Analysis of the Correlation of Physical, Topological, and Geometric Variables Present in the Phase Transition of a 2D Ising Model with Zero External Magnetic Field*

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I. INTRODUCTION

The atoms of certain materials have magnetic moments due to the spin of the electrons or the movement of the nucleus. In many materials, the magnetic dipoles of the atoms are randomly oriented, resulting in a total magnetic field of zero. There are other materials, such as ferromagnets, that exhibit a macroscopic magnetic field different from zero due to interactions between the magnetic dipoles. This phenomenon is observed at temperatures below a critical temperature T_c, also known as the Curie temperature. The temperature T_c is relevant because when the temperature of the ferromagnet reaches the critical temperature ($T = T_c$), it undergoes a phase transition. The phase transition is identified by observing changes in the physical properties of the system.

The Ising model dates back to the early 20th century when Willhelm Lenz conceived the problem for his student Erns Ising. In his doctoral thesis, Ising demonstrated that the system did not exhibit a phase transition in one dimension. Later, Lars Onsager showed the exact solution in two dimensions using the transfer matrix technique with zero field.

The Ising model is widely studied because it is the simplest statistical model that exhibits a phase transition. Its importance lies in its ability to simplify the nature of spins to create a system that can be solved exactly and compared with experimental data. The phase transition is considered second order.

The study of solid state focuses on the essential forms in which matter presents itself, i.e., its states of aggregation. It is characterized by a specific arrangement of the particles that compose it, allowing the matter to have a well-defined physical structure. For the Ising model, this specific arrangement refers to the magnetic moments of the spins in the crystalline lattice, as the model considers a regular lattice of spins that can have two possible states: up ($+1$) or down (-1). This is the simplification present in the model, as it considers the spin as a scalar quantity and not as a vector quantity.

For studying these systems composed of many particles, they are usually divided into three different types of ensembles: microcanonical, canonical, and grand canonical. The canonical ensemble describes a system in contact with a thermal reservoir, allowing energy exchange with the surroundings at a constant temperature but not matter. The volume it occupies and the number of particles are constant. This is the ensemble with which we study the Ising model because the number of particles present in the lattice remains constant. The temperature in the model is an external variable that is kept constant, and the system exchanges energy with the thermal bath

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* A footnote to the article title

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while seeking equilibrium.

Near the critical temperature, changes in the physical properties of the system occur, characterizing the system's criticality. At low temperatures, the magnetic moments tend to align, causing the system to exhibit macroscopic magnetization. The system's magnetization changes abruptly when crossing the critical temperature, decreasing as the temperature increases ($T > T_c$). Another quantity that exhibits abrupt changes is the magnetic susceptibility. Magnetic susceptibility measures the system's response to an external magnetic field. At temperatures close to $T \approx T_c$, magnetic susceptibility increases, indicating the system's sensitivity to small perturbations.

To analytically observe and analyze the thermodynamic properties of the system for temperatures close to T_c, it is necessary to study the system's behavior in the thermodynamic limit. This limit refers to the number of particles (spins) in the system being infinitely large. In the context of the Ising model, the thermodynamic limit implies increasing the size of the spin lattice to infinity while maintaining the spin density constant. Mathematically, we denote it as $N \to \infty$, where N is the number of spins in the lattice. Taking this limit makes the phase transition more clearly and precisely observable because statistical fluctuations are reduced. These changes can be observed in the macroscopic properties of the system, such as magnetization, internal energy, and magnetic susceptibility.

Simulating the dynamics of the spins in a lattice for the Ising model is computationally complex. These systems are commonly simulated using the Monte Carlo method and the Metropolis algorithm. The Monte Carlo method is based on the `Central Limit Theorem`, which allows complex distributions to be approximated by generating random samples. The sampling integration in this method allows the expected value of the distribution of interest to be approximated by generating random samples and averaging their values. On the other hand, the Metropolis algorithm is based on the use of `Markov chains`, where the conditional probability of each value only depends on the previous value. The `detailed balance principle` ensures that the Markov chain converges to thermodynamic equilibrium.

Other quantities of interest in the study of the Ising model come from network theory. A square lattice in the Ising model can be represented by assigning nodes to each spin site in the lattice, while the interactions between them can be reflected as connections. The temporal evolution of the magnetic orientation of the spins allows the Ising model to be approached using dynamic models on networks. These models enable identifying and characterizing different phases of the system, especially phase transitions. This way, we can analyze how these connections influence the system's physical properties.

We refer to magnetic domains in an Ising model as the spatial arrangement of regions with uniform magnetic orientations in the material. The topology of the present magnetic domains allows studying the topology of the ferromagnetic material through its spatial distribution, average size, and how they evolve in response to changes in the system's temperature.

