UNIVERSIDAD DE GRANADA

Facultad de Ciencias

Computational Physics

Volunteer 1: Simulation of the Ising model with the Kawasaki dynamic

Summary

The results show how the spin exchange dynamics influences the formation of magnetic domains and the evolution towards thermal equilibrium as a function of the number of Monte Carlo steps. In addition, non-zero magnetisation was studied to better understand the phase transitions in the Ising model. All the plots and program used can be found in the GitHub repository: Kawasaki.

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Degree in physics

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1. Dinåmica del modelo.

Simulate the dynamics of this model for various temperature values. Repre- sent several frames associated with various temperatures.

For this section a spin value of N=32 is set to facilitate convergence. We started with zero magnetization, which is nothing more than placing the same number of spin +1 as spin -1, and we also fixed the spins at the edges of the y-direction, to facilitate the observation of the magnetic domains, obtaining the following initial conditions: The following are shown below

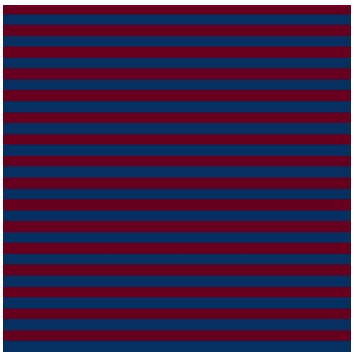


Figure 1: Initial conditions: zero magnetisation, fixed y-spins. associated frames at

different temperatures:

1.1. Equilibrium temperature: 1K.

For T=1 K, it is observed that the higher the number of Monte Carlo steps, the more the system evolves towards the equilibrium state, characterised by the formation of magnetic domains, areas where all the spins are aligned, +1 or -1:

- For figure 2, where the system has only been allowed to evolve 1000 Monte Carlo steps, it can be seen that the fragmentation and dispersion of the domains indicate that the system is in the early stages of evolution towards equilibrium. The spins are beginning to redistribute towards the most favourable energy state, but more defined domains are still some time away.

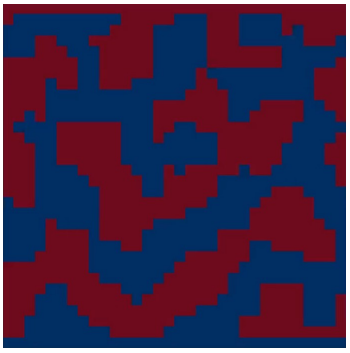


Figure 2: T=1, 1000 MC Steps.

- For figure 3, it can be seen how 100000 Monte Carlo steps are sufficient for the spins to have had multiple interactions, resulting in the consolidation of domains in
  The system is closer to equilibrium. The system is closer to equilibrium, although there could still be more restructuring and domain growth with more steps.

Figure 3: T=1, 100000 MC Steps.

- For figure 4, where the system has been allowed to evolve for a million Monte Carlo steps, large band-like domains are seen, indicating that the exchange dynamics has allowed the spins to reorganise almost completely. This pattern is indicative that the system has reached a state where energy has been minimised, the equilibrium. Consequently, any further changes in the domains will be much slower and less significant.

Figure 4: T=1, 1000000 MC steps.

1.2. Critical temperature: T_c

At the critical temperature, a state characterised by fluctuations is observed, where the magnetic domains show a highly variable structure. The system is far from equilibrium, and the configuration is dominated by a mixture of small and medium-sized aligned regions, reflecting the critical nature of the temperature. Despite increasing Monte Carlo steps, the system does not tend towards defined domains, because the critical temperature is a transition point to

from when the spontaneous magnetisation observed in the previous section ceases to occur. Therefore, the system will continue to show characteristics of critical fluctuations, since the equilibrium domains begin to transition to a state of disorder.

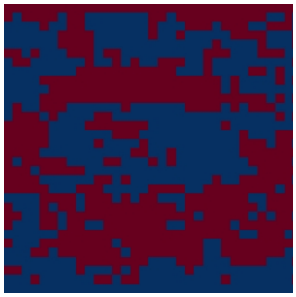


Figure 5: $T_c = \frac{2}{\sqrt{2}}$, 1000 MC steps

Figure 6: $T_c = \frac{2}{\sqrt{2}}$, 100000 steps MC

Figure 7: Comparison of Monte Carlo simulations with different number of steps. $T_c = \frac{2}{\sqrt{2}}$, N=32.

1.3. Temperature above T_c : T=5 K.

For a temperature above T_c , it is observed that spontaneous magnetisation no longer occurs, regardless of the number of Monte Carlo steps. Due to the high temperature, the spins are randomly oriented, without forming domains.

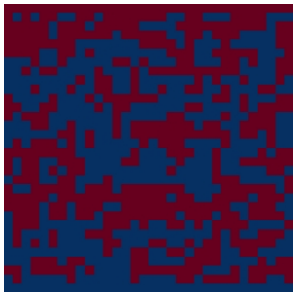


Figure 8: T=5K, 1000 MC steps.

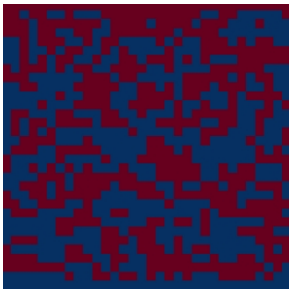


Figure 9: T=5K, 100000 MC steps.

