Numerical Simulations of the 2D Ising Model

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Abstract

The aim of this project was the simulate the well known Ising Model from statistical mechanics in 2 dimensions and investigate the thermodynamic properties of such a system. Using python the metropolis algorithm was used to simulate a pseudo-infinite system by use of periodic boundary conditions (PBCS). It was found that systems simulated at temperatures below the theoretical critical/curie temperature of ≈ 2.2691853 K, spontaneous magnetisation of the system was possible in ferromagnetic materials in a first order phase transition. Without the use of the above conditions it was found that no spontaneous magnetisation occurred yet the system still evolved to states of minimum energy. For anti-ferromagnetic materials it was found magnetic spins tended towards anti-parallel states. It was found that an external magnetic field of constant magnitude 5 had no effect on the critical temperature for a system adhering to PBCS, only affecting the equilibrium energy of the system. Systems adhering to a different neighbouring scheme where all immediate neighbours were considered were found a have a higher critical temperature of ≈ 5.3 K.

1 Introduction

1.1 The 2D model

The Ising model is a model of ferromagnetism from statistical mechanics. The 2D Ising model is in fact the only non trivial example of a phase transition that can be worked out with rigorous mathematics [2]. In the model, elements of a lattice are given discrete spin values of ± 1 and interactions are assumed to occur only between nearest neighbours. From here on, the spin value of sight i will be denoted bu σ_i. The Hamiltonian of the system is given by the simple equation [1]

$$H(\sigma) = -J_{ij} \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_j \sigma_j \qquad (1)$$

where $\langle i, j \rangle$ denotes the sum over the spins of the nearest neighbours of a given sight. B denotes the magnetic field in which the material is placed. For the initial simulation carried out in python the magnetic field is taken to be 0, however we will later attempt to investigate the effect of a constant magnetic field. The exchange energy J is assumed to be identical for all of the sights (in fact it is taken to be 1), hence the Hamiltonian can be reduced to

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

for 0 magnetic field simulations, with the J appearing with a minus in front by convention.

Included below is a figure demonstrating the nearest neighbours of a given sight in a 2D square lattice.

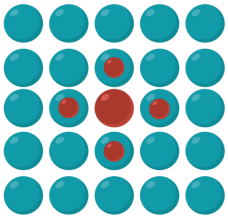


Figure 1: The central red lattice point has its nearest neighbours highlighted in red.

1.2 Periodic Boundary Conditions

One of the condition for the occurrence of a phase transition in the Ising model is that the 2D material be infinite in size. As this is not possible for practical simulations we employ periodic boundary conditions. These allow for sights at the edge of the system to be considered nearest neighbours with sights at the opposite edge of the system. A graphical representation of the idea is given in the graph below.

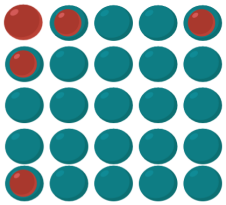


Figure 2: Periodic boundary conditions

Simulations with and without the use of periodic boundary conditions are carried out to show the usefulness of the practice to demonstrate phase transitions.

1.3 Phase Transitions/Spontaneous Magnetisation

One of the phenomena we wish to investigate in the simulation is that of a phase transition. As can be seen from the form of eq(1), for a ferromagnetic material the states of the system which has the least energy are those in which all of the spins are aligned, and of course the opposite is true for anti-ferromagnetic materials. It is found that at a critical temperature, materials may undergo spontaneous magnetisation. At higher temperatures this is not possible as the thermal noise is always too great and the particles in each sight frequently have enough energy to flip their spins even at an energy cost.
The critical temperature for he 2D Ising Model has the theoretical and accepted value

$$T_c \approx 2.2691853 \text{ K}$$

and is derived from the Kramers-Wannier duality [2]. For a proof of the existence of spontaneous magnetisation in two dimensions see "Huang, Kerson: Statistical Mechanics, Chapter 12".

1.4 Calculated values

The main quantities we wish to extract from our model after the simulation has been run is are the

1. Energy
2. Magnetisation

3. Heat Capacity
4. Magnetic Susceptibility

The energy is calculated as in eq (1), with the magnetisation defined as the average value of all the spins.

$$M = \frac{1}{N}\sum_{i=1}^{N}\sigma_i \tag{2}$$

Heat Capacity
The specific heat capacity is given by a known formula from statistical mechanics

$$C_v = \frac{\sigma_E^2}{kT^2} \tag{3}$$

where σ_E^2 is the variance of fluctuations in E. It is worth noting here that in using natural units during the simulation I set the vale $k = 1$

Magnetic Susceptibility
This is calculated similarly to the specific heat capacity and is defined as

$$\chi = \frac{\sigma_M^2}{kT} \tag{4}$$

1.5 Ferromagnetic Materials

The usual assumption when one is discussing the Ising model is that a ferromagnetic model is being discussed. Ferromagnetic materials are those in which neighbouring sites tend toward the same spins. In fact Ising models can be characterised by the sign of the interaction term J.

$J > 0 \rightarrow$ Ferromagnetic
$J < 0 \rightarrow$ Anti-ferromagnetic
$J = 0 \rightarrow$ Non-Interacting

Ferromagnetic materials tend towards neighbouring sights adopting parallel spins whilst ferromagnetic materials do the opposite, as illustrated below.

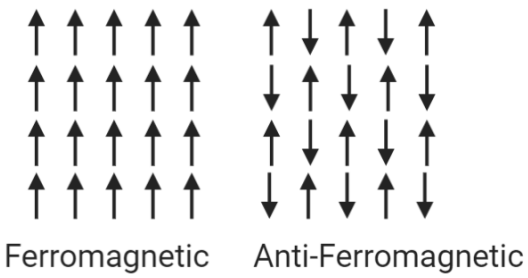


Figure 3: Positive or negative J leads to different tendencies

In terms of the simulation we give ferromagnetic materials a positive interaction energy J, and a negative value for anti-ferromagnetic materials. These values take ± 1 in this simulation.

2 Methods

2.1 The metropolis algorithm

To simulate the Ising model we employ the Metropolis algorithm. This algorithm. The steps of the algorithm are summarised as follows.

1. A square (size N*N) lattice of random states i.e Spin $= \pm 1$ is generated.
2. Periodic boundary conditions are applied to the calculation of the energy of each sight due to the finite size of the system.
3. A sight is chosen at random and its energy is calculated along with the energy of the sight if it were to flip its spin. The difference in these energies is dE.
4. If $dE < 0$, i.e energy is lowered by a spin flip, then the sight flips its spin. If $dE > 0$ then the spin is flipped iff $\exp(-\Delta E/k_B T) > y$, with y a random number on the interval [0,1]

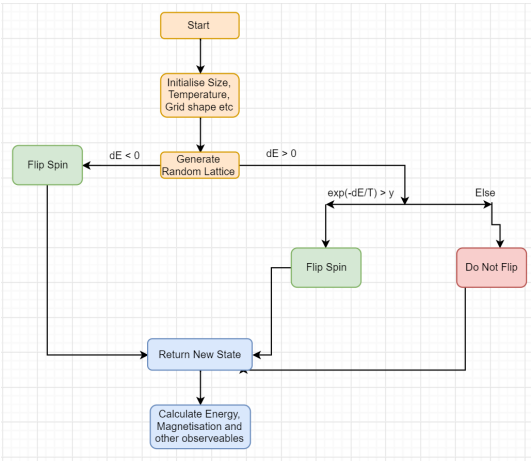


Figure 4: Chart highlighting the main steps of the algorithm

2.2 Code Structure

The problem was simulated by creating a class structure that would create an initial configuration of spins states. Various functions within the class could then be called upon to run sweeps of the simulation and extract data. Within the attached note-

book commented out lines discuss the workings of the code.

