Simulation of the Two-Dimensional Ising Model: Metropolis Algorithm and Phase Transitions[*]

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In this work, we simulate the two-dimensional Ising model using the Metropolis algorithm to study phase transitions in magnetic systems. The simulations include an analysis of the system under different temperature regimes—low, medium, and high—to observe phase transitions and compare them with the theoretical critical temperature. Additionally, we explore thermodynamic properties such as magnetization and magnetic susceptibility near the critical temperature. The results clearly show a phase transition from a ferromagnetic phase, where spins align at low temperatures, to a paramagnetic phase, where spins are disordered at high temperatures. The obtained values of the critical exponents ($\gamma = 1/8$ for magnetization and $\varepsilon = 7/4$ for susceptibility) agree well with theoretical predictions, validating the accuracy of the simulations. We also study the effects of initial conditions (hot and cold starts) on the system's equilibrium, observing that a disordered initial state requires more time to reach equilibrium.

I. INTRODUCTION

The one-dimensional Ising model is one of the few interacting particle systems for which an exact solution is known, and it is undoubtedly the simplest of all. This model is of great interest for several reasons. On one hand, it was key in the historical understanding of ferromagnetism and phase transitions, playing a crucial role in this context. On the other hand, the one-dimensional solution method developed by Ising, later extended to two dimensions by Onsager, has laid the foundation for many modern methods in the statistical physics of critical phenomena. Finally, it is now recognized that the Ising model, along with its generalizations, is useful for describing a wide range of phenomena, not only in physics but also in various areas of biology [2].

In this work, we aim to simulate a network of $L \times L$ spins using the Metropolis algorithm through Monte Carlo methods. These simulations include analyzing the system at low, medium, and high temperatures. In this way, we aim to observe a phase transition and compare it with the theoretical value of the temperature at which this change occurs. Additionally, we study the behavior of thermodynamic properties near this critical temperature.

II. BACKGROUND

A. Two-Dimensional Ising Model

The 2D Ising Model is a fundamental tool in statistical physics for studying phase transitions, particularly the ferromagnetic transition in magnetic materials. The Ising model was invented by physicist Wilhelm Lenz (1920), who conceived it as a problem for his student Ernst Ising to demonstrate that the system exhibited a phase transition. Ising (1925) showed that no such phase transition exists in one dimension, solving it in his 1924 thesis [3].

In the two-dimensional Ising model, we consider a grid or *lattice* of $L \times L$ sites, where each site i has a spin s_i that can take one of two values: $s_i = \pm 1$, referred to as spin up ($s_i = +1$) or spin down ($s_i = -1$). These spins interact with their nearest neighbors on the lattice. The objective is to study how the spins align under different temperatures and how they change when an external magnetic field is applied. To describe the behavior of the system, the total energy, or Hamiltonian, of the system is expressed as:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i \tag{1}$$

Where:

- J is the interaction constant between neighboring spins.
  - If $J > 0$, the interaction is ferromagnetic, meaning the spins tend to align in the same direction.
  - If $J < 0$, the interaction is antiferromagnetic, meaning the spins tend to align in opposite directions.
- $\langle i, j \rangle$ denotes the sum over pairs of neighboring spins.
- H is the external magnetic field applied to the system.
- s_i and s_j represent the spins at sites i and j, which take values ± 1.

The macroscopic behavior of the system can be analyzed through the partition function Z, which contains all the statistical information of the system. The partition function is defined as:

$$Z = \sum_s e^{-\beta H}$$

where $\beta = 1/k_B T$, with k_B being the Boltzmann constant and T the temperature. The partition function is crucial because it allows the calculation of other quantities of interest, such as free energy, magnetization, susceptibility, among others. These quantities can be calculated as follows.