Figure 10: Comparison of Monte Carlo simulations at T=5K with different number of steps.

2. Magnetisation.

Obtain the magnetisation curve per particle calculated per domain as a function of temperature for various sizes of the system, averaged over a sufficient number of Monte Carlo steps, so that the error is reasonably small. This domain averaging is performed - in case of zero initial magnetisation - by calculating the magnetisation in each of the halves (upper and lower) of the system.

In this section, for different sizes, namely N=10, 16, 32 and 64, the magnetisation of the top and bottom as a function of temperature, in the range of T=[0, 5.8], is calculated. For the calculation, the expression has been used:

$$mdomain = \left\langle \frac{2}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} s(i,j) \right| \rangle \quad (1)$$

The figures obtained are shown below, showing the upper and lower magnetisation and their sum, which, as can be seen, is always zero, since we are working with zero magnetisation and in the Kawasaki model, since there are only exchanges of spins, the total magnetisation is always constant.

It is important to note that as N increases, the number of Monte Carlo steps decreases, since the compilation time increases exponentially with the number of spins.

All errors associated with the calculations are within a 99,74 % confidence interval.

- For N=10, 100.000 Monte Carlo steps were taken (figure 11). It can be seen that for temperature T=[1, 1.2], the magnetisation is maximal. This makes sense because at that temperature is where more magnetic domains exist, i.e., more spins are aligned and therefore there is more magnetisation. As the temperature increases, the system loses spontaneous magnetisation and in the two halves it tends to 0.

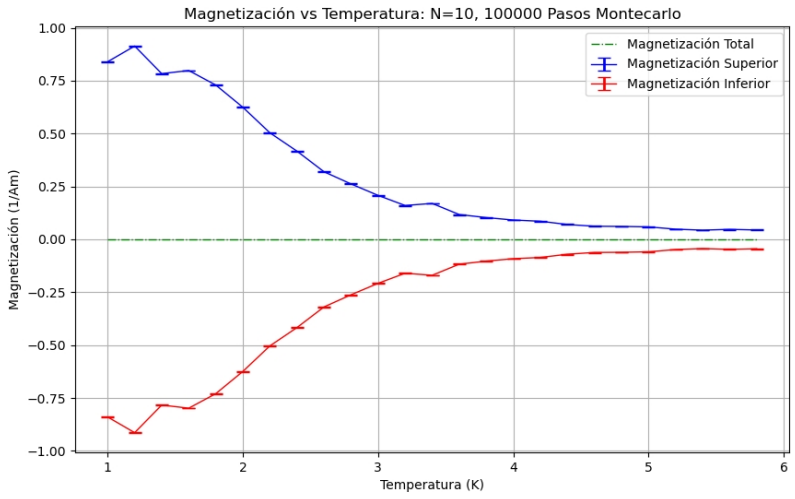
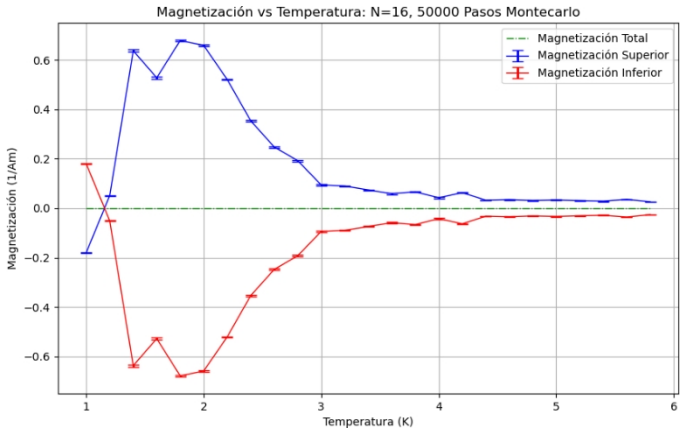


Figure 11: Upper, lower and total magnetisation. N=10, 100000 Monte Carlo steps. Confidence 99,74 %.

- Once again, for N=16, (figure 12), it can be seen that at high temperatures ($T > T_c$), the magnetisation tends to 0. In this case, the magnetisation at T=1 is not the maximum, this may be due to the fact that N has been increased and the Monte Carlo steps have been reduced, and therefore less time is available to reach equilibrium. Even so, the global behaviour of the system follows the expected behaviour.



Figure√1 2: Upper, lower and total magnetisation. N=16, 50000 Monte Carlo steps. It can be estimated $T_c \approx 2$ 2. 99,74 % confidence

- For N=32, 50000 Monte Carlo steps (figure 13), the expected behaviour is again observed, with spontaneous magnetisation $\rightarrow$ 0 for $T > T_c$ and maximum for T=1.

