École Centrale Supelec

Hexagonal 2D Ising model : Antiferromagnetic frustration

Élèves :
Adrien Lamoureux
Paul Rousset-Rouard

Encadrant :
Fabien Brieuc

November 14, 2024

Contents

Introduction

The goal of the project was to simulate by the Monte-Carlo Metropolis method a 2D hexagonal lattice system of $N = n^2$ magnetic moments which have two possible states, $+\mu$ or $-\mu$ (along the axis perpendicular to the lattice plane). For each simulation, the system is supposed to evolve at a constant temperature T (so we are simulating in the canonical ensemble). In order to simulate an infinite lattice, we used the Born-von Karman periodic boundary condition. The order parameters we are interested in are the mean energy, the mean magnetization and the heat capacity of the system.

We considered only first neighbors interaction, and so the Hamiltonian of the system is (in the absence of an exterior magnetic field) :

$$H = \frac{J}{2} \sum_{i=1}^{N} \sum_{j \text{ first neighbors of } i} \mu_i \mu_j$$

J is called the exchange constant. The case $J < 0$ corresponds to a ferromagnetic material, whereas the case $J > 0$ corresponds to an antiferromagnetic material. Let us the justify quickly the second appellation : at very low temperatures, the system want to minimize its energy so if we look at the Hamiltonian, the product of spins must be negative, meaning that each moment tends to antialign with its first neighbors, hence the name antiferromagnetic, in opposition to ferromagnetic where all the magnetic moments tend to align in the same direction.

In order to realize more efficient and accurate simulations, we manipulate dimensionless (and normalized) quantities. We identify a characteristic energy $H^* = J\mu^2$, and so we get dimensionless magnetic moments μ^*, whose values are either $+1$ or -1.

The energy associated to a given temperature T is $k_B T$, so we can define a normalized temperature $T^* = \frac{k_B T}{J\mu^2}$ and a normalized heat capacity $c_V^* = \frac{\partial H^*}{\partial T^*} = \frac{c_V}{k_B}$.

The dimensionless Hamiltonian therefore becomes :

$$H^* = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \text{ first neighbors of } i} \mu_i^* \mu_j^*$$

We finally define the magnetization of the lattice by :

$$M^* = \frac{1}{N} \sum_{i=1}^{N} \mu_i^*$$

Our tutor first advises us to do the simulation on a square lattice, as it would be

much more simple to check if the code is giving the expected results. Once our code was working, we made the simulation on the hexagonal lattice for which the antiferromagnetic frustration phenomenon appears. Finally, we discussed the influence of an external magnetic field on the system.

1 2D square lattice simulation

In this section, we will explain our implementation of the Metropolis algorithm for the Ising model (on Python), as well as present results for the square lattice case.

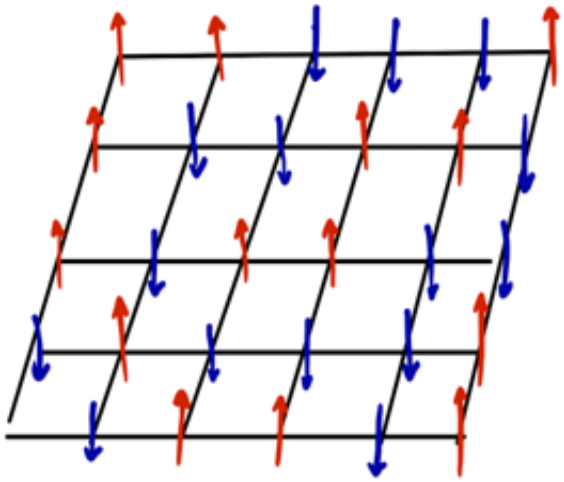

Figure 1: Square 2D Ising model

1.1 Implementation of Monte-Carlo Metropolis

The principles of the Monte-Carlo simulation is to generate a Markov chain using a $\mathbf{\Pi}$ matrix, that will visit the canonical ensemble configuration space. That $\mathbf{\Pi}$ matrix is called the transition matrix, and must :

1. be stochastic
2. be ergodic
3. be relatively "big"
4. verify the micro-reversibility condition.