2.3 Extracting the data

When extracting the values of energy, magnetisation etc from the model it is first important to allow the model to "warm" up first, as during the first number of sweeps there are large fluctuations in the state of the model before it reaches equilibrium. When extracting data of a 10x10 lattice 75 sweeps were performed to allow the model to reach equilibrium and then 100 sweeps were performed after that, with the average values of energy after each of these sweep taken for out plots.

2.4 Plotting the initial states

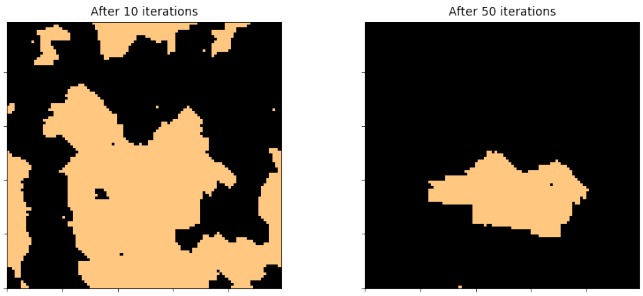
The first problem was to create a 2D square grid of states and find a way to visually represent them. This was done using the "meshgrid" function from the Numpy scientific library as well as the random class from the same library. Refer to the "init" and "grid-figure" functions within the class of the attached Jupyter notebook to see the implementation.

Figure 5: Plot of the initial states using np.meshgrid. Each pixel of the same colour has same spin orientation. Grid is 100x100.

3 Results

3.1 Evolution of ferromagnetic material

The first type of material investigated was a ferromagnetic material. For these types of materials we expected that the spin states will converge to align with one another. This was in fact found to be the case as can be seen below.

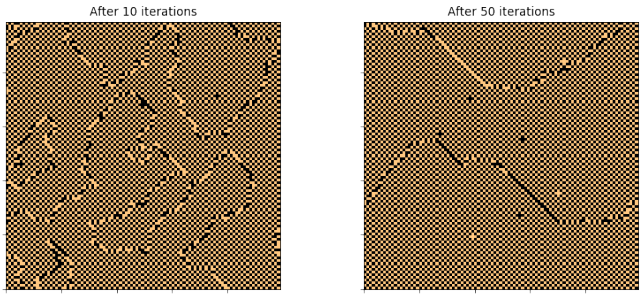


(a) System after 10 sweeps (b) System after 50 sweeps

The above simulations were run for temperature $T = 1$ K, which was deliberately chosen as it is lower than the critical value of $T_c \approx 2.269$ K. If the simulation was ran above this temperature the spins would tend not to align and the configuration would remain in a random state. For a visual aid to picture the evolution above, please refer to the included GIF file attached to submission.

3.2 Evolution of anti-ferromagnetic material

The value of J was then set to -1 to simulate the conditions of an anti-ferromagnetic material. The plots again yielded results as expected as the spins seemed to tend toward anti-parallel states. Again the simulation was run at a temperature of $T = 1$ K.



(a) System after 10 sweeps (b) System after 50 sweeps

Looking above it is seen there seems to be a graining pattern that becomes visible through the anti ferromagnetic model. I suspect this is a product of the fact that the simulation is not a true model of random evolution as the algorithm used checks the candidacy of a single sight to flip spin before moving on to the next sight in the list of sights. Included in the appendix of figures at the end of the report are larger scaled versions of the above plots along with the results for a greater array of iterations.

3.3 Magnetisation Times

A plot was made to demonstrate the magnetisation of the ferromagnetic material at temperatures below the critical/curie temperatures. As can be seen the system magnetises very quickly for simulations run at a temperature of T=1 K and does not tend to converge at all for temperature T=3 K.

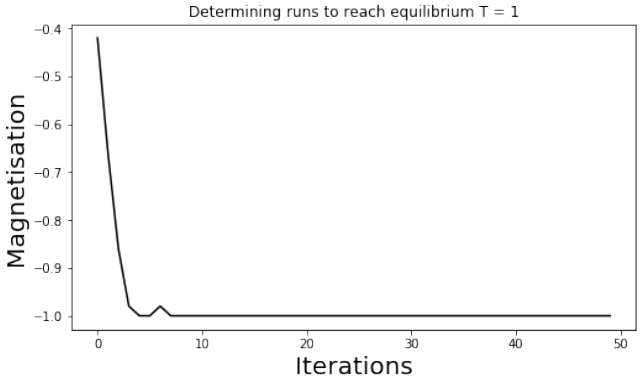


Figure 8: Magnetisation vs Sweeps for T=1 K

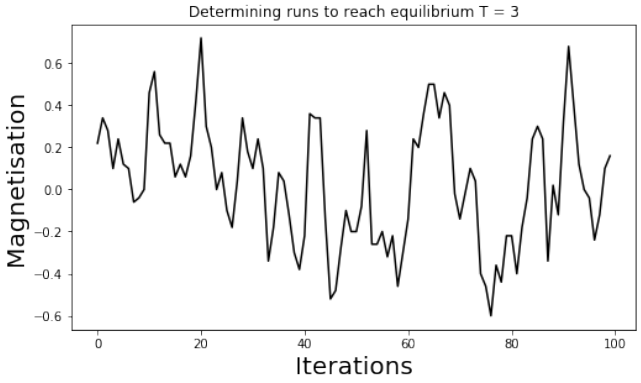


Figure 9: Magnetisation vs Sweeps for T=3 K

For temperatures near the critical point, the system seemed to tend towards becoming magnetised quickly but then proceeded to hover around the point of having all spins aligned.

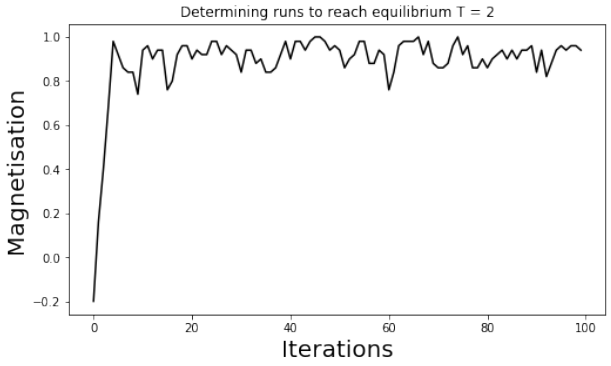


Figure 10: Magnetisation vs Sweeps for T=2

Identical plots were made for the anti-ferromagnetic model and can be seen to converge towards 0 magnetisation, implying all neighbouring spins becoming anti parallel.