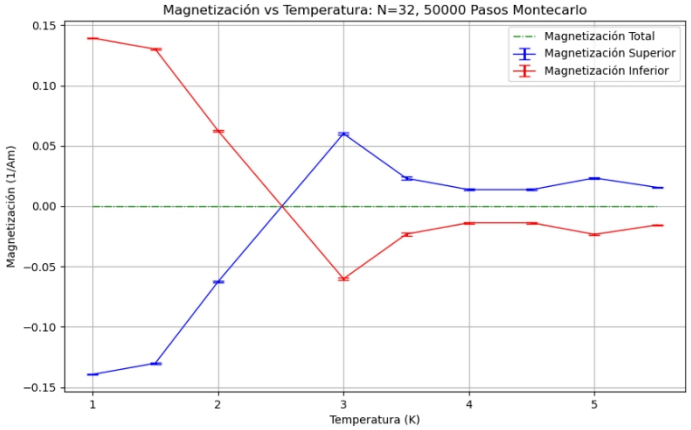


Figure 13: Upper, lower and total magnetisation. N=32, 50000 Monte Carlo steps. Confidence 99,74 %.

- For N=64, 50000 Monte Carlo steps were made again (figure 14), but reducing the temperature range. Again, the same behaviour can be discerned for the other sizes, although the magnetisation is on average larger, as this system is larger in dimensions and needs more time to stabilise.

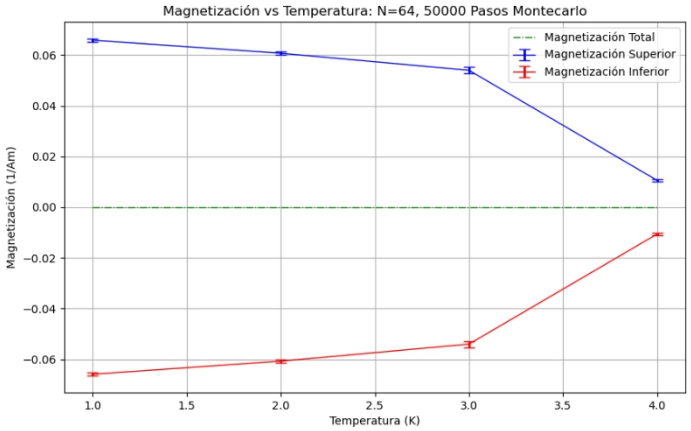


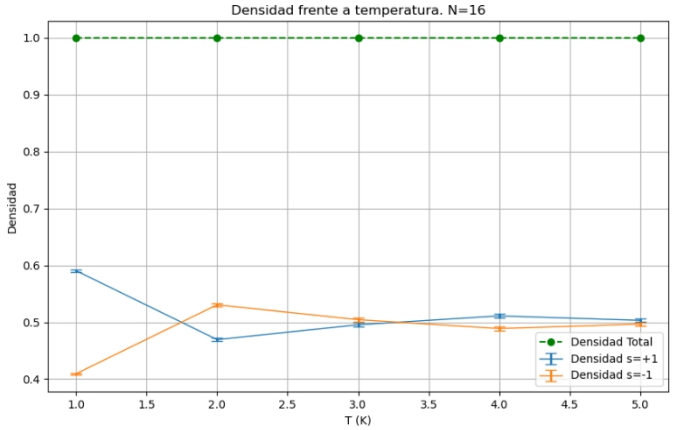
Figure 14: Upper, lower and total magnetisation. N=64, 50000 Monte Carlo steps. Confidence 99,74 %.

3. Average particle density per column.

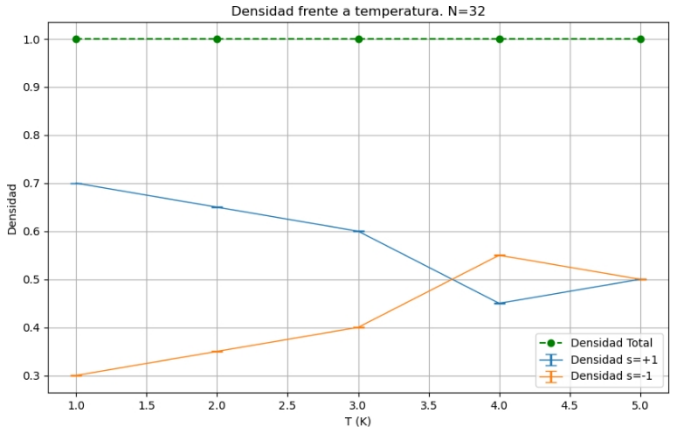
Calculate the mean particle density in the y-direction as a function of temperature and for different sizes.

In this section, the +1 spin density and the -1 spin density per column, as a function of temperature, are calculated for different sizes. It is important to note that the total density is always 1, which indicates that the whole column is taken into account and the analysis is complete. For both figure 15b and 15c it can be seen that for low temperatures there is much more density of +1 spin than -1 spin; this makes sense, since at these temperatures, as we have seen in previous sections, the magnetisation is maximal, therefore there would be two domains, one for the +1 spin and one for the -1 spin. where the majority of the column is occupied by spins of the same type.

