Magnetic Phase Transitions in Lattice Magnet Configurations Modelled by the 2D Ising Model and Monte-Carlo Markov Chain Algorithms

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Overview

Magnetism and Inter-Particle Interactions

- The spin-state of particles induces magnetic moments.
- A system of such particles involves inter-particle interactions due to the relative orientation of their magnetic moments as a result of their respective spin states.
- A system of magnetized particles also interacts with external magnetic fields.
- The response of a system to such stimuli is also dependent upon the parameters under which it evolves.
- The combination of these effects results in the system's configuration.

Magnetism and Inter-Particle Interactions

Throughout this project, we consider a system of equally spaced atoms that are magnetized as a result of the spin of their constituents. Principles of quantum mechanics motivate the classification of the atoms' spin states in two categories, which we label $+1$ and -1.

Most materials can be classified as **diamagnets**, **paramagnets,** or **ferromagnets** depending on the inter-particle and external field interactions involved. We subject our system to fluctuations in temperature and external field and evaluate its evolution and tendency toward particular states, or configurations.

The 2D Ising Model

- Powerful mathematical problem that we use to represent our system and formalize our problem.
- Generalizable to far more applications than magnetic systems.
- Lattice sites that take one of two states represent our atoms.
- Restriction to 2D due to complexity, posing a limitation on our project.

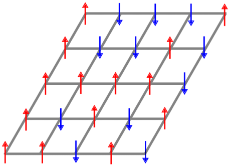


Figure: 2D Ising Model Lattice

Objectives

Throughout this project, we exploit the numerical implementation of the 2D Ising model in order to:

- demonstrate **phase transition**, namely the shift from paramagnetism to ferromagnetism under the Curie temperature.
- recover behavior aligning with Curie's law.
- recovering behavior predicted in real life by physical laws governing system evolution such as hysteresis cycles.
- generalize our model to situations involving a continuum of magnetization states.

Logical Guiding Questions

- How does the system evolve?
- How does phase transition manifest itself?
- How do we measure system characteristics to detect phase transition?

The Hamiltonian

We need to extract energy from a given configuration. The Hamiltonian, in this framework, derives from statistical physics and writes:

$$\mathcal{H} : \begin{cases} \{-1, 1\}^N & \longrightarrow \mathbb{R} \\ \quad \sigma & \longmapsto \mathcal{H}(\sigma) = -E \sum_{<i,j>} \sigma_i \sigma_j \; - \; J \sum_{i=1}^{N} h_i \sigma_i \end{cases}$$

The Partition Function & Configuration Probabilities

Whether a configuration is physically favorable or not depends on the **partition function** defined below:

$$Z : \begin{cases} \mathbb{R}_{>0} & \longrightarrow \mathbb{R} \\ T & \longmapsto \sum_{\sigma \in \{-1,1\}^N} e^{-\frac{1}{k_B\, T}\, \mathcal{H}(\sigma)} \end{cases}$$

The probability of a configuration occurring is then defined as:

$$\mathbb{P}(\sigma) = \frac{1}{Z(T)}\, e^{-\frac{1}{k_B\, T}\, \mathcal{H}(\sigma)}$$

Measuring Quantities

The quantities we are interested in measuring to track the system's behavior and identify transition are:

- the magnetization.
- the magnetic susceptibility.
- the heat capacity.
- the energy.

Important Note on Measurables

Because of the complexity of the computation of Z, especially with an ever-evolving temperature, the measurement of these quantities is done through stochastic integration, the process of which is very thoroughly outlined along with many interesting details on the theoretical background as well as the specifics of the numerical implementation involved in the project.

We only mention that the quantities, in this framework, are defined as continuous applications on Z, which can be shown to be equivalent to statistical measures of random variables that are functions of σ distributed according to the partition function. This motivates Monte-Carlo integration and the use of statistical limit theorems to average values over r.v. realizations.

The Free Energy

A very interesting quantity that will not reappear in the subsequent slides is the free energy defined as:

$$\mathcal{F} : \begin{cases} \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R} & \longrightarrow \mathbb{R} \\ (\beta, E, J) & \longmapsto \lim\limits_{N \to +\infty} \dfrac{1}{N\beta} \ln Z(\beta, E, J) \end{cases}$$

- Analog of the Helmholtz free energy: $F = U - TS$..
- Dictates Spontaneity.
- Nice Interpretation for Phase Transitions.
- Used by Onsager to analytically solve the Ising model in 2D.
- Thermodynamic Limit! (need discontinuities...)