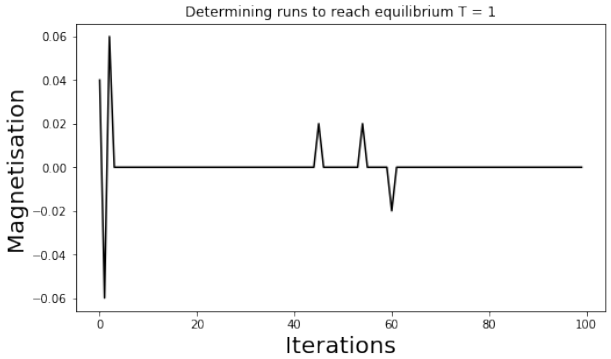


Figure 11: Magnetisation vs Sweeps for T=1

All figures 8 to 11 were taken from simulations of 10x10 square lattice Ising models.

3.4 The Critical point

As previously stated the critical point of the 2D Ising model is mathematically derived as $T_c \approx 2.269$ To investigate if the code produced this value correctly the average magnetisation per site of the ensemble was plotted after a given number of updates to the system. The plot below shows the results.

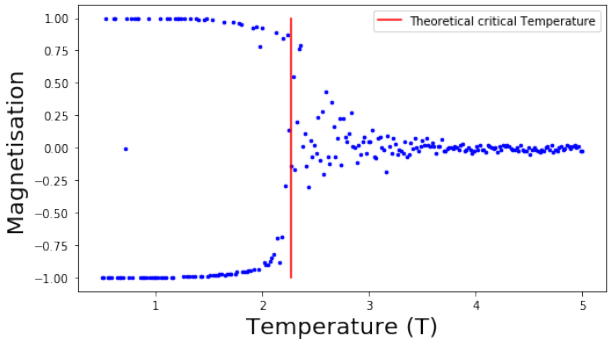


Figure 12: Average magnetisation vs temperature

It is clear from the plot that there is a change in the behaviour of the material when it reaches the region near the critical temperature. It is also worth noting that the simulation shows no preference between the system tending towards all sights becoming spin up or spin down below the curie temperature. It is also evident that the tending of the system towards having all sights spin up or down is independent of temperature, which could be erroneously implied from figures 8 and 10.

3.5 Thermodynamic Quantities

The average values of the heat capacity and magnetic susceptibility of the were recorded for a 10x10 ferromagnetic square lattice and the results are as below. Also included are plots of the average energy and magnetisation at equilibrium. 75 runs of the simulation were allowed to reach equilibrium and the average was taken over 150 subsequent sweeps of the system.

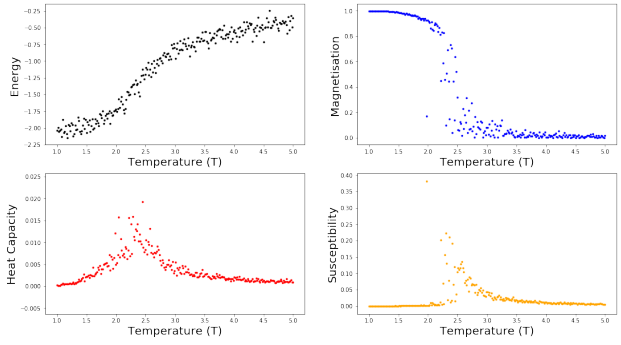


Figure 13: Average energy (black), magnetisation (blue), heat capacity (red) and magnetic susceptibility (yellow) of ferromagnetic material in equilibrium.

From these figures it is also clear of the occurrence of a phase transition occurring near the curie temperature. Whilst difficult to see given the relatively large gaps in temperatures for which the plots were produced, the discontinuity that is visible in the plots of heat capacity and magnetic susceptibility are indicative of a first order phase transition. Continuous plots would have been indicative of second order or higher. Similar plots for the anti-ferromagnetic model were produced and are included in the attached glossary of images.

3.6 Varying Neighbour Schemes

The neighbour scheme was changed in the simulation from nearest neighbours to all neighbours. A visual representation of this is provided in the image glossary. PBCS was still enabled yielding the following graph that shows the effect of the scheme on the critical point.

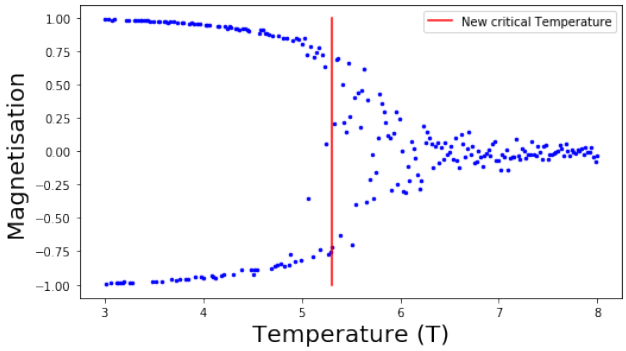


Figure 14: Critical temperature in new neighbour scheme

The system still did spontaneously magnetise but the critical point was found to have increased to ≈ 5.3 K.

3.7 Effect of external field

By applying an external field of strength = 5 T to the simulation, it was found that no effect was had on the critical temperature of the system and it was found to still magnetise below T = 2.269 K. Plot identical to figure 12 was produced to show this effect. Left to the glossary as nothing new to show.

3.8 Finite volume evolution

All relevant simulations were run again but with the periodic boundary conditions (PBCS) turned off, which would mean the behaviour of the finite sized grid could be investigated. Included below is

a plot similar to Figs 8 to 11 which shows this non convergence. All other plots relevant to the simulation without PBCS are included in the glossary.

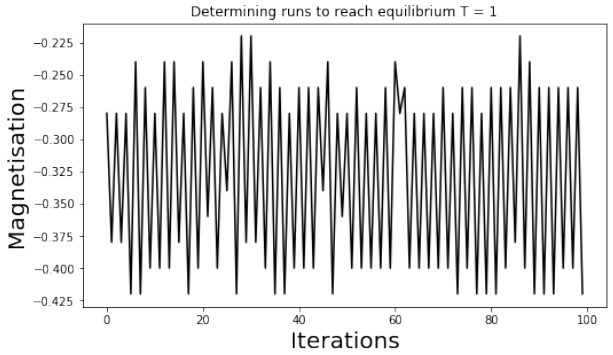


Figure 15: No spontaneous magnetisation.

The magnetisation of the system appears to oscillate randomly about the magnetisation of the system in its initial state (chosen at random).

To investigate the evolution of the finite volume system, this plot was produced next to a similar one tracking the change if energy of the system as the evolution occurred. The evolution seemed to be much more erratic in the finite volume case, nevertheless evolution occurred in a way such that the energy of the system was minimised.

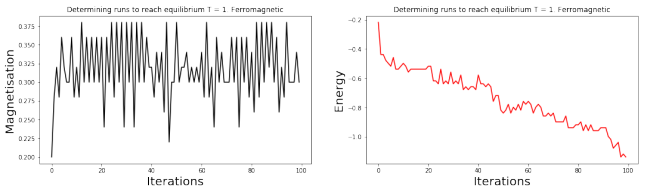


Figure 16: Magnetisation is erratic whilst energy still decreases

4 Conclusions

It was found that for a ferromagnetic 2D square lattice with periodic boundary conditions that that the Ising Model simulated via the metropolis algorithm could spontaneously magnetise if the temperature was set to below the theoretical critical temperature of ≈ 2.269 K.