The matrix $\mathbf{\Pi}$ can be decomposed as $\mathbf{\Pi} = \alpha\mathbf{P}$, where α is called the underlying matrix of the Markov chain. The choice of α is arbitrary, provided it is symmetrical and stochastic. The matrix $\mathbf{P}$ represents the probability of accepting the new configuration starting from a given configuration.

In our case, the 2D square lattice can be modeled as a $\mathbf{n}$ x $\mathbf{n}$ matrix of magnetic moments ($\mathbf{n}$ is the number of atoms on one side of the lattice). If (i, j) is the position of a magnetic moment, then its first neigbors are in position $(i + 1, j)$, $(i - 1, j)$, $(i, j -$

1) and $(i, j+1)$. We then use the Born-Von Karman periodic boundary conditions to simulate an infinite 2D lattice and the probability of accepting a new configuration j from a configuration i is given by $min(1, \exp(-\frac{H_j^* - H_i^*}{T^*}))$.

A choice of ours was to choose at each simulation step to flip a random magnetic moment of the **n** x **n** matrix. Each magnetic moment is flipped with the same probability, so that the underlying matrix of the Markov chain is symmetrical and stochastic. In the case of the 2D square lattice, each atoms has 4 first neighbors, and the energy needed to flip a random magnetic moment μ^* is equal to :

$$\Delta = 2\mu^* \sum_{i \text{ i first neighbors of } \mu^*} \mu_i^*$$

with μ^* being the new orientation of the random magnetic moment chosen. It is important to note that the choice of flipping only one moment works well for small matrices of magnetic moments, but for larger matrices, it is more efficient to flip 2 or more magnetic moments at a time, as the configuration space will be visited quicker. Understanding this is a key ingredient to faster Monte-Carlo Metropolis simulations, as the energy evaluation of new configurations becomes a trivial calculation.

1.2 Results for a square lattice

In the ferromagnetic case (where the magnetic moment tends to align in the same direction at low temperatures), i.e. $J < 0$, the mean magnetization should be equal to -1 or +1 when below the Curie point, and 0 above. Same for the energy, which should be equal to $-2n^2$ at very low temperature, and demonstrate a brutal jump at the Curie point. Consequently, the heat capacity should theoretically diverge at the Curie point.

To observe this 2nd order transition from paramagnetic to ferromagnetic, we plot (see **Figure 2**) the average energy, the mean magnetization (in absolute value), and the heat capacity when the temperature varies around the Curie point. The heat capacity is calculated according to the formula $c_V^* = \frac{<H^{*2}> - <H^*>^2}{T^{*2}}$. In the algorithm we wrote, the variance of the mean energy is calculated starting from the 10,000 simulation step to get a better convergence, as the mean energy will less fluctuate. The mean magnetization is plotted in absolute value for a better visualization of the transition.

For the antiferromagnetic case, we expect the transition from a global order where magnetic moments are anti-aligned at low temperatures to a paramagnetic phase where there is no global order at high temperatures. If we only look at the magnetization as the sum of the magnetic moments, we would observe no change from the antiferromagnetic regime to the paramagnetic regime as we can see on the **Figure 3** for the magnetization plot.

This can be solved by looking at the alternated sum of the magnetic moments $\mu_{11} - \mu_{12} + ... - \mu_{21} + \mu_{22} - ....$ This is what we plotted on **Figure 4** and what will be plotted in all the following graphs regarding at an antiferromagnetic case.

In both ferromagnetic and antiferromagnetic cases, one can observe a transition

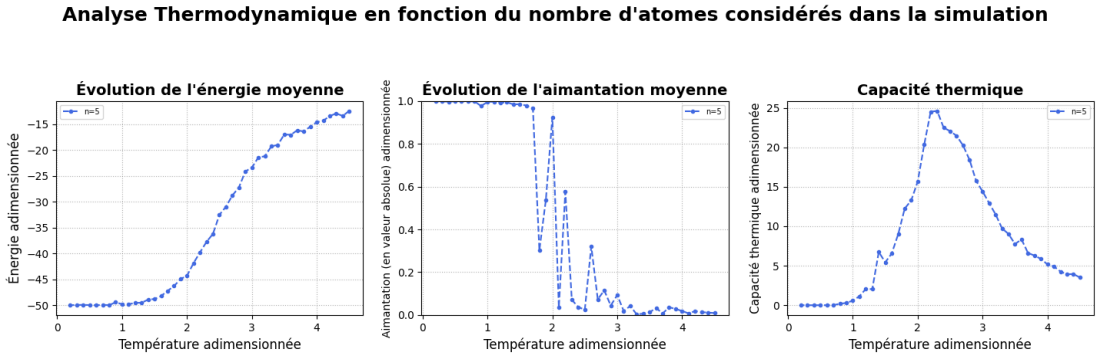

Figure 2: Results of Monte-Carlo Metropolis simulation for a 2D square lattice of 25 atoms and 50 000 simulations steps in the ferromagnetic case.