The Discrete Case

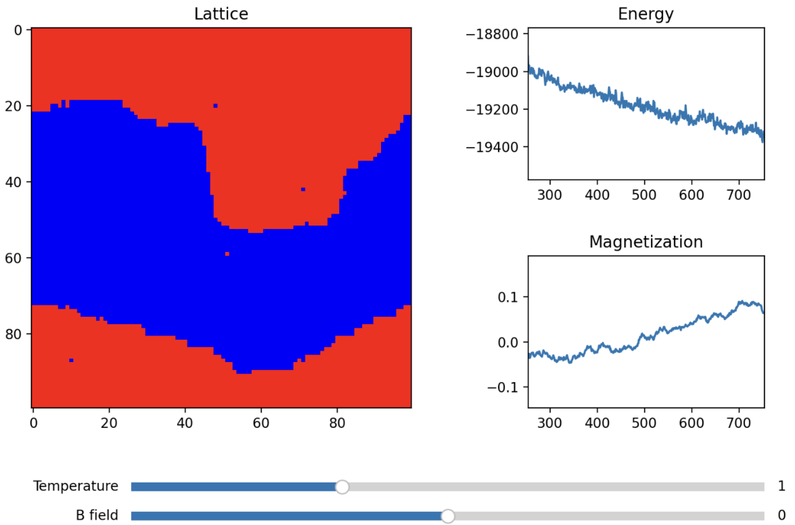
We model our problem with a lattice containing $N = L \times L$ nodes. Each of these nodes contains a spin $\sigma_{i,j} \in \{\pm 1\}$.
We use a Hamiltonian of the form:

$$\mathcal{H} = -E \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J \sum_i \sigma_i$$

and compute the acceptance probability as:

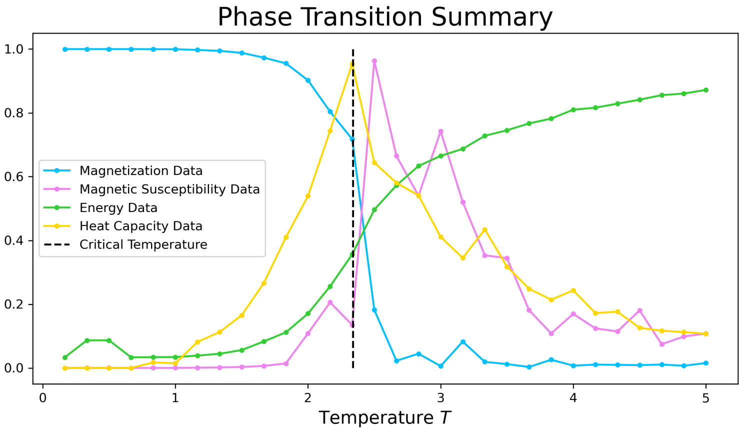
$$p \sim e^{-\Delta \mathcal{H} / k_B T}$$

Implementation



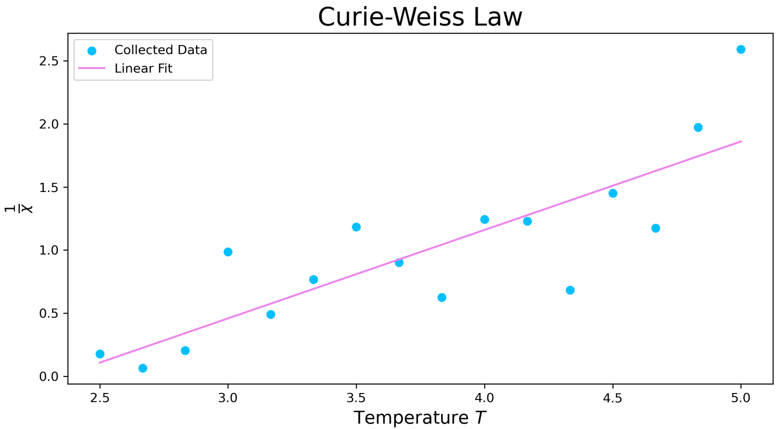
The Phase Transition

We run simulations of the model and observe the dependence of the different measurables on the temperature.
We determine $T_C \approx 2.34$, compared to $T_{C,theory} = 2.27$.



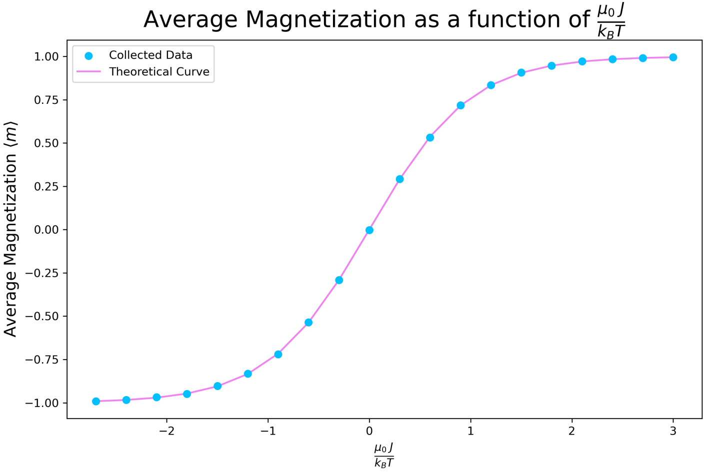
Curie-Weiss Law

We confirm experimentally the Curie-Weiss law by plotting the inverse of the susceptibility against the temperature.