Ferromagnetic materials were found to also evolve but to do so such that all spins in the system tended to become anti-parallel as expected.

It was found that without the use of periodic boundary conditions the system did not tend towards a state of any particular symmetry with respect to the spins, although it did still evolve such that energy was decreased.

A constant magnetic field was found to have no effect on the critical temperature of a ferromagnetic material, only serving to altar the energy at which the material reached equilibrium.

When a new neighbouring scheme which involved all neighbours was simulated, the critical temperature of a ferromagnetic material with PBCS was found to increase to ≈ 5.3 K, suggesting increasing the number of particles with which one particle can interact increases the critical temperature of such a material.

5 References

[1] Huang, Kerson (1987), Statistical mechanics (2nd edition), Wiley, ISBN 978-0-471-81518-1

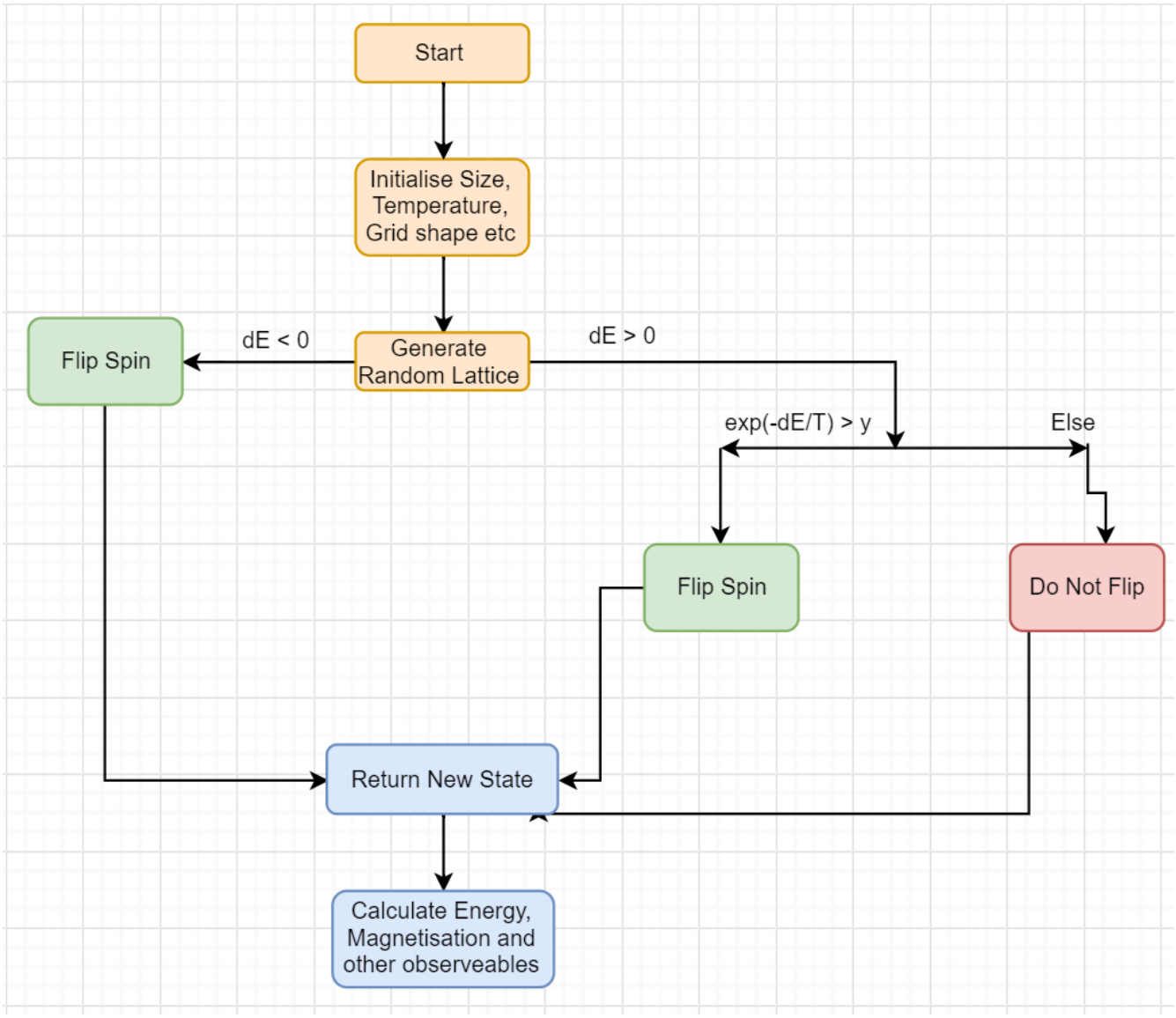
[2] https://www.maths.tcd.ie/bouracha/reports/2-dimensional-ising-model.pdf

[3] arXiv:cond-mat/9511003

[4] Styling of graphs included in Figure 13 were taken from https://rajeshrinet.github.io/blog/2014/ising-model/

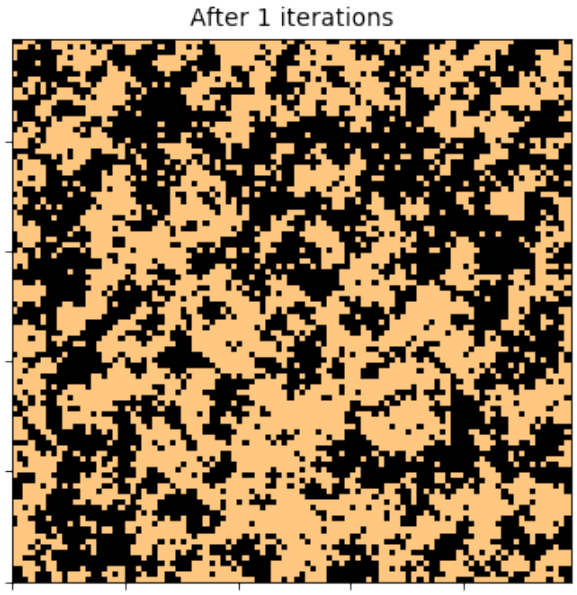
[5] Import tool used to import IsingModel class in Jupyter notebook can be found at https://stackoverflow.com/questions/20186344/ipynb-import-another-ipynb-file

