Investigating Phase Transitions Using The Classical Ising Model

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Abstract

The Ising Model is a mathematical model of ferromagnetism [1] that consists of discrete variables representing the magnetic dipole of particles arranged in a lattice. Such variables can have values of ±1 in the Classical Model and any superposition of these in the Quantum model.

Materials undergoing a phase transition below a certain critical temperature will undergo a change in the collective ferromagnetic properties.

The project aims to simulate a 2D ferromagnetic lattice and determine its critical temperature, T_c, above which the lattice is completely disordered and net magnetisation drops to zero.

The investigation shows that :

- The critical temperature of a 2D lattice where a change of state occurs is around 2.3K
- At higher temperatures magnetisation tends to zero (see graph1, graph 2 and third series of snapshots)
- The stable state (all spin up or all spin down) is achieved quicker in the presence of an applied external magnetic field

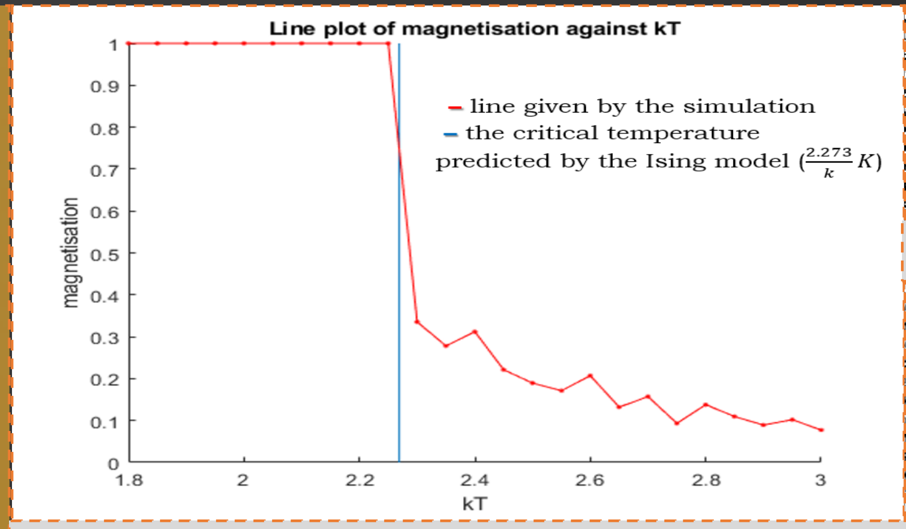


Figure 2: Magnetisation vs kT with lattice size 25x25. For each studied temperature, 10 values were found and the mean value has been plotted. At each measurement, magnetisation was recorded after

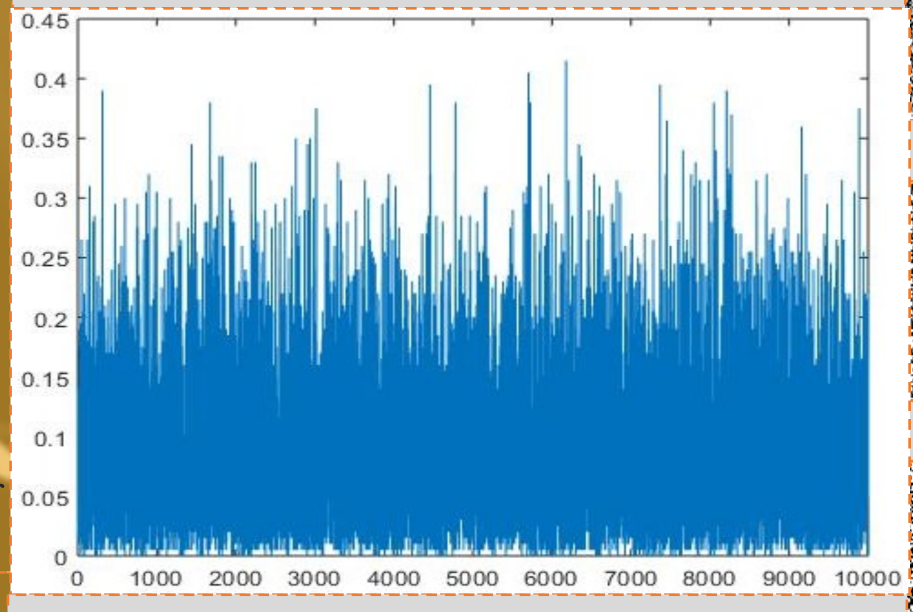
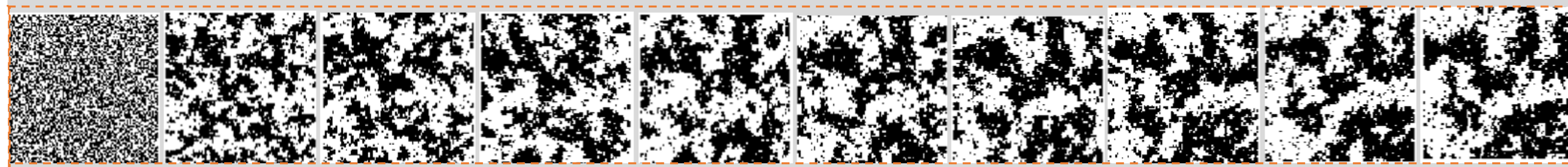
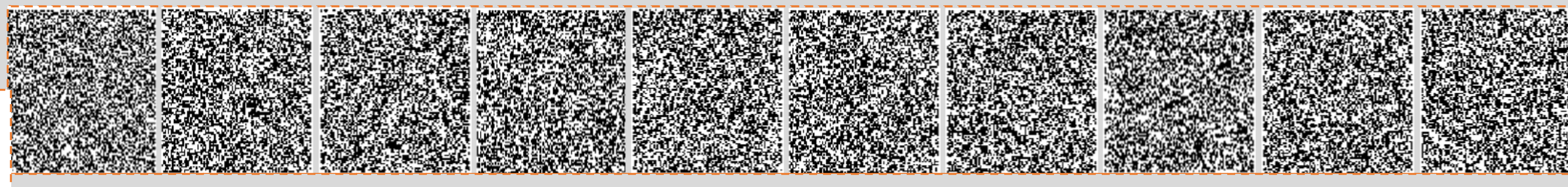