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Magnetization
Magnetization is the measure of the net magnetic moment of the system and is calculated as:

$$\langle M \rangle = \frac{1}{L^2} \sum_i s_i \tag{2}$$

Specific Heat C_v
The specific heat is a measure of how the system's energy changes with temperature and is related to energy fluctuations. It can be calculated as:

$$C_v = \frac{\partial \langle E \rangle}{\partial \beta} = \frac{\beta}{T} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{3}$$

Magnetic Susceptibility χ
Magnetic susceptibility indicates the degree of sensitivity of a material's magnetization to an applied magnetic field. It can be obtained from:

$$\chi = \frac{\partial \langle M \rangle}{\partial H} = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{4}$$

Phase Transition
In the 2D Ising model, the phase transition occurs at a critical temperature T_c where the system transitions from a magnetized state (spins aligned, $M \neq 0$) to a disordered state (zero magnetization, $M = 0$). For the model without a magnetic field ($H = 0$), Lars Onsager solved the model exactly [1], finding that the critical temperature is given by:

$$k_B T_c = \frac{2J}{\ln(\sqrt{2}+1)} \tag{5}$$

B. Metropolis Algorithm

The Metropolis algorithm is a technique used to simulate physical systems such as the 2D Ising Model, particularly when calculating thermodynamic properties through Monte Carlo methods. This algorithm is especially effective for studying systems with many possible configurations, where directly calculating the partition function would be computationally difficult or even impossible.

The goal of the Metropolis algorithm is to create system configurations that align with the Boltzmann distribution at a given temperature. The idea is to explore the configuration space efficiently, generating more probable configurations more frequently than less probable ones, which facilitates the calculation of average properties such as energy, magnetization, and others. This algorithm can be described more illustratively in Figure 1, where the new state S_1 represents flipping a random spin in the system (i.e., changing $+1$ to -1 or vice versa).

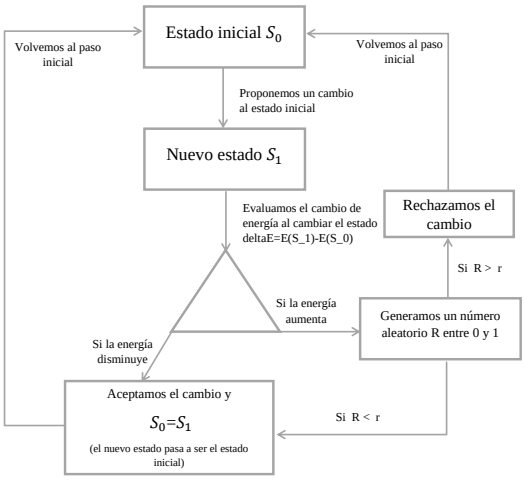

Figura 1: Metropolis Algorithm

In the algorithm, r is the change in energy (probability) when transitioning between states, and it is given by:

$$r = \frac{p(S_f)}{p(S)} = e^{-\beta(E(S_1)-E(S_0))} = e^{-\beta \Delta E} \tag{6}$$

C. Implementation of the Algorithm to Calculate Thermodynamic Properties

In Python, we implemented the Metropolis algorithm described in 1 and calculated the energy, magnetization, specific heat, and susceptibility according to (1), (2), (3), and (4), respectively. We calculated these physical quantities for low to high temperatures to observe where the phase transition occurs.

Conditions

- $L = 10$
- $J = 1$
- $H = 0$
- Thermalization time: $2^{13} = 8192$. Repetitions of the Metropolis algorithm until the system reaches equilibrium.
- We considered two cases: A hot start, with all spins in the grid random, and a cold start, where all spins are the same (either $+1$ or -1).
- For this configuration, the theoretical critical temperature is $T_c \approx 2.26918$

D. Behavior of Specific Heat C_v and Susceptibility χ Near the Critical Temperature T_c

Magnetization near (but still below) the critical temperature is given by

$$\frac{\langle M \rangle}{L^2} \sim (T_c - T)^{\gamma} \tag{7}$$

with $\gamma = 1/8$ and $T \in [T_c - 0.5, T_c - 0.01]$ with a total of 80 values in that interval. Using the Metropolis algorithm, we analyze the magnetization in this temperature range, where we plot $\langle M \rangle$ against $T_c - T$ to numerically determine the value of γ.