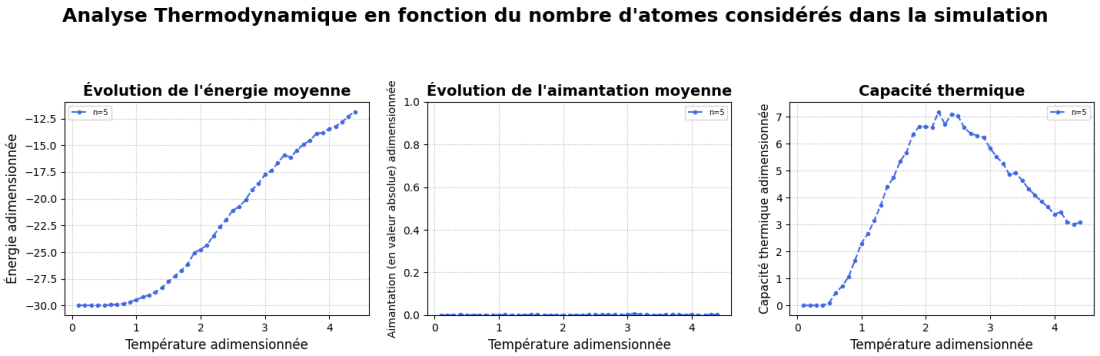

Figure 3: Results of Monte-Carlo Metropolis simulation for a 2D square lattice of 25 atoms and 50 000 simulations steps in the antiferromagnetic case. The magnetization is taken as the simple sum of the magnetic moments.

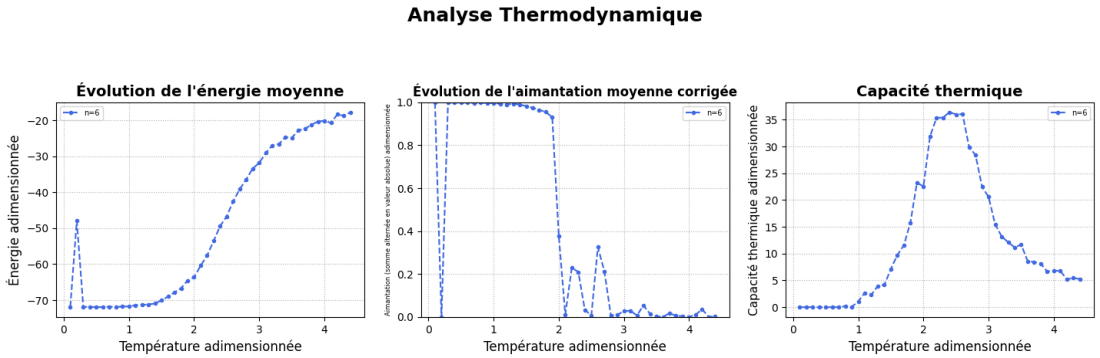

Figure 4: Results of Monte-Carlo Metropolis simulation for a 2D square lattice of 36 atoms and 50 000 simulations steps in the antiferromagnetic case. The magnetization is now taken as an alternated sum (in order to see the transition).

temperature around $\mathbf{T^* = 2}$.

2 Frustration phenomenon for an hexagonal lattice

In this section, we will explain how we simulated an hexagonal lattice (**Figure 5**) and the simulation results we observe.