Figure 3: Net magnetisation above T_c for 10,000 different 20x20 lattices after 1,000 iterations. As can be seen, magnetisation rarely jumps above 0.4, even in the presence of domain walls.

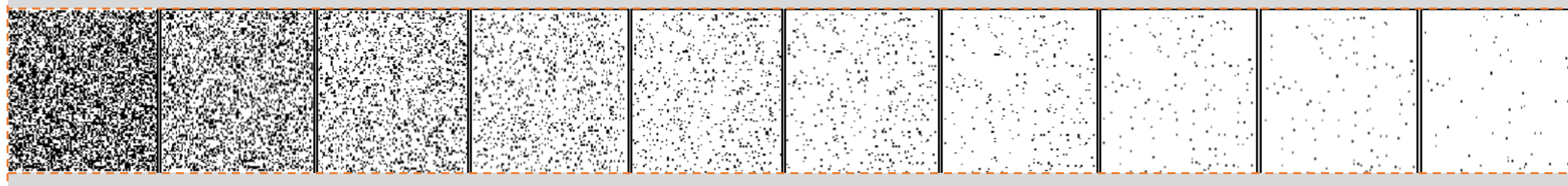
Figure 5: Snapshots taken every 100,00 iterations. Lattice size : 100x100 kBT = 0.0001



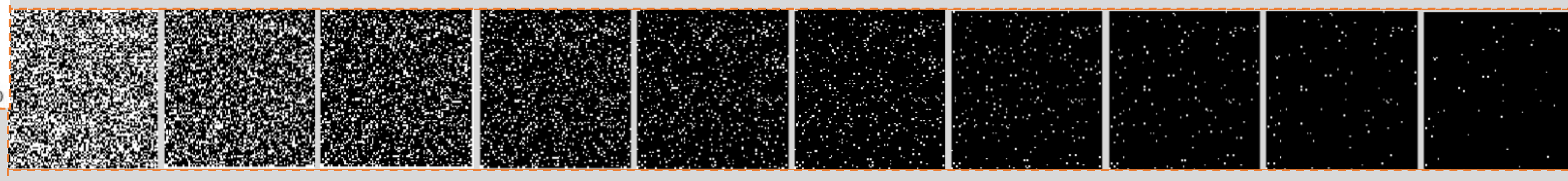
Snapshots taken every 100,00 iterations. Lattice size : 100x100 kBT = 2.270



Snapshots taken every 100,00 iterations. Lattice size : 100x100 kBT = 10



Snapshots taken every 5,000 iterations. Lattice size : 100x100 External Field: 4T kBT = 0.0001



Snapshots taken every 5,000 iterations. Lattice size : 100x100 External Field: -4T kBT = 0.0001

Weiss Domains

When a ferromagnetic material is cooled below its critical temperature it will spontaneously divide itself into small regions, Weiss Domains, where spins within the regions are aligned however the net spins of different regions are not aligned.

This is seen in the data when the net magnetisation of the lattice is neither 0 nor 1 but a number in between.