In exactly the same way, the susceptibility near the critical temperature behaves as

$$\frac{\chi}{L^2} \sim |T_c - T|^{\varepsilon} \tag{8}$$

with $\varepsilon = 7/4$ and the same temperature range near the critical temperature. Similarly, we numerically determine the value of ε.

E. Log-Log Fit to Determine γ and ε

Since we need to determine the value of the exponents in the functions (7) and (8), we will have a problem of the form

$$y = x^n$$

where the unknown to determine is the value of n. It is convenient to work with the function in a $\log - \log$ system, since

$$\log(y) = n \log(x)$$

Thus, the problem reduces to performing a linear fit in which we must determine the value of the slope n, which is precisely the exponent we need.

III. RESULTS

A. Hot Start

The graphs 2, 3, 4, and 5 (in red) correspond to the physical quantities: energy, magnetization, specific heat, and magnetic susceptibility, respectively. These correspond to a hot start in the grid, meaning that the spins are oriented randomly (spins 'up' and 'down' distributed randomly), representing a disordered paramagnetic state with an average magnetization close to zero. Since the system is initially disordered, it may take longer to reach the ordered state, especially with simulations that have limited time (as in our case, where we choose a low thermalization time).

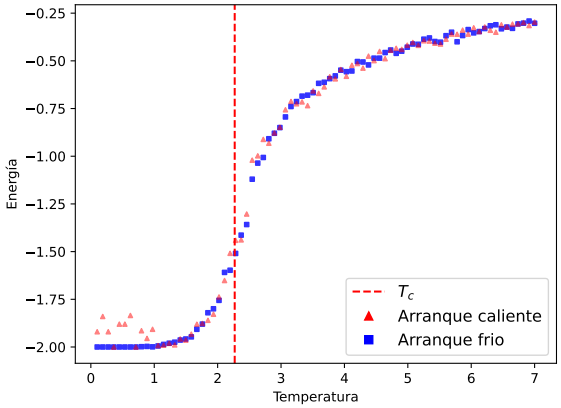

Figura 2: Average energy vs temperature for a hot start in the lattice.

At low temperatures, the spins should tend to align, as evidenced in the magnetization graph 3. However, since the system started in a disordered state, it is difficult for the system to reach equilibrium, and we observe a tendency to reach a total magnetization of $+1$ (ferromagnetic phase) at low temperatures. However, this is not fully achieved due to the hot start of the system.

On the other hand, all the graphs show a sharp change right at the theoretical critical temperature $T_c \approx 2.26918$. This was expected and serves as evidence of the correct functioning of the simulations. This indicates that there is a *phase transition* between the ferromagnetic phase (low temperatures), where all spins are aligned, and the paramagnetic phase (high temperatures), where the spins are completely disordered, reflecting a high entropy state.

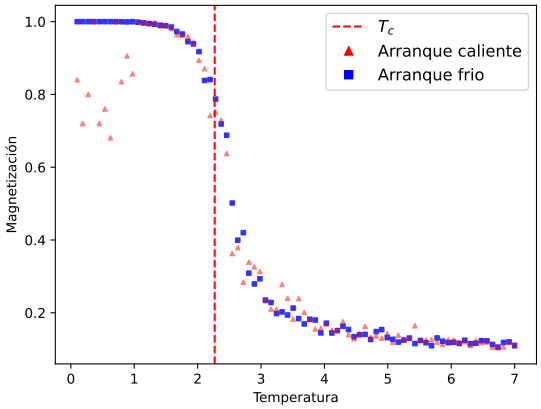

Figura 3: Average magnetization vs temperature for a hot start in the lattice.