Studying the square lattices of an Ising model using graphs allows us to study geometric variables of the spin lattice. Quantities such as the Forman-Ricci curvature provide information about the incidences of vertices present in a graph, thus relating connectivity and local structure with geometry. On the other hand, the Ollivier-Ricci curvature allows us to understand the topology and geometry of the graph, as it is based on the distance measure between its vertices. This quantifies the geometric and metric structure of the lattice.

II. THEORETICAL PRELIMINARIES

- Toca hablar de: Modelo de Ising, en que consiste matematicamente, fisicamente y en teoria de redes. Hacer énfasis en la trasición de fase. Solución analítica para el caso 1D, el rol del campo magnético. Las fronteras.

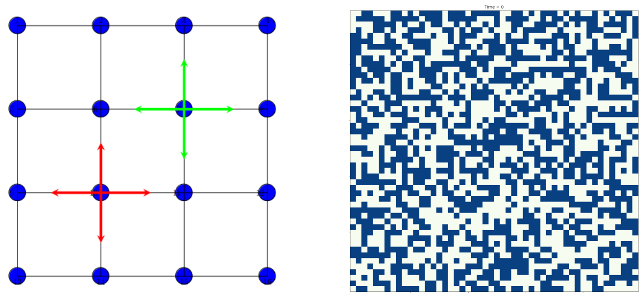
- Los dominios y las variables topologicas. La relación con las redes, en particular los grafos.

- ¿Es natural o esperable que las variables topológicas capturen información de la transición de fase? ¿Hay otros trabajos en esta dirección? ¿En qué aciertan y en qué fallan? ¿Qué hay de nuevo en nuestro enfoque? (Ojo: la curvatura)

- ¿Qué captura la curvatura en este caso? ¿Tiene algo que ver con el flujo magnético en los dominios? ¿Es la curvatura de FR más sensible, menos sensible que las medidas convencionales para deterctar las transiciones de fase? ¿Cómo se define sensibilidad? En caso, es a nivel computacional.

- In 1D, the model is analytically solvable, showing no phase transition at finite temperature. In network theory, the Ising model can be extended to describe phenomena such as opinion dynamics. The role of the magnetic field introduces asymmetry, favoring one spin orientation, while boundary conditions significantly affect the system's behavior. Topological variables, such as those related to domain structures a crucial role in understanding the global properties of the system, particularly in relation to network theory. It is natural to expect that these topological variables capture phase transition information, as they reflect changes in the system's global structure. The curvature of Forman-Ricci can potentially offering greater sensitivity in detecting phase transitions. Curvature may capture the spatial distribution of magnetic domains and could be more sensitive than conventional measures, particularly in detecting subtle geometric changes, where sensitivity is defined computationally as the ability to detect small structural changes.

Let us consider a set Λ that contains the sites of the configuration. For each site present in this representation $k \in \Lambda$, we have a discrete variable $\sigma_k \in \{-1, +1\}$ that represents the aforementioned spin variable.



(a) Nearest neighbors (b) Initial state

FIG. 1: Ising model with nearest neighbor J interactions for the square lattice. Blue and white area mean $s = +1$ and $s = -1$ respectively.

We define the spin configuration as $\sigma = \{\sigma_k \mid k \in \Lambda\}$. For two adjacent sites $i, j \in \Lambda$, there is an interaction J, which we call the interaction factor. There is also an external magnetic field B interacting with each site $j \in \Lambda$. The Hamiltonian for such a model can be written as:

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \cdot \mu \sum_j \sigma_j \tag{1}$$

The magnetization of the Ising configuration can be calculated as the sum of the spins at each site of the lattice. Suppose we have a lattice of size $L \times L$ with spins represented by variables s_{ij}, where i and j indicate the coordinates of the site. The magnetization M is calculated as:

$$M(\sigma) = \sum_{i=1}^{L} \sigma_i \tag{2}$$

where σ_i can take the values $+1$ or -1, depending on the orientation of the spin at site (i).

The geometry of the model is schematically illustrated in 1.

A. Analysis

We have two cases that naturally draw attention: the case where $T \ll T_c$ and the case where $T \gg T_c$.

1. $T \ll T_c$

   It is expected that at temperatures close to absolute zero, the system tends to occupy its minimum energy state and a nonzero magnetization value. This minimum energy state can be inferred from equation 1, which represents the microstate where all spins are oriented in the same direction, exhibiting an ordered phase. This is because the factor J represents the magnitude of the interaction between adjacent spins in the system, and the negative sign induces a ferromagnetic interaction, minimizing the system's energy when the spins are aligned.

   In contrast, the dependence of magnetization on temperature starts with a maximum value and decreases sharply as the system approaches temperatures near the critical temperature (T_c).