Summary of metropolis algorithm used

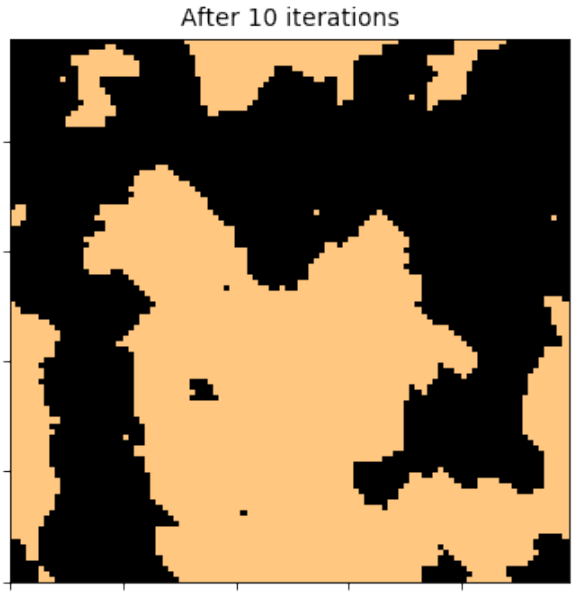


(a) Metropolis algorithm

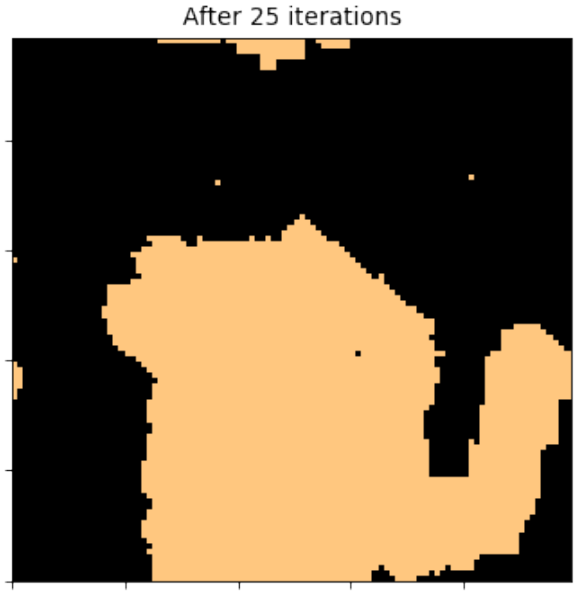
Evolution of the Ferromagnetic system with PBCS



(a) System after 1 sweep



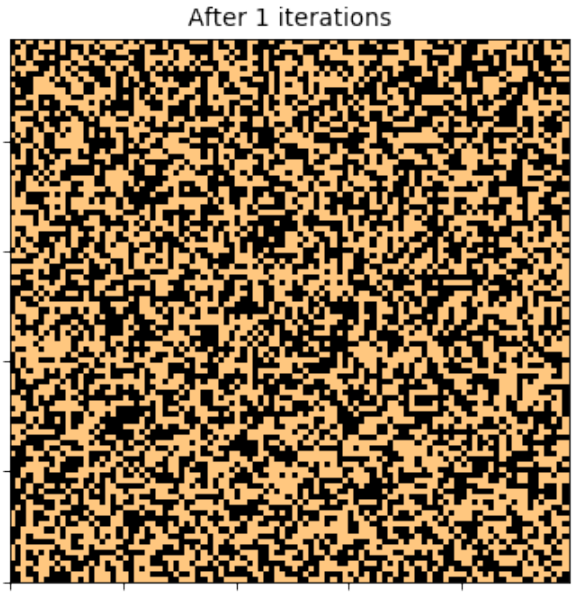
(b) System after 10 sweeps



(c) System after 25 sweeps

(d) System after 50 sweeps

Evolution of the Ferromagnetic system with PBCS off



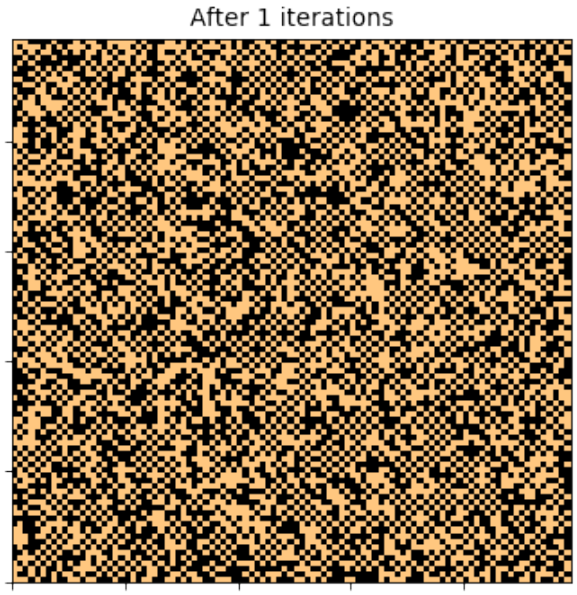
(a) System after 1 sweep

(b) System after 10 sweeps

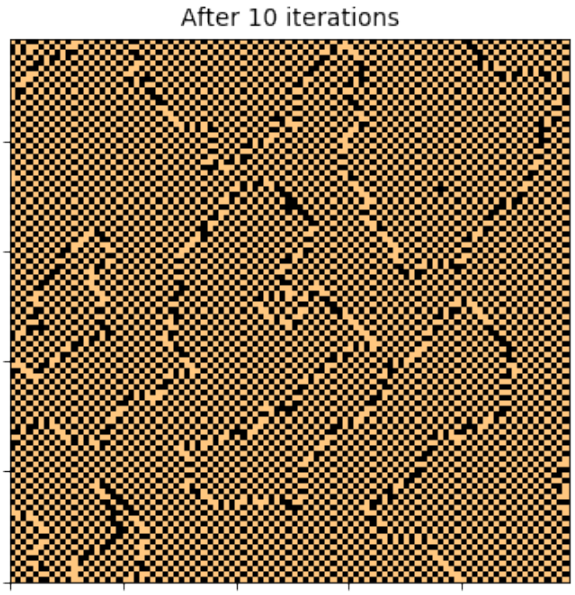
(c) System after 25 sweeps

(d) System after 50 sweeps

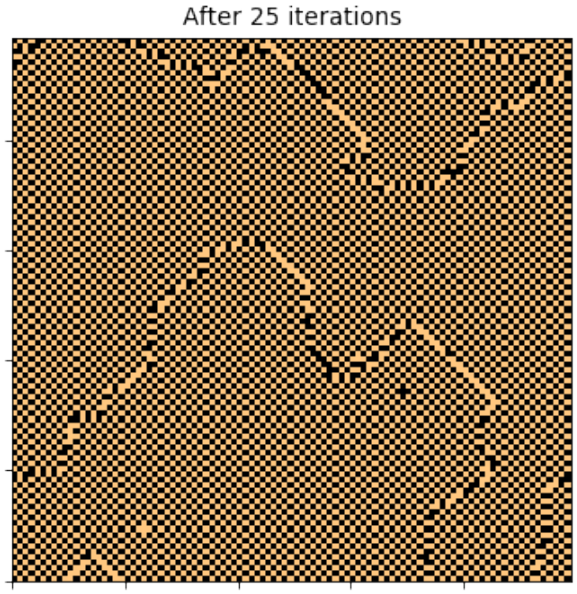
Evolution of Anti-ferromagnetic material with PBCS.