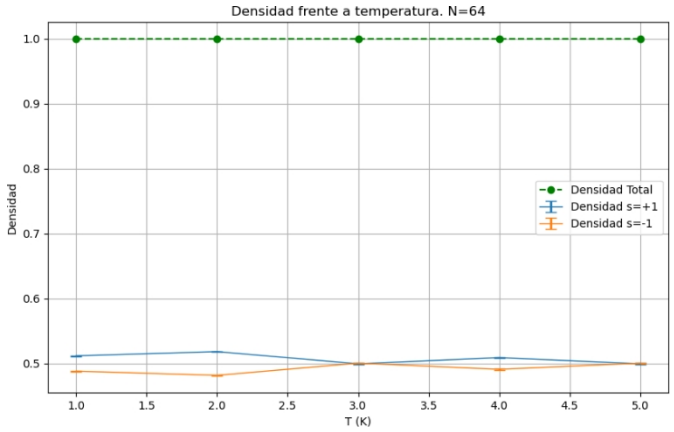
As the temperature rises and the system loses its spontaneous magnetisation, the densities +1 and -1 are practically equal, due to the randomness of the system and its disorder, the spins take any value homogeneously.



(a) Density of spin +1, spin -1 and their sum. N=16. 10000 Monte Carlo steps. Confidence 99.74 %.



(b) Density of spin +1, spin -1 and their sum. N=32. 10000 Monte Carlo steps. Confidence 99.74 %.



(c) Density of spin +1, spin -1 and their sum. N=64. 50000 Monte Carlo steps. Note that as N is higher, there is difficulty in convergence at low temperatures. Confidence 99.74 %.

Figure 15: Comparison of spin densities for different N values.

4. Average energy per particle.

In this section, the average energy per particle is calculated with the following expression, averaged over the total Monte Carlo steps:

$$e = \frac{\langle E(s) \langle E(s) \langle E(s) \rangle}{N} \quad (2)$$

As can be seen in figures 16, 17, 18 and 19, there is a minimum energy for T=[1, 1.2], which makes sense, since this is the equilibrium temperature, where the lowest possible energy is achieved.

For 2-3 K, there is a series of fluctuations, indicating a phase transition. In the critical temperature range, the system experiences large fluctuations in energy due to the competition between the order caused by spin interactions and the disorder induced by thermal energy.

During the phase transition, small perturbations can change the state of the system from an ordered to a disordered configuration and vice versa. This results in an increase in energy.

At high temperatures $T > T_c$ K, the thermal energy dominates and the spins are randomly oriented. In this disordered state, the energy of the system is higher compared to the ordered state, and it increases uniformly.

For N=16 and N=32: The energy shows a sharp increase and fluctuations at lower temperatures, which could correspond to finite size effects or phase transition effects. [1]or phase transition effects.

For N=64: The curve appears smoother and the phase transition behaviour is more evident, with a clear change in slope around T 2.5-3, which is closer to the expected critical temperature for the 2D Ising model.

For N=128: The curve becomes fully homogeneous and follows the usual behaviour, all finite-size effects are removed from the system, albeit at the cost of error due to the computational cost of making N=128.

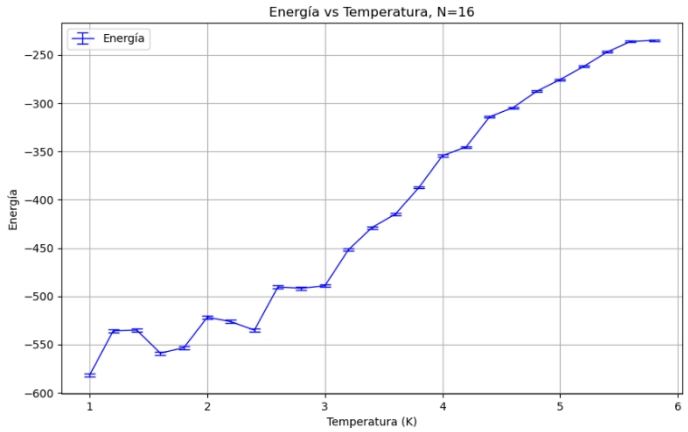


Figure 16: Average energy per particle. N=16, 100000 Monte Carlo steps. Confidence 99.74 %.

[1]The finite size of the system (N=16, N=32, N=64) may cause deviations from the expected behaviour of an infinite system. These effects could manifest themselves as more pronounced fluctuations or less marked transitions, which can be seen in the curves.

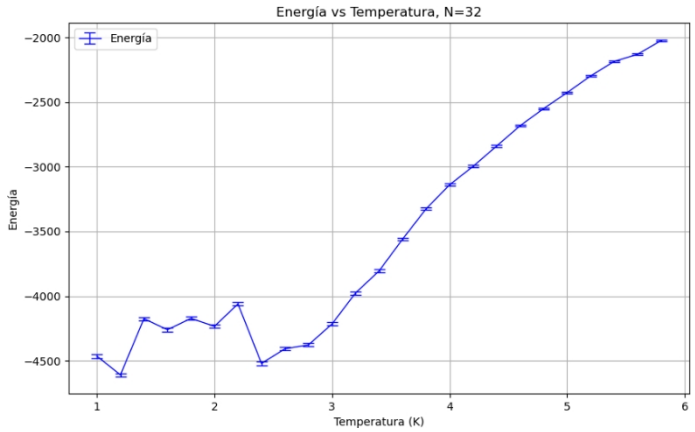


Figure 17: Average energy per particle. N=32, 100000 Monte Carlo steps. Confidence 99.74 %.

