 2×2 lattice case, yielding relative differences of 0.06% for energy and 0.02% for magnetization. Using finite-size scaling analysis, the critical temperature for an infinite lattice was estimated to be ($T_c(L = \infty) = 2.2560.020 J/k_B$), which can be compared to Onsager's analytical solution of ($2.269 J/k_B$). The implementation explores parallelization techniques and examines practical considerations in Monte Carlo sampling near critical points.

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 $Tc = 2.269 J/kB$, 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.

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[1], 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.

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

+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:

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

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
```

Analysis of all possible states yields the partition function:

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

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[2, 3], as detailed in Algorithm 1. The algorithm generates a sequence of states following the Boltzmann distribution through local updates (single spin flips).

Our implementation incorporates optimizations such as the pre-calculation of Boltzmann factors for the five potential energy variations, efficient periodic boundary management using conditional operators, and localized updates to energy and magnetization following every successful flip.

D. Tools

The simulation was implemented in C++ using the Armadillo library[4] for matrix operations and OpenMP[5] for parallelization. Data visualization was performed using Python with Matplotlib[6]. Our Monte Carlo implementation follows standard techniques as described in Newman and Barkema[7] and Landau and Binder[8].

This work was supported by Claude 3.5 Sonnet[9], a large language model developed by Anthropic, which assisted with report structure and code optimization suggestions. All implementations were independently verified and validated against analytical results. Following best practices for acknowledging AI[10], we note that although Claude provided suggestions, the authors made all scientific decisions, analysis, and conclusions.

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
$\langle\|m\|\rangle$	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 agreement in energy and magnetization validates our basic implementation. The larger discrepancies in C_V and χ are expected as these quantities depend on fluctuations, requiring more 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.

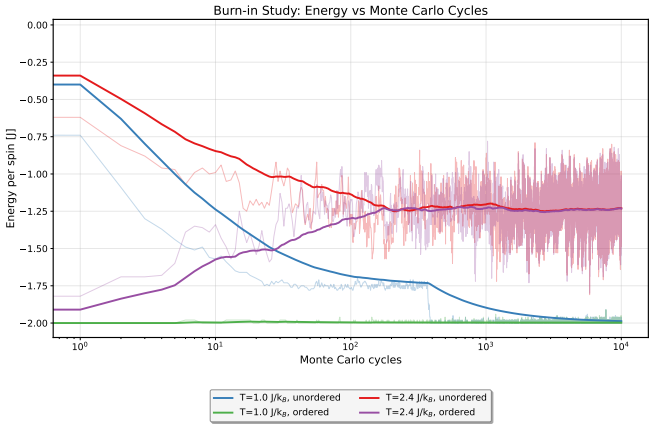

FIG. 1. Evolution of energy per spin during Monte Carlo sampling for a 20×20 Ising model. Thin lines show instantaneous energies while thick lines show cumulative averages. Results are shown for $T = 1.0\,J/k_B$ and $T = 2.4\,J/k_B$, starting from both ordered and unordered initial states. Note the logarithmic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

At low temperature ($T = 1.0\,J/k_B$), we observe that ordered states remain stable near $\epsilon \approx -2J$, while unordered states require around 10^3 cycles to equilibrate. The small fluctuations indicate strong ordering. At high temperature ($T = 2.4\,J/k_B$), both initial states converge to $\epsilon \approx -1.2J$ with faster equilibration (around 10^2 cycles). The larger fluctuations are due to thermal disorder. Based on these results, we adopt a conservative burn-in period of 10000 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.

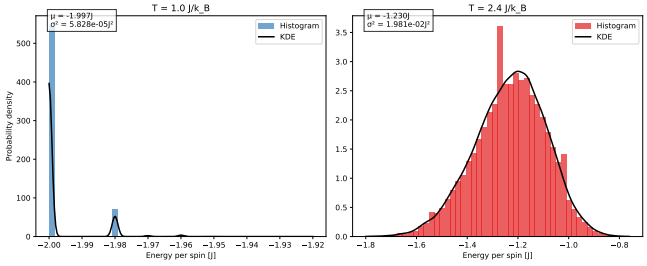