Scaling of the Magnetization

When subjecting the lattice to a fixed temperature T and varying the magnitude of the external field, we obtain the following plot:



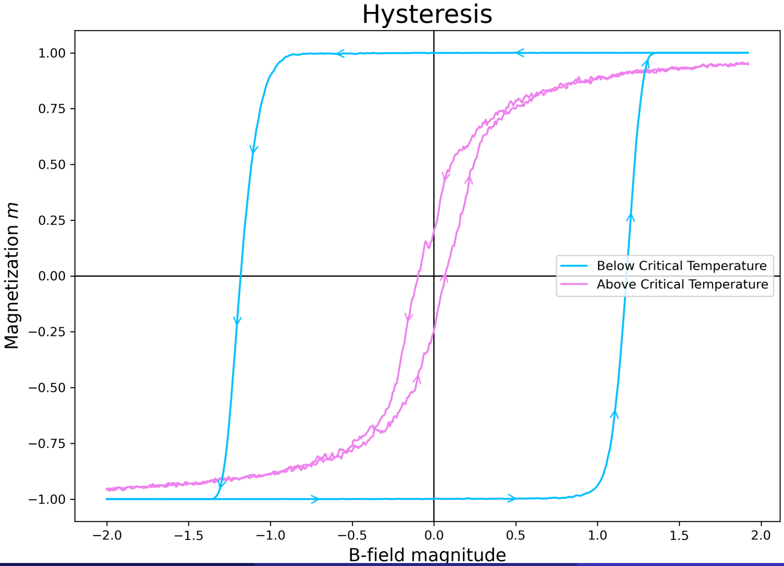
Hysteresis

Ferromagnets display a behaviour called hysteresis when their temperature is below the Curie temperature.
We can reproduce this behaviour easily in our simulation:

- Start from a random initial spin distribution
- Increase the external field until the magnetization is saturated
- Decrease the external field until the magnetization is saturated again
- Increase the field again until it is saturated

During one of those cycles, record the magnetization, and plot it as a function of the magnitude of the field.

Hysteresis



Hysteresis
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization m
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
B-field magnitude
Below Critical Temperature
Above Critical Temperature

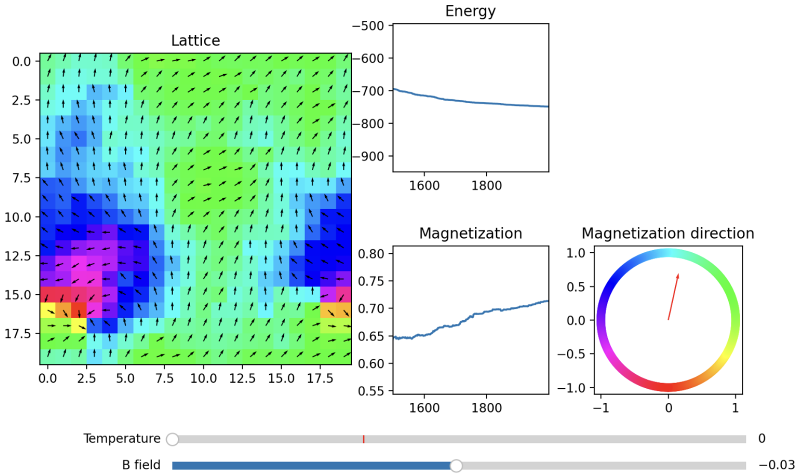
Second Implementation: The Continuous Case

We modify our model: instead of spins being binary, i.e. directed "up" or "down", we consider a continuum of spin values corresponding to a direction in the plane.

This modifies our Hamiltonian as such:

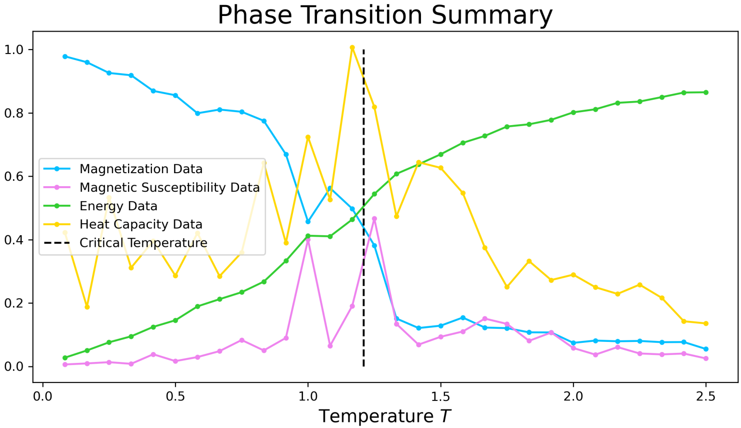
$$\mathcal{H} = -E \sum_{\langle i,j \rangle} \cos(\pi(\sigma_i - \sigma_j)) - J \sum_i \cos(h_i - \sigma_i)$$