2. $T \gg T_c$

   Above T_c, the value of $\beta \to 0$ and $\mathbb{P}(E) \to \frac{1}{Z}$. In this case, since $\kappa_B T \gg J$, the thermal part dominates compared to the interaction between spins, reducing the ferromagnetic alignment and increasing the system's energy as the factor β decreases in the probability distribution of states. Thus, for very high temperatures, equation tends towards very small energy values, so the expected value of $\langle E \rangle \to 0$ as can be seen in Figure

   Above T_c, a paramagnetic phase is observed, that is, disordered, characterized by a random distribution of spins and the convergence of magnetization to zero due to the increase in the system's entropy.

For the analysis of the behavior of these two quantities, the temperature interval was divided using the same process as for the physical variables. In this way, we obtain two intervals as shown below.

1. $T \ll T_c$

   We know that for temperatures lower than T_c, the system tends to occupy its minimum energy state, characterized by an alignment of the spins in the same direction. Thus, the number of domains for this temperature range stabilizes in the set of values `DN`$\in \{0, 1\}$. Meanwhile, the average domain size is in a set with values `MDS`$\in \{0, 255\}$.

   As the temperature values approach T_c, the topological variables undergo abrupt changes. On one hand, `DN` increases due to the transition to a paramagnetic phase, characterized by a random distribution of spins, which breaks the homogeneity in the number of domains for temperatures farther from T_c. This is highlighted in Figure , where it is observed that the number of domains grows abruptly for the aforementioned case. Similarly to magnetization, `MDS` undergoes an abrupt change due to the phase transition, since the random distribution of spins results in the domain sizes always being different from the minimum energy state. If the minimum energy state is represented by all spins oriented in the positive direction, `MDS` experiences an increase. In the opposite case, which is what we are reporting in these results, it shows a decrease for temperature values close to T_c, as observed in Figure

2. $T \gg T_c$

   For these temperature values, the system is in a paramagnetic phase. With a random distribution of spins, `DN` tends to increasingly larger values due to the increase in the system's entropy.

   On the other hand, we can observe the convergence of `MDS` to values close to 1. This is related to the value of magnetization because, as magnetization tends to zero due to the random distribution of spins, with spins being equally distributed, the average domain size tends to be the smallest possible.

Another quantity reported during the simulations was two topological variables: the number of domains and the average domain size. To characterize these quantities, topological domains were defined as sets of adjacent spins of positive value (Figure Ring boundary conditions were taken into account to calculate the number and size of each of them. The variable mean domine size was calculated as the ratio of the sum of the size of each domain present in the network to the total number of domains. The evolution of these quantities as a function of temperature can be seen in Figures

III. PHYSICAL VARIABLES: RESULTS

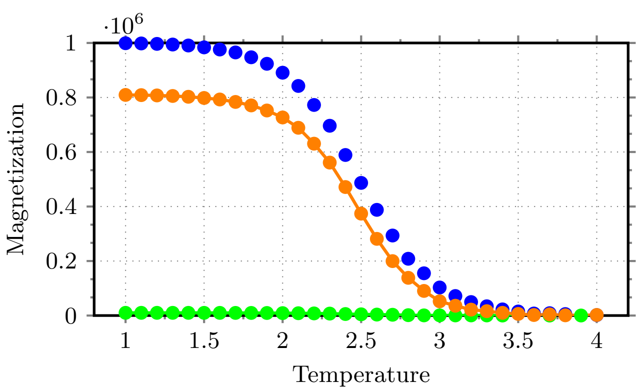


FIG. 2: Magentization as function of discrete values of temperature. Agregar la grafica de valores per sitio.

IV. TOPOLOGICAL VARIABLES: RESULTS

V. DISCRETE CURVATURE

- Erick, calcula detalladamente, el número máximo de aristas que puede tener el sistema con nxn nodos.

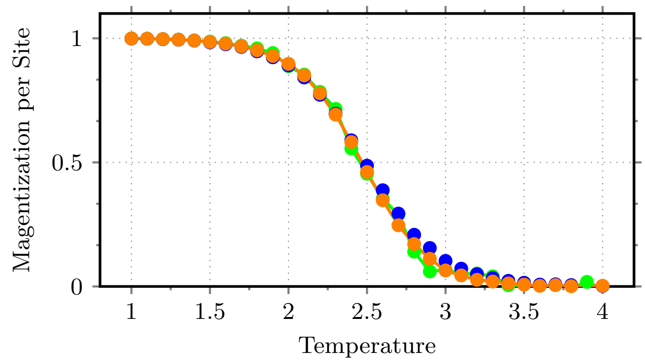


FIG. 3: Magnetization per Site as function of discrete values of temperature.