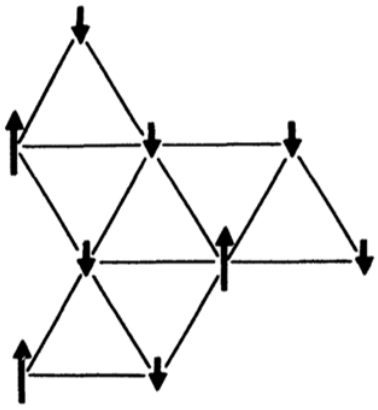

Figure 5: Hexagonal 2D Ising model

2.1 Degenerescence of the ground state

In an hexagonal lattice, each magnetic moment now has 6 neighbors. Therefore, we also simulated the lattice with a **n** x **n** matrix but now, if (i, j) is the position of a spin, we also consider the $(i-1, j+1)$ and $(i+1, j+1)$ spins as first neighbors.

With this configuration, one can quickly see a problem for the antiferromagnetic case as it is impossible to reach a configuration where each spin is anti-aligned with all of its first neighbors (see **Figure 6**).

As a consequence of this frustration, there is not a unique configuration of the ground state at very low temperatures for an antiferromagnetic.

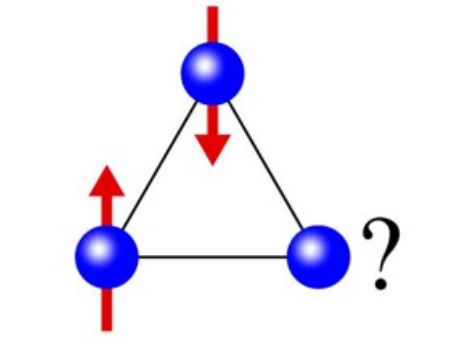

Figure 6: The spins can't anti-align with all of their neighbors, they are said to be "frustrated".

2.2 Antiferromagnetic frustration : simulation

As we said, for an antiferromagnetic, the hexagonal lattice is interesting since it represents a simple example of frustrated system. There is theoretically no phase transition at finite

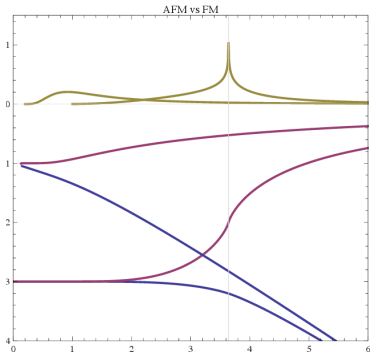

Figure 7: Theoretical thermodynamic values for antiferromagnetic and ferromagnetic hexagonal lattice. The heat capacity is in the top position (in yellow), the energy in purple and the per spin free energy in blue. We notice that the energy in the antiferromagnetic case is a third of the ferromagnetic in the low temperatures. Graph issued from Codello, Allessandro.

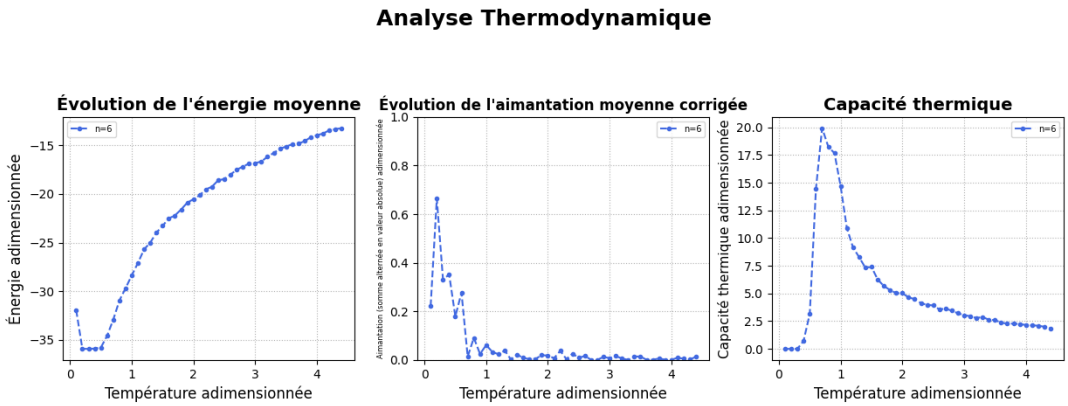

Figure 8: Results of Monte-Carlo Metropolis simulation for a 2D hexagonal lattice of 36 atoms and 50 000 simulations steps in the antiferromagnetic case. The magnetization is now taken as an alternated sum.