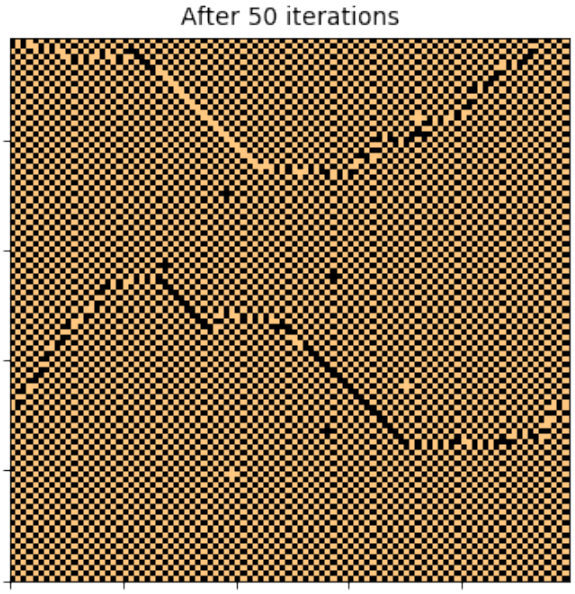
(a) System after 1 sweep



(b) System after 10 sweeps

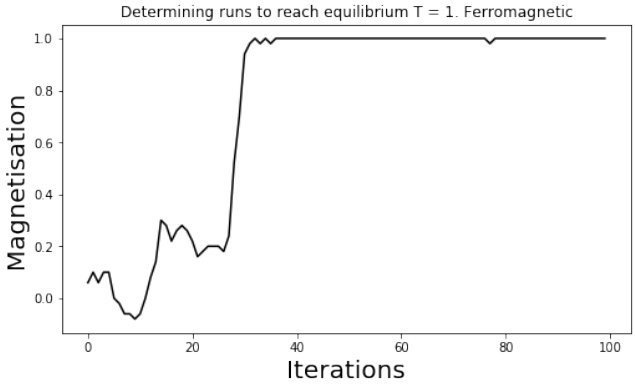


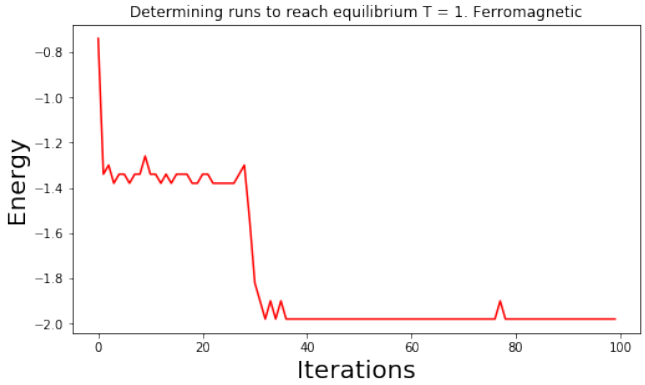
(c) System after 25 sweeps



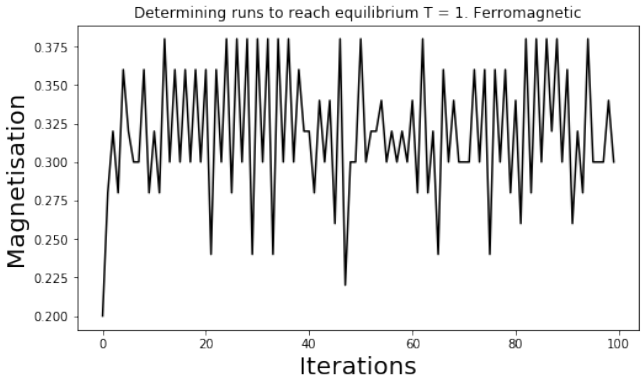
(d) System after 50 sweeps

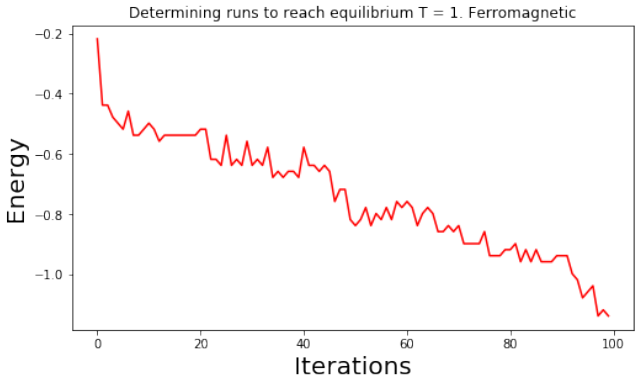
Magnetisation times of Ferromagnetic material with PBCS and without including energy evolution.





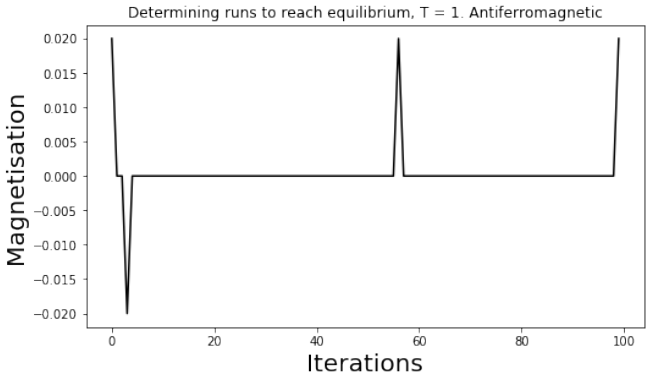
(a) PBCS used.

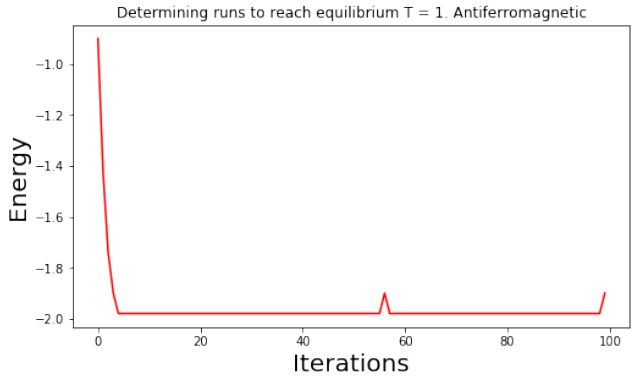




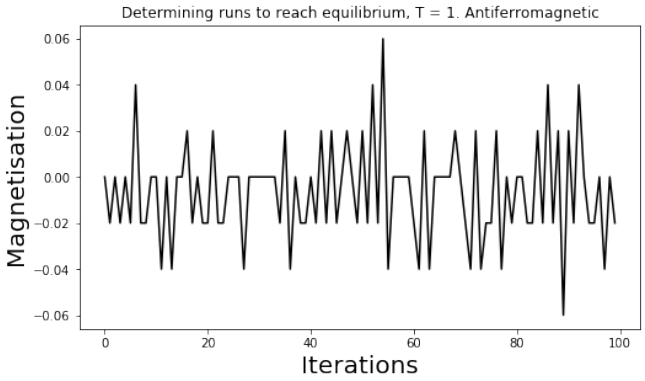
(b) No PBCS can be seen to not converge despite energy decrease

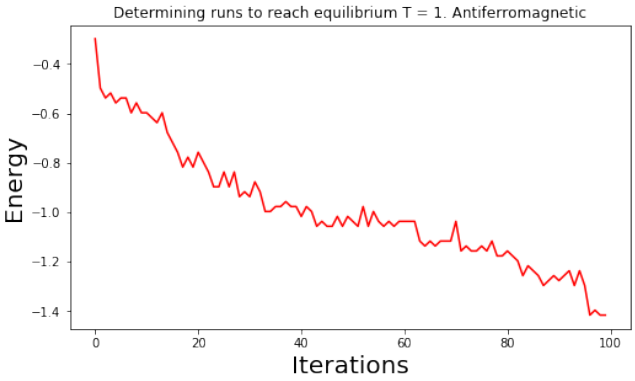
Magnetisation times of Anti-ferromagnetic material with PBCS and without including energy evolution.