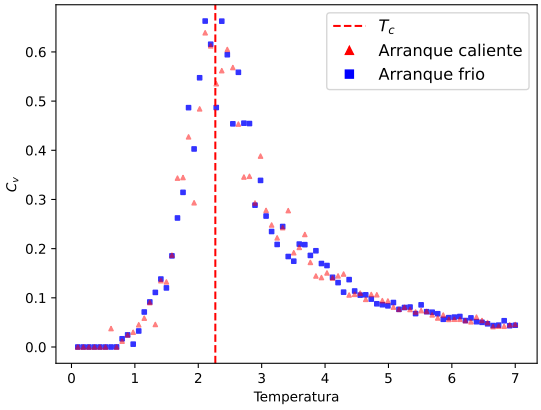

Figura 4: Specific heat vs temperature for a hot start in the lattice.

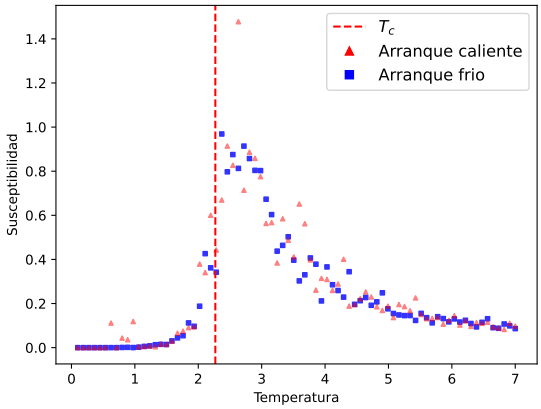

Figura 5: Magnetic susceptibility vs temperature for a hot start in the lattice.

B. Cold Start

The graphs 2, 3, 4, and 5 (in blue) correspond to the physical quantities calculated this time with a cold start. That is, in this case, the spins are perfectly aligned at the start (all $+1$). The differences in contrast with the hot start are evident, especially at low temperatures, where, for example, the magnetization is perfectly $+1$ at temperatures below T_c (figure 3, in blue). This was also anticipated because we started with a completely ordered configuration (a low-entropy state), so the system is already in equilibrium.

In each of the graphs, a phase transition is also evident exactly at T_c. The specific heat shows a peak at the critical temperature, indicating that the system experiences maximum energy fluctuations, as defined by C_v in (3). A small variation in temperature causes a large change in the internal energy of the system, reflecting a high capacity to store or release heat.

C. Ferromagnetic Phase Transition

Here, what we are now interested in is studying how the magnetization and magnetic susceptibility behave near the critical temperature, where a ferromagnetic to paramagnetic phase transition occurs.

1. *Magnetization near the critical temperature*

As discussed in the previous section, the goal is to determine the exponent of the fit in order to find the behavior of the magnetization near T_c. In figure 6, we plot the magnetization for values near T_c, with the red curve indicating the theoretical fit. In figure 7, in a log $-$ log plot, we perform the linear fit and find that $\gamma = 0.125$, which is in complete agreement with the theoretical value of $\gamma = 1/8$.

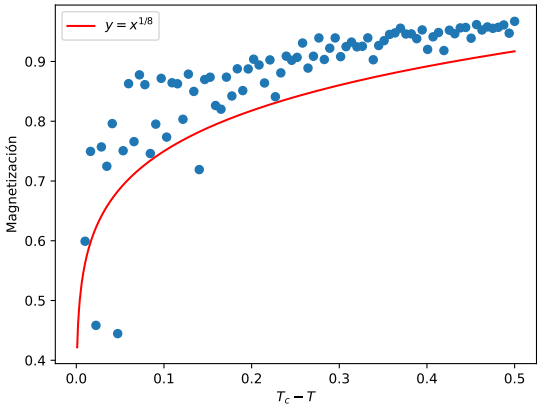

Figura 6: Magnetization near the critical temperature (blue) and theoretical fit (red).