This makes it difficult to ascertain when exactly a "change of state" has occurred. To mitigate against this, the magnetisation is rounded up to 1 if it is at or above 0.4. This is justified by the large probability of the lattice being uniform, given enough iterations. This is particularly obvious in figure where n is very large. A 1000 iterations

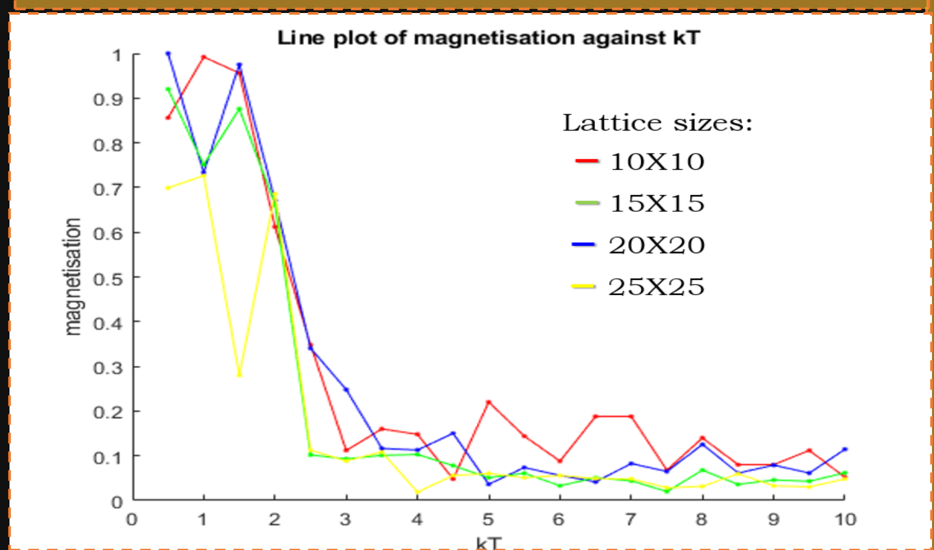


Figure 1: Magnetisation vs kT with varying lattice sizes

Applications

In physics [5]:

1. Describing phase transitions in magnetics
2. Describing "change of physical state" phase transitions
3. Describing lattice binary mixtures
4. Variations of the model can model complex lattices such as fcc or bcc lattices[3]

Outside physics [6]:

The Ising Model can be used to explain properties of living organisms on all scales. Examples include:

1. Analysis of complex genetic models to simulate gene interaction and interdependence
2. Critical transitions occurring from the dynamics of ecological populations. In ecology, long-range synchronization of oscillations in spatial populations may elevate extinction risks.
3. Simulating population dynamics may lead to insights related to cultural segregation, herd behaviour in people as well as social behaviour in other animals. This can be seen in Figure 4 where populations will clump together, forming domains.

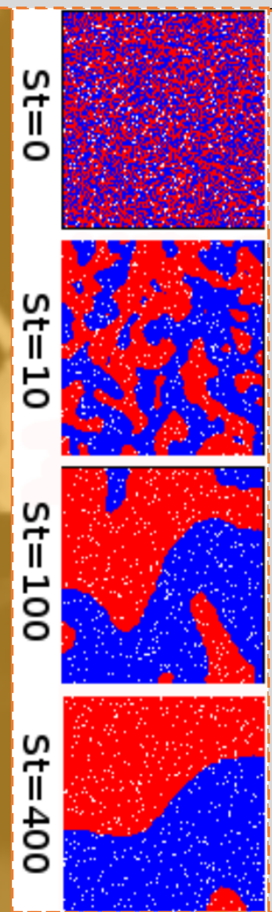


Figure 4: Modelling Segregation with the Ising Model, Temperature in this case will be replaced by tolerance. The figure shows how the 'segregation' develops through the iterations (St) [7]. Note the similarly to the domain behaviour in 2D lattices.

Initiation of programme

Begin with an initial temperature T → Create nxn matrix → Assign random spins (-1 or +1) to each cell

Change of spins in the matrix

Select a random cell and calculate its energy, H_μ which depends on the spins of its neighboring cells: $H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_j \sigma_j$. J is assumed to be one and h is the external magnetic field (see diagram above; the last two sequences have non-zero h). → If the energy calculated (H_μ) is greater than the energy when spins are reversed (H_v) then flip the spin. However, include a probability of $e^{-\beta(H_2-H_1)}$ to change the spin also when if $H_v > H_\mu$, $\beta=\frac{1}{k_bT}$ → Repeat this process by i iteration times

Magnetisation calculation

After the last iteration, calculate the magnetization of the total system which is the sum of the of the average spin around each cell in the array. To normalise it, the sum can be divided by n^2 → Record the absolute value of the normalized magnetization → Repeat part 1, 2 and 3 for different temperatures with increments of 0.5K or 1K

Plotting graphs

Plot graph of magentisation vs temperature

Iteration loop to model the change of states in the matrix

Loop for different temperatures

Conclusions

The project successfully calculated the critical temperature beyond which a phase transition occurs for a 2D lattice with an error of 0.882%. Of course, real lattices are not 2D and so the findings of this project should be applied with care in the real world. While the current code simply sums up the magnetisations of each lattice site[2], this is cumbersome and sets an upper limit on the lattice size. A different approach, looking at the relative stability of each lattice site and summing those up instead, should allow bigger lattice sizes and therefore more reliable data. The project also does not consider the quantum case where spins can be 0,1 or any superposition of these, nor does it apply periodic continuity. This means that the results are only accurate for whole classical lattices that are not part of a bigger lattice where the fringe sites have less neighbours.

References

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