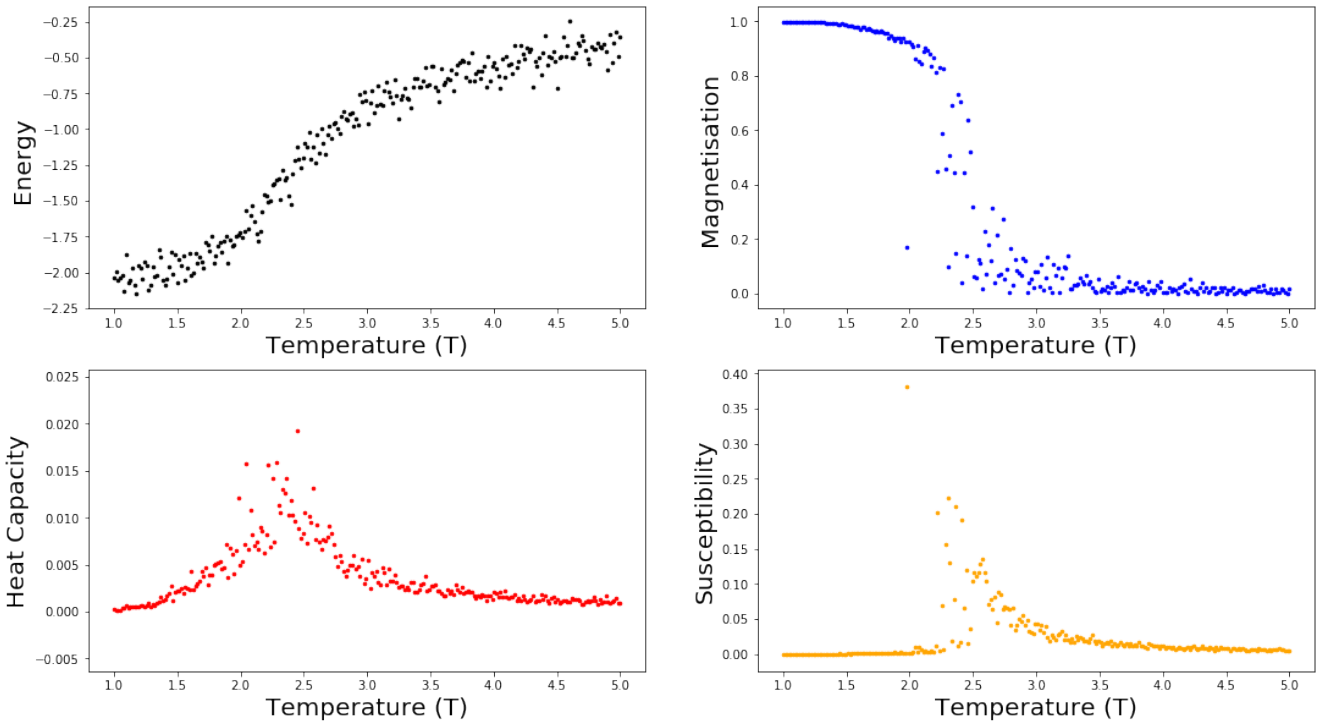
(a) PBCS used.