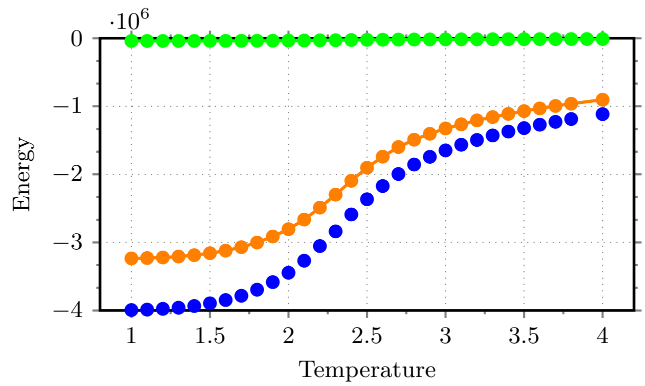


FIG. 4: Energy as function of discrete values of temperature.

Let n denote the number of vertices in the network. Given the initial conditions, we know that the degree of each vertex can be at most 4. Thus, the maximum number of edges that can be present in a network with n vertices is given by:

$$\frac{4n}{2}$$

- el rango de valores de curvatura.

Vertex	**Minimum curvature value**	**Maximum curvature value**
10000	0	20000
160000	0	320000
490000	0	980000
810000	0	1620000
1000000	0	2000000

TABLE I: Minimum and maximum curvature values for different matrix sizes.

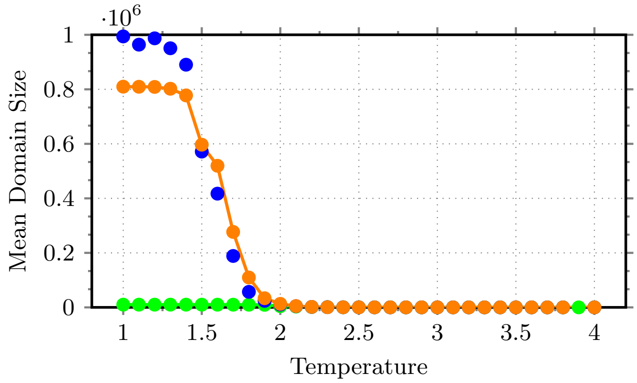


FIG. 5: Mean Domain size as function of discrete values of temperature.

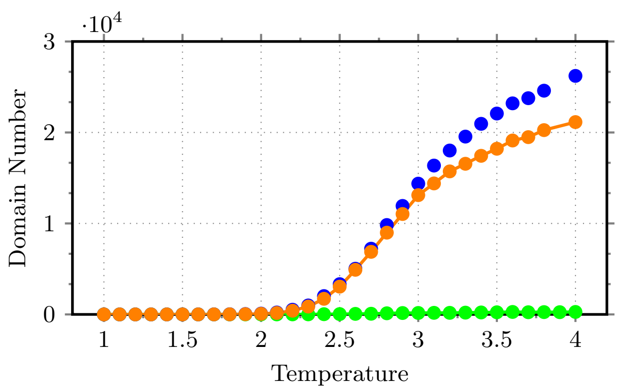


FIG. 6: Mean doamain size as function of discrete values of temperature.

VI. CURVATURE NUMERICAL RESULTS

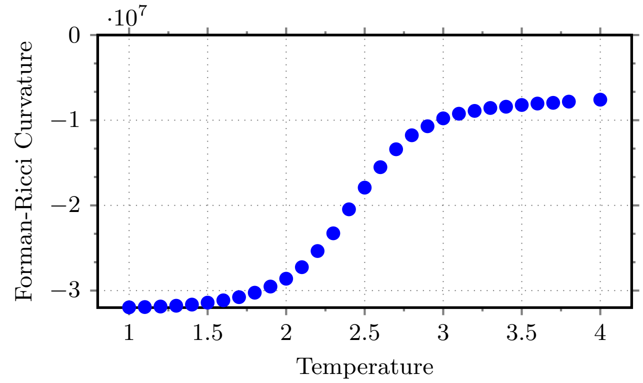


FIG. 7: Forman-Ricci curvature as function of discrete values of temperature. Spin matrix has dimension 1000×1000.

Dada una red real, ¿será que ésta puede verse como un dominio magnético en un modelo de Ising 2D? Indicaría la curvatura de FR una forma de exlorar esto?

VII. CONCLUSIONS

ACKNOWLEDGMENTS

Thanks to

Appendix A: Data availability

Source data are provided with this paper. The experimental data used in this paper are also publicly available in a Github repository at https://github.com/erick-rios/ising-model-analysis/tree/main.

Appendix B: Code availability

The code used to generate the corresponing matrices, the physical, topological and geometric variables asociated to them are available at https://github.com/erick-rios/ISINGenerator.

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