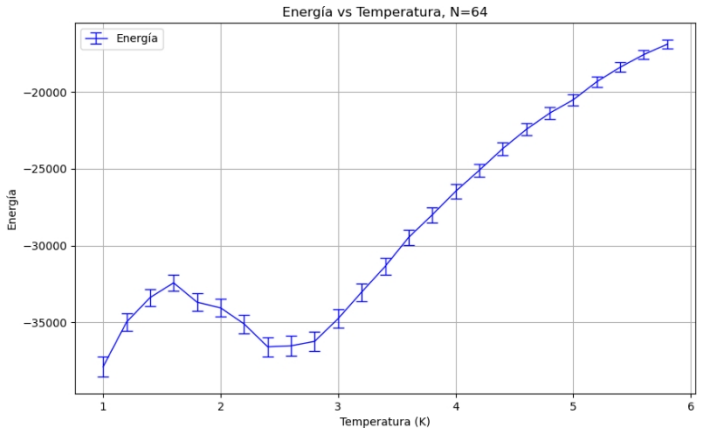


Figure 18: Average energy per particle. N=64, 50000 Monte Carlo steps. Confidence 99.74 %.

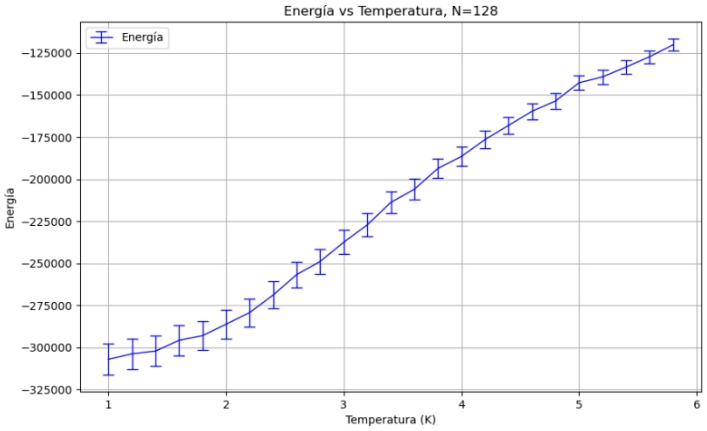


Figure 19: Average energy per particle. N=128, 1000 Monte Carlo steps. Confidence 99.74 %.

5. Average density in y-direction

Calculate average particle density in the direction and for various temperatures.

In this section, the density of each spirit is defined as:

$$\sigma_i = (s_i + 1)/2 \tag{3}$$

We can then interpret the system as a lattice gas, where $\sigma_i = 1$ indicates presence of particle and $\sigma_i = 0$ indicates absence.

The total density would then be:

$$\rho = \frac{1}{N} \sum_i \sigma_i \tag{4}$$

Therefore, we can plot a dependence between the total density and a fixed position 'y'. Figures 20, 21 are obtained for different sizes.

As can be seen, the highest and lowest densities are found at temperature T=1 K, this is in agreement with what has been said before, at the equilibrium temperature, there are very large magnetic domains, therefore in a row where there is a +1 spin domain the density will be, in its majority, 1, while in the case of -1 spin, it will be close to 0.

As can be seen, at higher temperatures, the density is *approximately constant*, which indicates the absence of magnetic domains, since there is spin disorder and equal density of the two.

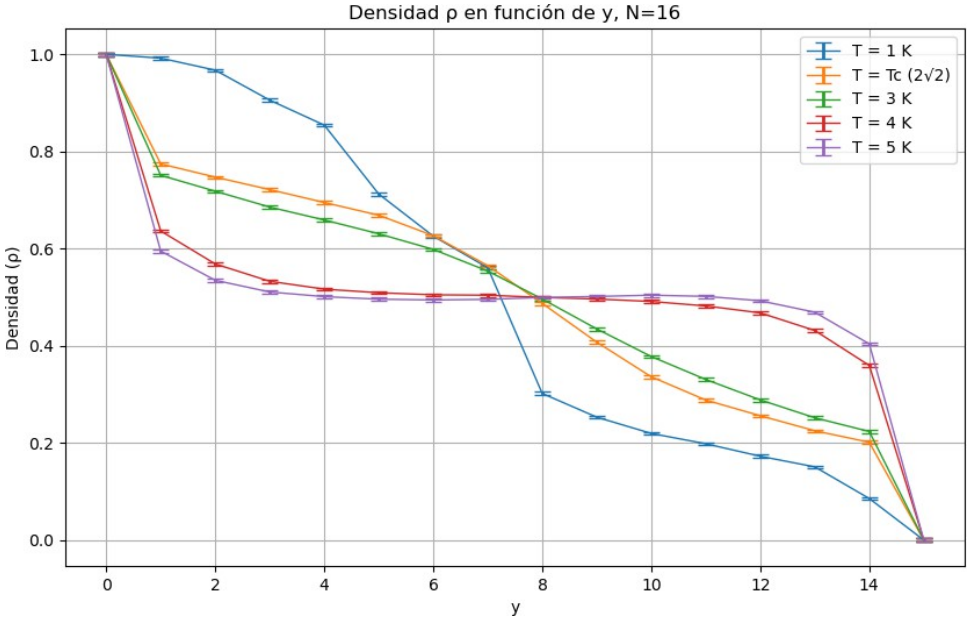


Figure 20: Average particle density in the direction and for different temperatures. N=16. 120000 MC steps. Confidence 99,74 %.