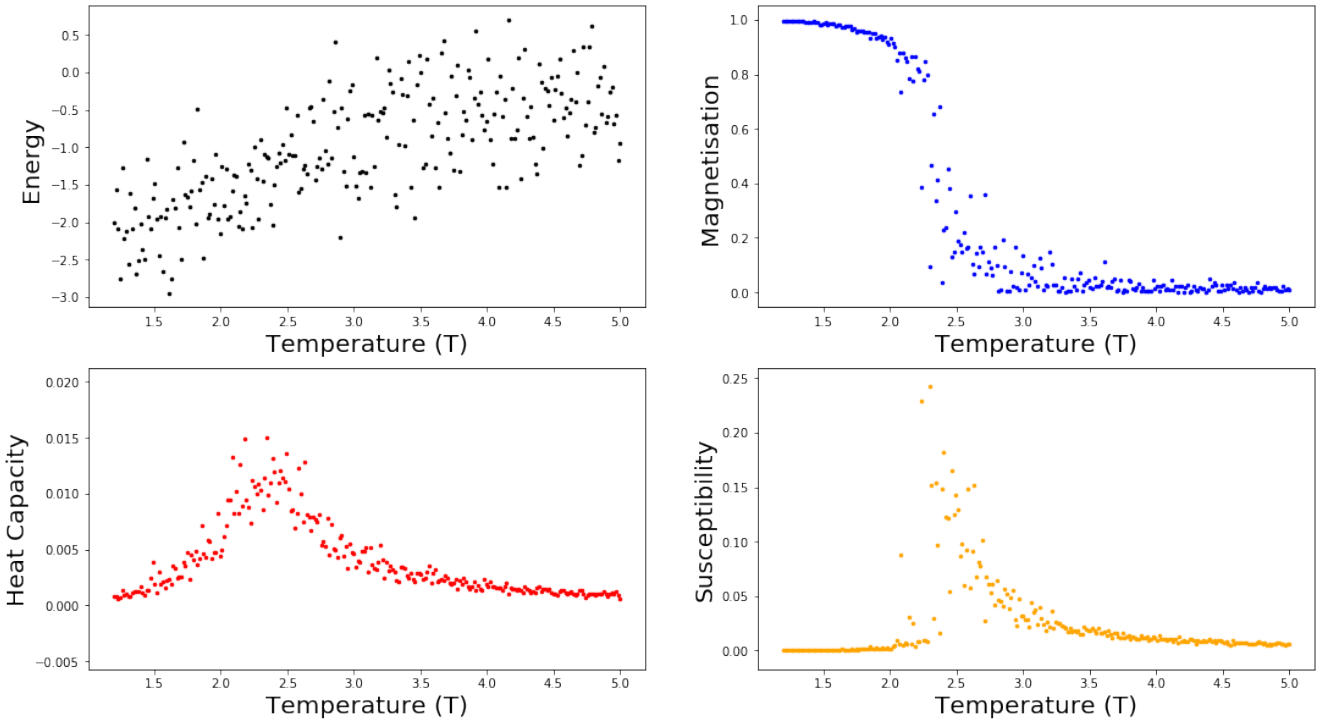


(b) No PBCS can be seen to not converge despite energy decrease

Thermodynamic quantities of ferromagnetic materials with and without PBCS

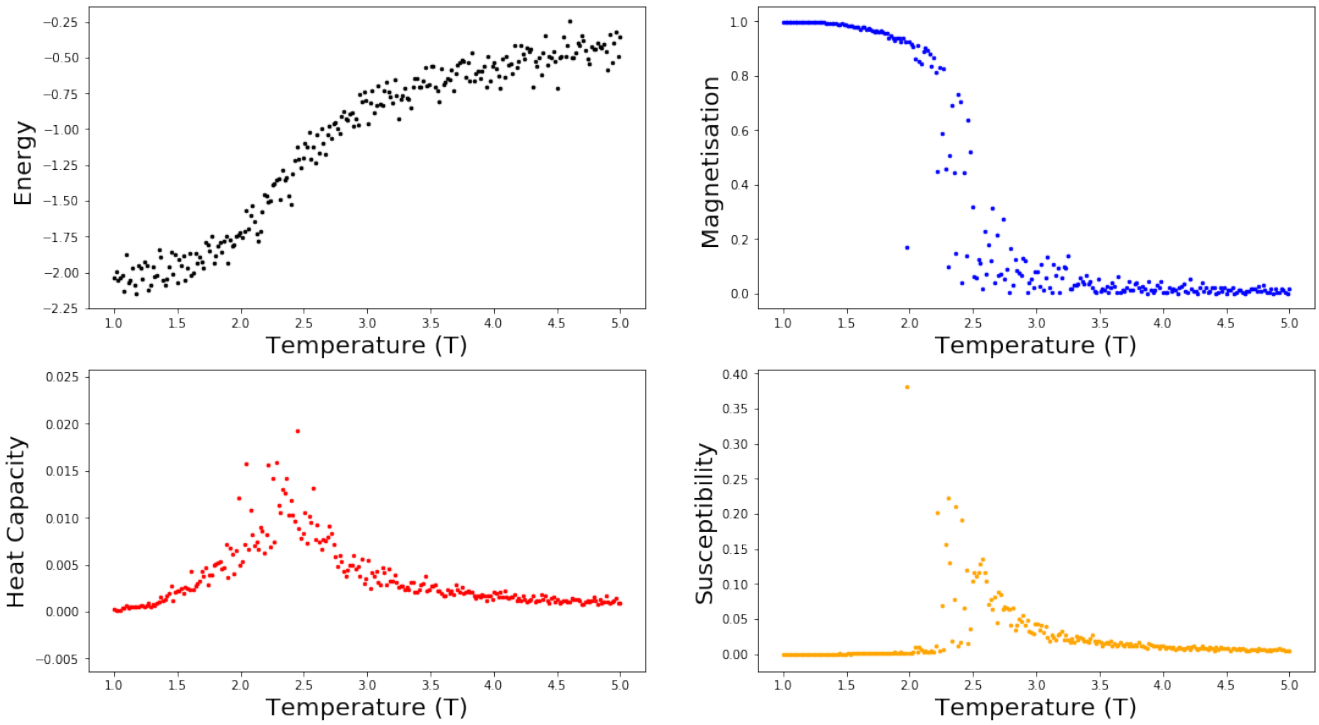


(a) Ferromagnetic PBCS



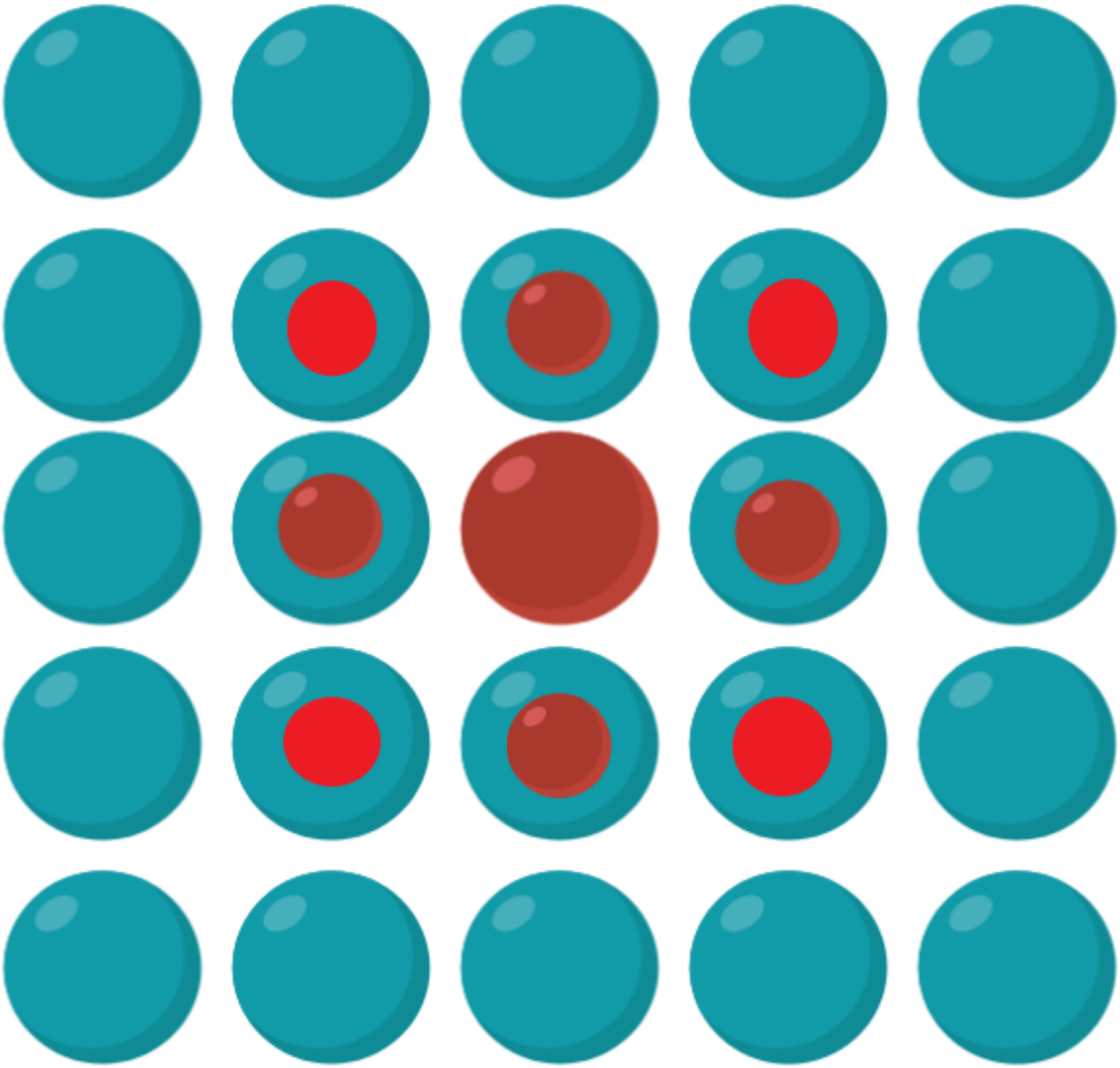
(b) Ferromagnetic no PBCS

Anti-ferromagnetic material with PBCS



(a) Anti-ferromagnetic, PBCS on.

All neighbour scheme investigated that raised the critical temperature



(a) All-neighbour scheme investigated