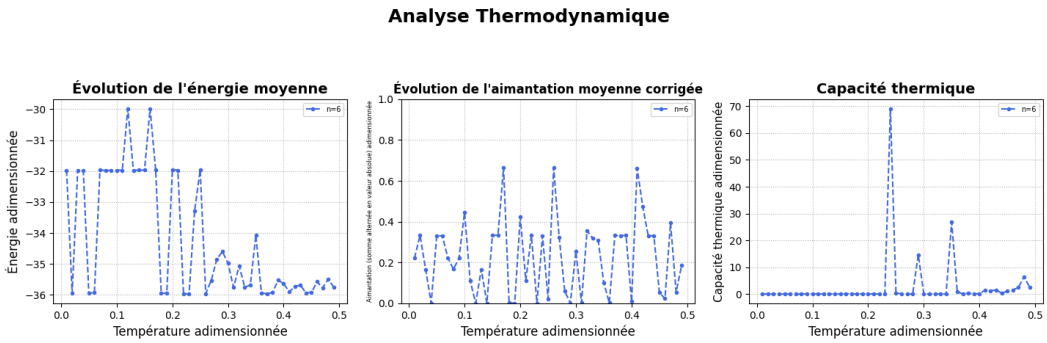

Figure 9: Results of Monte-Carlo Metropolis simulation for a 2D square lattice of 36 atoms and 50 000 simulations steps in the antiferromagnetic case. The magnetization is now taken as an alternated sum (in order to see the transition). Zoom on very low temperatures. The simulation steps taken were too little for such low temperatures, resulting in results that do not conform to theory.

temperature and the model is always disordered, even at T = 0 where the ground state is frustrated and the system has a non–zero entropy.
As the system has no clear ground configuration anymore, one can observe with the simulations that the magnetization is chaotic at these temperatures, and the transition seems to happen at lower temperatures than before (theoretically zero).

The low temperature internal energy in the antiferromagnetic case is supposed to be equal to a third of the low temperature energy in the ferromagnetic case in an hexagonal lattice according to theory. For our simulation with 36 atoms, we obtain an energy of -36 (see **Figure 8**), which is coherent because it is a third of $\frac{-36*6}{2} = -108$.

As we get closer to zero temperature, the simulation needs more and more steps to converge, which explains why **Figure 9** displays an internal energy not perfectly equal to -36.

3 Influence of a magnetic field : hysteresis loop

3.1 Modelisation

When a magnetic field is applied B perpendicularly to the lattice place, a new term appears in the Ising Hamiltonian :

$$H = \frac{J}{2} \sum_{i=1}^{N} \sum_{j \text{ first neighbors of } i} \mu_i \mu_j - B \sum_{i=1}^{N} \mu_i$$

Written with dimensionless quantities, our energy of interest is :

$$H^* = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \text{ first neighbors of } i} \mu_i^* \mu_j^* - B^* \sum_{i=1}^{N} \mu_i^*$$

with $B^* = \frac{B}{J\mu}$.

Theoretically, as we increase the norm of the magnetic field, the term depending on it in the Hamiltonian is supposed to become dominant, and so the spins will tend to align in the direction of the field (see **Figure 10**).

3.2 Hysteresis loop

The phenomenon happens for an antiferromagnetic at a temperature near the transition, when we loop on the intensity of the magnetic field. This means we start from no magnetic field, then increase it until a saturation value, and then decrease it until an other (negative) saturation value before returning to 0.

The most important thing here is to keep the state in which the system ends for the precedent value of the field. In this manner, one can see the appearance of an hysteresis loop (see **Figures 11**, **12** and **10**), which physically means that when saturation

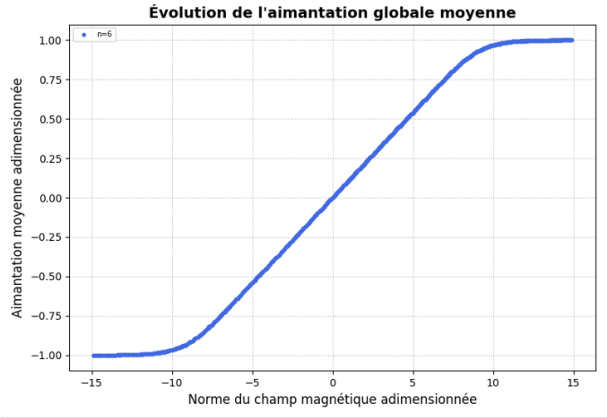

Figure 10: 2D Monte-Carlo Metropolis simulation results of an hysteresis loop in a antiferromagnetic for an 36-atoms hexagonal lattice. No residual magnetization is observed.