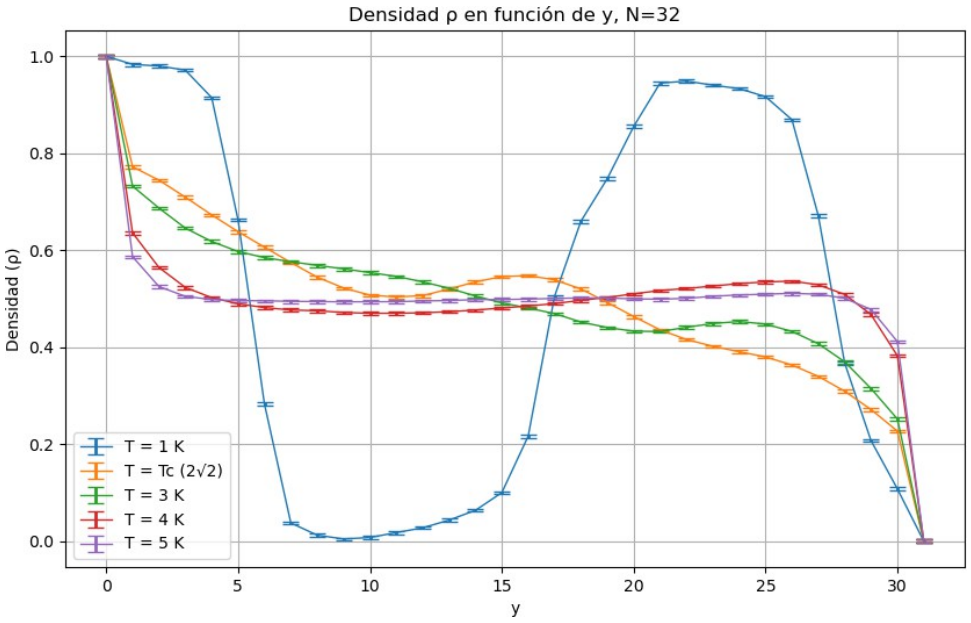


Figure 21: Average particle density in the direction and for different temperatures. N=16. 120000 MC steps. Confidence 99,74 %.

6. Non-zero magnetisation.

Carry out points 1-6 above starting from a non-zero magnetisation. Recall that the magnetisation per particle can take values between -1 and 1, i.e. $m \in [-1, 1]$**. Therefore, if we fix** $m = m_o$ **the average 'per domain' of the magnetisation will be realised, in this case, by averaging separately the fraction** $x = (1 + m_o)/2$ **with x (**$\in [0, 1]$**) lower of the system, and the fraction 1 - x upper of the system. Thus, for T** $\to$ **0, we will have:**

$$m = x(+1) + (1 - x)(-1) = m_o \tag{5}$$

We note that if $m_o = 0$ **we have that x = 1/2, i.e. we have to average the magnetisation separately in the lower half and in the upper half of the system, as we explained in section 2. Plot the magnetisation versus temperature curve and check that it is discontinuous below a critical temperature. This discontinuity will become more pronounced as the size of the system increases.**

6.1. Dynamics for non-zero magnetisation.

This section discusses the plots in the figure itself.

Figure 22: T=1, 500000 MC steps. Non-zero magnetisation. Each magnetic domain is formed at the equilibrium temperature. The fact that there are more spins of one type than others only affects the size of certain domains.

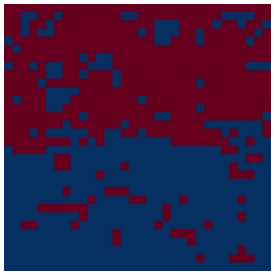


Figure 23: $T=T_c$, 500000 MC steps. In this figure, the transient nature of the critical temperature can be clearly seen, as there are two domain banks, up and down, which are transitioning, as the spontaneous magnetisation is lost, to a state of disor- den, gradually losing the magnetic domains.

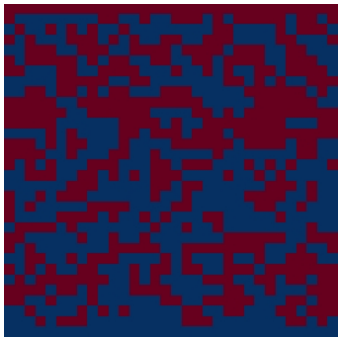


Figure 24: T=5, 500000 MC steps. In this figure one can see the total absence of magnetic domains, there is no spontaneous magnetisation due to temperature and therefore there is total dis-order.

6.2. Non-zero and critical temperature

The magnetisation of the two halves as a function of temperature is shown below.
Two types of plots have been made:

- Using a random mesh for each temperature. That is, a different magnetisation m_o for each temperature.
- Always using the same mesh, thus having the same m_o for all T.

Now, by restricting the mesh to two parts of figure 25, it can be seen that it is indeed discontinuous below the critical temperature, but that it is continuous above it.