Implementation



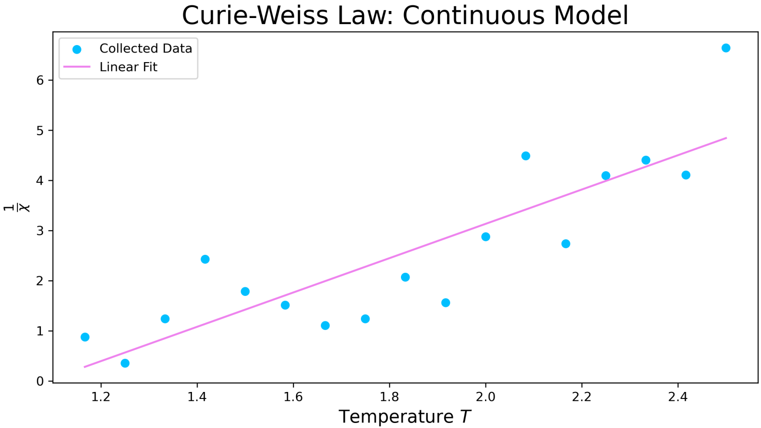
Phase Transition?

We run the simulation and observe the dependence of different measurables on the temperature.
We observe similar behaviour to the standard Ising model. We infer the critical temperature $T_C \approx 1.21$.



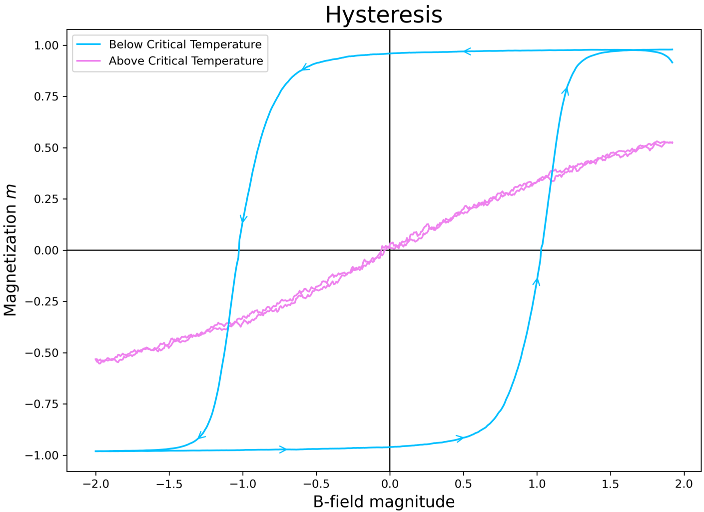
Curie-Weiss Law?

We observe a correlation, as in the standard Ising model.

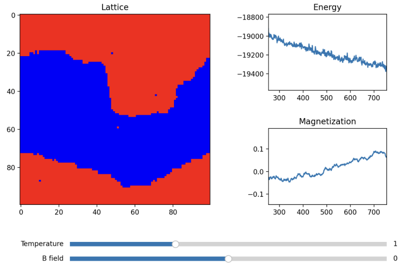


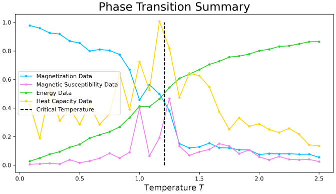
Hysteresis?

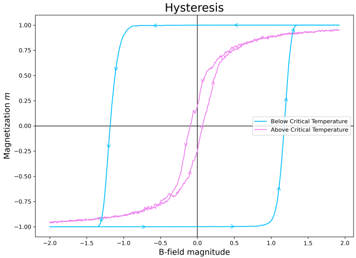
The phenomena of Hysteresis holds in the continuous model.

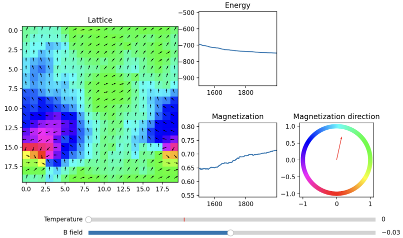


Conclusion


Lattice
Energy
Magnetization
Temperature
B field


Phase Transition Summary
Magnetization Data
Magnetic Susceptibility Data
Energy Data
Heat Capacity Data
Critical Temperature
Temperature T


Hysteresis
Below Critical Temperature
Above Critical Temperature
Magnetization m
B-field magnitude


Lattice
Energy
Magnetization
Magnetization direction
Temperature
B field