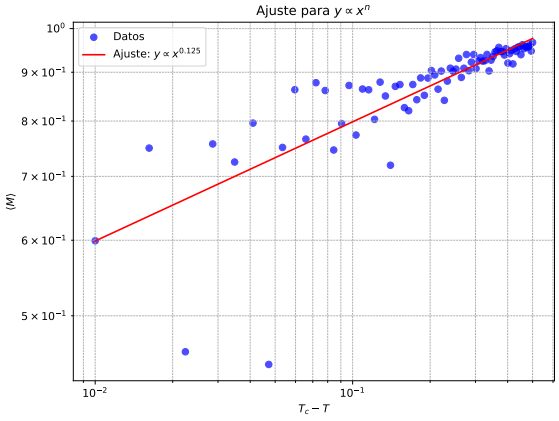

Figura 7: Linear fit for magnetization near critical temperature on a graph log $-$ log

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2. *Susceptibility near the critical temperature*

Analogously to the magnetization at T_c, in figure 8 we observe how the susceptibility varies near the critical temperature, with the solid curve indicating the theoretical behavior. On the other hand, in the plot 9, where the fit is performed, we obtain a value of $\varepsilon \approx 1.736$, which matches well with the theoretical value of $\varepsilon = 7/4 = 1.75$.

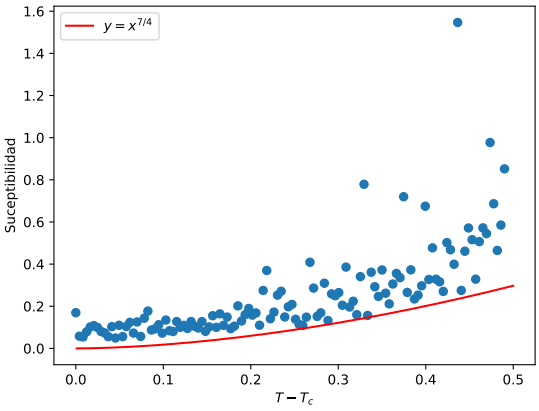

Figura 8: Susceptibility near critical temperature (blue) and theoretical fit (red)

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IV. CONCLUSIONS

We have simulated the two-dimensional Ising model using the Metropolis algorithm to study phase transitions in magnetic systems. From these simulations, we have observed clear changes in the thermodynamic properties near the theo-

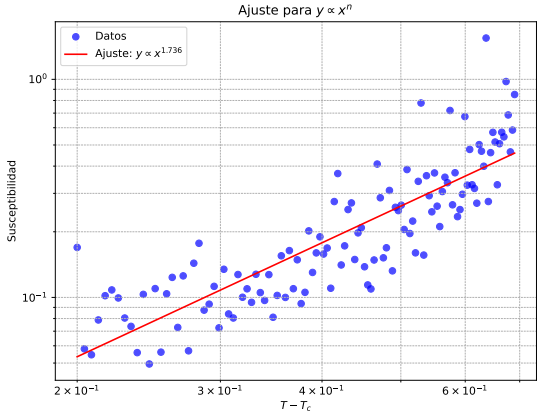

Figura 9: Linear fit for susceptibility near critical temperature on a graph $\log - \log$

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retical critical temperature $T_c \approx 2.26918$, which provides clear evidence of a phase transition. Additionally, this confirms the correct implementation of the algorithm and its usefulness for describing these physical phenomena.

The system transitions from a ferromagnetic phase at low temperatures, where the spins are aligned, to a paramagnetic phase at high temperatures, where the spins are disordered. The magnetization and magnetic susceptibility exhibited behavior consistent with the theoretical values of the critical exponents ($\gamma = 1/8$ and $\varepsilon = 7/4$), which validates the accuracy of our simulations.

Furthermore, the study of the system's initial configurations (cold start and hot start) demonstrated how the initial condition can affect the thermalization time and convergence to equilibrium. In the hot start, the system takes longer to reach an ordered configuration due to the greater initial disorder of the spins.

V. APPENDIX

The code can be found at the following link.

[1] Stephen J. Blundell and Katherine M. Blundell. *Concepts in Thermal Physics*. Oxford University Press, Oxford, 2 edition, 2010.

[2] Sergio A. Cannas. El modelo de ising, 2010. Notas de Termodinámica II, FaMAF, Universidad Nacional de Córdoba.

[3] Wikipedia, la enciclopedia libre. Modelo de ising. https://es.wikipedia.org/wiki/Modelo_de_Ising, 2024. Consultado el 27 de noviembre de 2024.