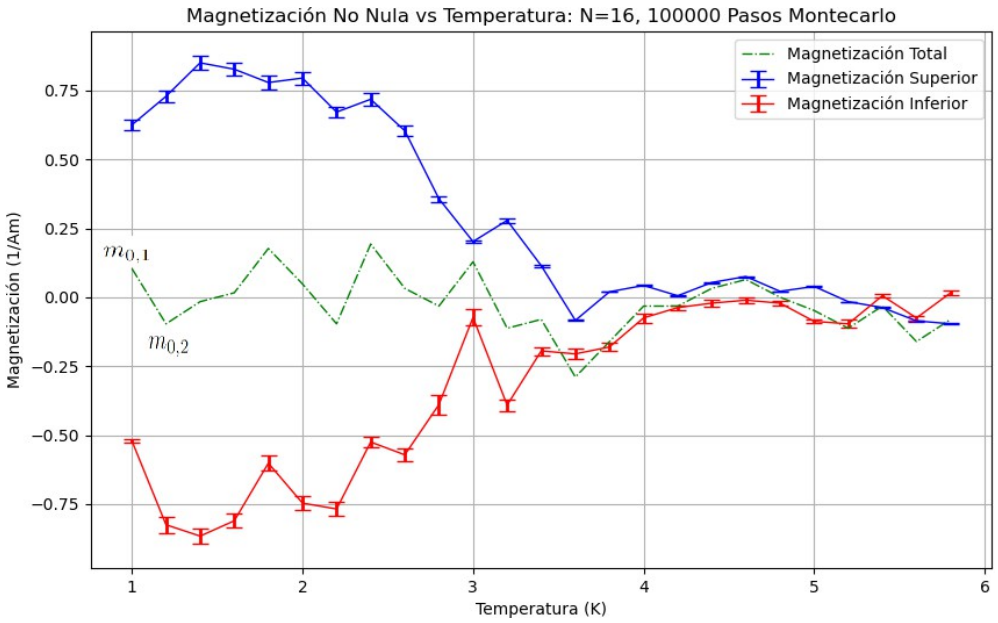


Figure 25: Non-zero magnetisation as a function of temperature for random meshes. N=16. 1000000 MC steps. Confidence 99,74 %.

Now, for fixed magnetization, limited by N x, we have figure 26, where the discontinuity already mentioned before the critical temperature is observed again. As N increases, this discontinuity becomes larger. It is important to note that the T_c changes with the size of the system. [2].

[2]The other sections can be found in the Annex, for lack of space.

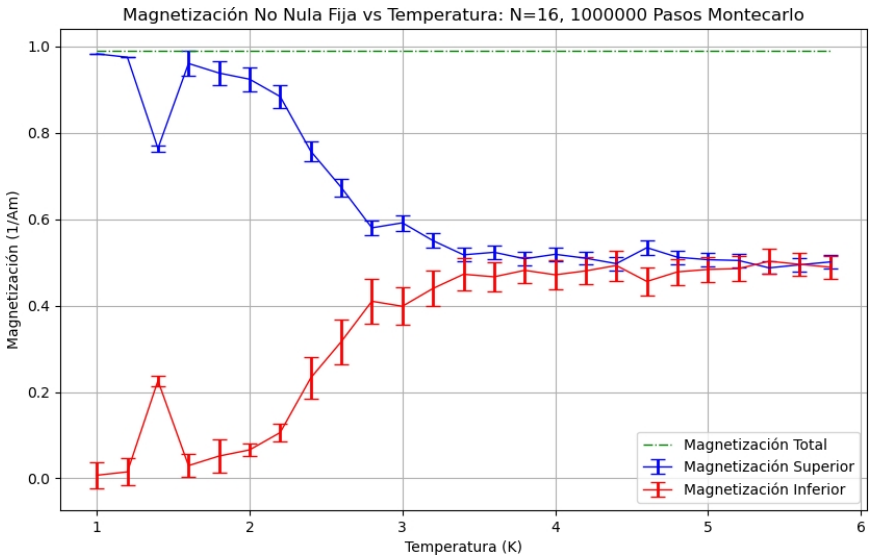


Figure 26: Non-zero magnetisation as a function of temperature for fixed magnetisation grid. N=16. 1000000 MC steps. Confidence 99,74 %.

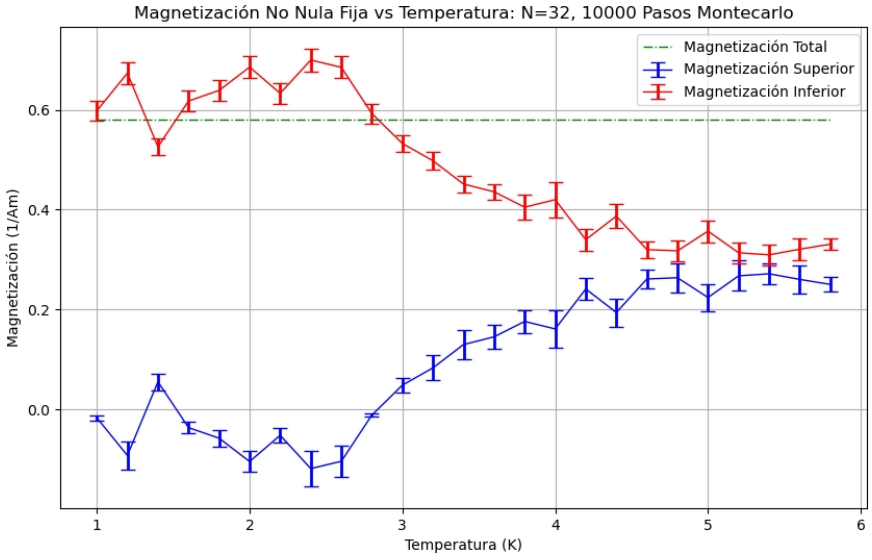


Figure 27: Non-zero magnetisation as a function of temperature for fixed magnetisation grid. N=32. 10000 MC steps. Confidence 95,44 %.