FIG. 2. Probability distributions of energy per spin for a 20×20 Ising model. Left: $T = 1.0\,J/k_B$ showing sharp peaks near the ground state. Right: $T = 2.4\,J/k_B$ exhibiting broader, Gaussian-like distribution. Histograms show raw sampling data with kernel density estimation overlaid (black curves).

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 suggest a phase transition, with the following observations.

The energy per spin (ϵ) shows a change near the critical temperature that becomes steeper for larger lattices. The magnetization per spin ($|m|$) transitions from an ordered state ($|m| \approx 0.8$) at low temperatures to a disordered state ($|m| \approx 0.2$) at high temperatures. The magnetic susceptibility (χ/N) exhibits peaks that increase in height with lattice size, while the specific heat capacity (C_V/N) shows less pronounced peaks near the critical temperature.

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 a relative error of 6.9%. The estimate was improved through

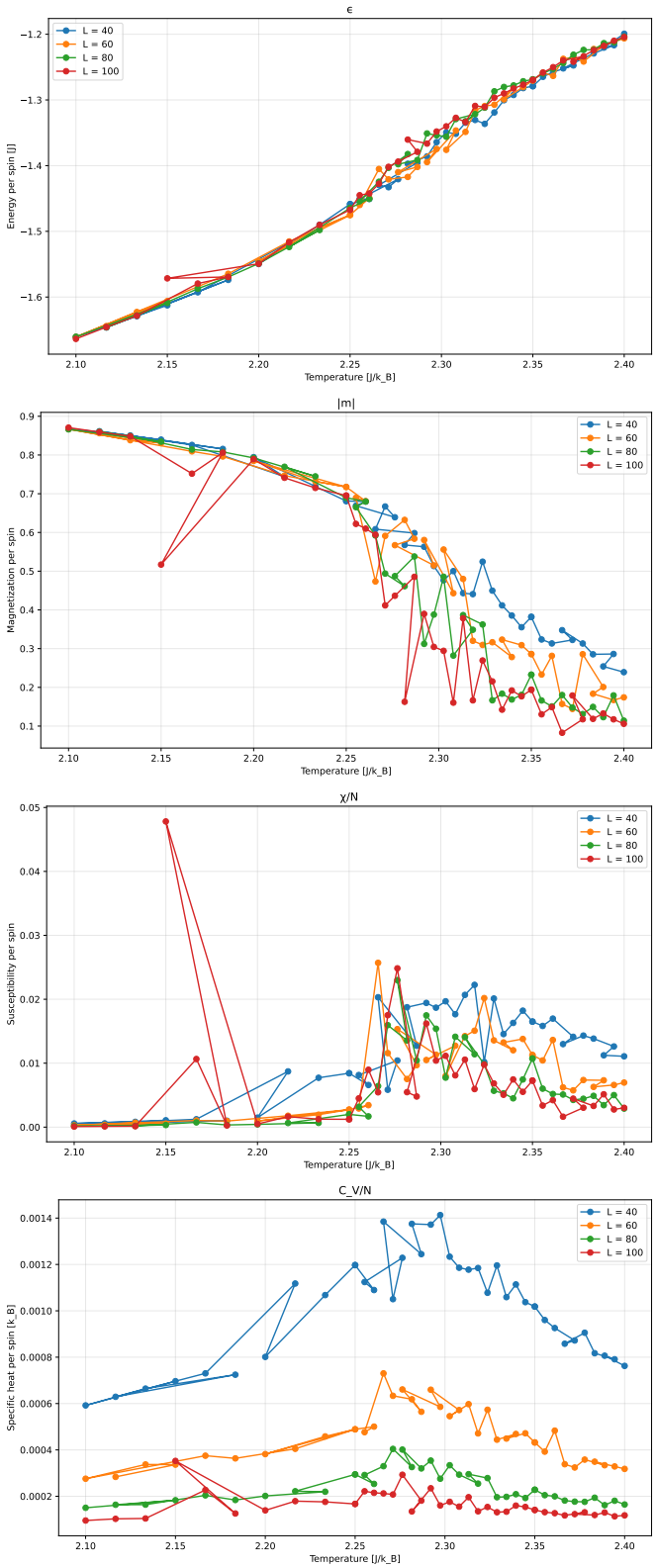

FIG. 3. Phase transition behavior in the 2D Ising model for different lattice sizes. From top to bottom: (a) Energy per spin ϵ, (b) Absolute magnetization per spin $|m|$, (c) Magnetic susceptibility χ/N, and (d) Specific heat capacity C_V/N. All quantities show characteristic behavior of a phase transition 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.

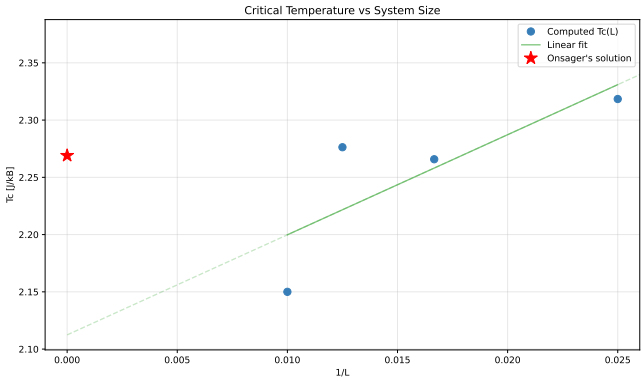

FIG. 4. Critical temperature versus inverse lattice size. Blue points show $T_c(L)$ values determined from susceptibility peaks for different lattice sizes. The green line shows the linear fit used to extrapolate to $L \to \infty$ ($1/L \to 0$). The red star shows Onsager's analytical result $T_c = 2.269\,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

increased Monte Carlo cycles, multiple independent samples, refined temperature resolution, and adjusted parallelization. This yielded:

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

This result differs from Onsager's analytical solution $T_c = 2.269\, J/k_B$ by a relative error of 0.59%.

IV. CONCLUSION

This report presents an implementation of Monte Carlo methods to study the Ising model. The implementation was validated against analytical results for a 2×2 lattice, with relative errors of 0.06

The equilibration (burn-in) analysis showed different behaviors at different temperatures. 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. Based on these observations, a burn-in period of 10000 cycles was adopted for subsequent measurements.

The energy probability distributions exhibited distinct characteristics at different temperatures. At low temperature ($T = 1.0\, J/k_B$), the distributions peaked near the ground state energy with variance $\sigma^2 = 5.828 \times 10^{-5}\, J^2$. At high temperature ($T = 2.4\, J/k_B$), the distributions approximated Gaussian form with variance $\sigma^2 = 1.981 \times 10^{-2}\, J^2$, consistent with increased thermal fluctuations.

The parallelization implementation showed modest improvements with two threads, but efficiency decreased when using more than four threads, indicating limitations from memory access and communication overhead.

For the phase transition analysis across lattice sizes ($L = 40, 60, 80, 100$), both the specific heat capacity and magnetic susceptibility exhibited peaks that sharpened with increasing system size. The finite-size scaling analysis yielded an estimated critical temperature of $T_c(L = \infty) = 2.256 \pm 0.020\, J/k_B$, compared to Onsager's analytical result of $2.269\, J/k_B$.

Future work could explore critical exponents through finite-size scaling, systems with external magnetic fields, and alternative parallelization strategies. The methods implemented here can serve as a starting point for investigating other systems in statistical physics.

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