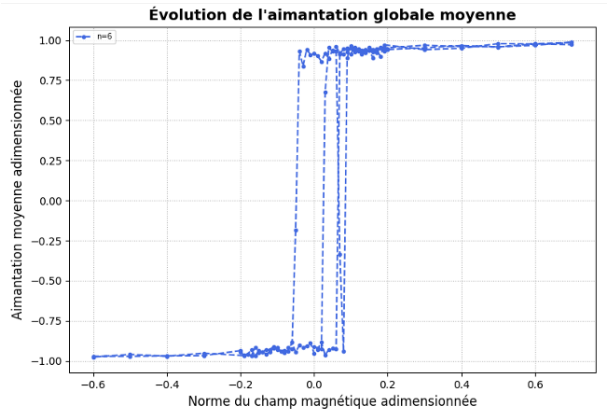

Figure 11: 2D Monte-Carlo Metropolis simulation results of an hysteresis loop in a ferromagnetic for an 36-atoms square lattice. A high residual magnetization is observed.

is reached, it is harder for the system to return in a lower energy state as we decreased the magnetic field : when all the spins are aligned at saturation, the material has more "magnetic inertia".

The hysteresis loop for an antiferromagnetic is not very visible, which is the expected behavior for a material whose spins tends to anti-align.

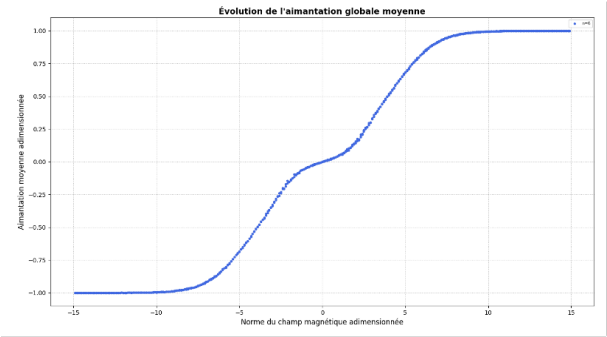

Figure 12: 2D Monte-Carlo Metropolis simulation results of an hysteresis loop in a antiferromagnetic for an 36-atoms square lattice. No residual magnetization is observed.

Conclusion

Through this project, we achieved a successful simulation of the 2D Ising model on both square and hexagonal lattices via the Monte Carlo Metropolis method. For the square lattice, our simulations delivered the expected results: a phase transition near the Curie temperature, with a clear shift from paramagnetic to ferromagnetic or antiferromagnetic order, depending on the sign of J. This provided an initial validation of our implementation.

In the case of the hexagonal lattice, the antiferromagnetic configuration allowed us to explore the phenomenon of geometric frustration. Unlike the square lattice, where long-range order can be established, the hexagonal lattice's structure prevents all spins from anti-aligning with their nearest neighbors, resulting in a system that remains disordered down to zero temperature. This behavior aligned with theoretical predictions, confirming the absence of a finite-temperature phase transition in frustrated systems.

Furthermore, when introducing an external magnetic field, we observed distinct hysteresis behavior across different configurations. In the ferromagnetic case on the square lattice, the field induced a notable residual magnetization, indicative of magnetic "inertia." In contrast, the antiferromagnetic hexagonal lattice showed no residual magnetization, reflecting its tendency to resist alignment under external influence.

Concerning the simulation, two major improvements could have been made. On one hand, we kept the same number of simulation steps regardless of the temperature while it is harder to reach equilibrium at high temperatures and easier at lower ones. On the other hand, we did not conserve the final state of a simulation at a given temperature to put it as the initial state of the next one. Adding this precision and simulating from high temperatures to lower ones could have given us better graphs regarding the theory, especially for the antiferromagnetic frustration phenomenon.

Bibliography

References

Codello, Alessandro (2015). "Chapter 5 Ising model and phase transitions". In.

Wannier, G. H. (1950). "Antiferromagnetism. The Triangular Ising Net". In: *Physical Review*.