7. Conclusion

The study carried out by Monte Carlo simulations of the Ising model with Kawasaki dynamics explains how temperature affects domain formation and magnetisation in a 2D spin system.

At low temperatures (1 K), the system tends to form well-defined domains, reaching equilibrium after a significant number of Monte Carlo steps.

At the critical temperature, the system exhibits considerable fluctuations, without forming clearly defined domains, reflecting the nature of phase transition at this point.

At temperatures above T_c , spontaneous magnetisation does not occur and the spins are randomly oriented.

These behaviours have been observed through the study of different observables.

For the magnetisation, it can be seen that at low temperatures the values of m per domain are maximal, since the spins are ordered by domains, however, as the temperature increases, the magnetisation decreases, because from the phase transition $at T_c$, the spontaneous magnetisation of the system is lost, and the disorder is maximised.

For the observable energy, it is observed that it rises with temperature. Before and during the critical temperature, energy fluctuations due to phase transition are found. These are finite size effects, negligible when $N \to \inf$.

For the observable +1 spin density, it is seen how, for low temperatures, absolute maxima or minima are found in the y-direction, since there would be large magnetic domains dominated by +1 type spins (maximum value) or -1 type spins (minimum value). At high temperatures, above T_c , quasi-constant +1 densities of value 0.5 are observed, since, due to disorder, the chances of finding +1 or -1 are equal.

For non-zero magnetisation, figures consistent with the theory have been obtained, with continuities in the magnetisation figures prior to T_c , clearly reflecting the phase transition.

A. Density averaged over all columns

In this part of the annex the density is averaged over all the columns, to check the correct functioning of the simulation used: The density *averaged over all the columns* would be, for zero magnetisation, always 0.5 for each type of spirit, and one in total, as shown in figure 28.

For non-zero magnetisation, there will be different values of density in the lattice, as is logical, figure **?**

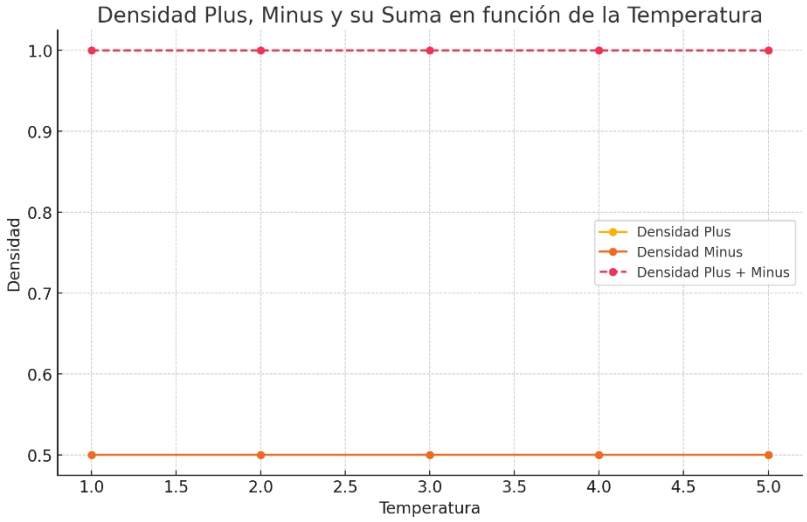


Figure 28: Density averaged between columns as a function of temperature. Zero magnetisation.

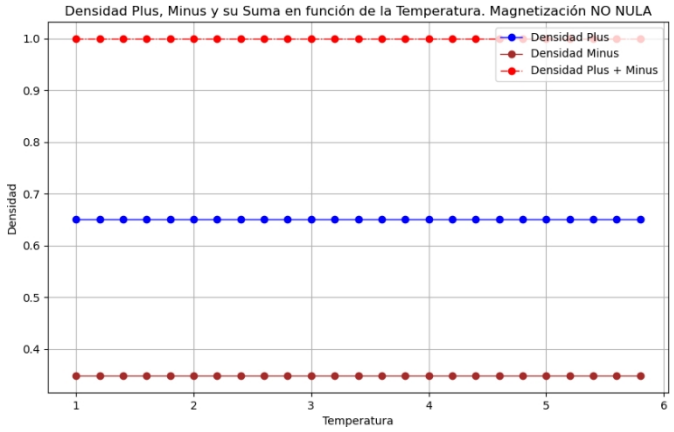


Figure 29: Density averaged between columns as a function of temperature. Magnetization NOT zero.

References

[1] Lavis, D. A., & Bell, G. M. (1999). Statistical Mechanics of Lattice Systems.

[2] Newman, M. E. J. (2013). Computational Physics. Createspace Independent Publishing Plat- form.

[3] For the calculation of observables: https://ergodic.ugr.es/cphys/LECCIONES/ising/ising-SLIDES.pdf