The 2D-Ising Model

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Abstract

The 2D Ising model for a square lattice was successfully carried out using the programming language, Python. This was achieved by implementing the Metropolis-Hastings algorithm (a Markov Chain Monte Carlo method) into the script to run a simulation of the system under changing conditions. Below the Curie Temperature, as sufficient time passed the initial randomly aligned spin sites in the lattice system settled into that of an ensemble of a single spin. Plots were successfully made for the system observables (average energy, average magnetisation, heat capacity and magnetic susceptibility) as a function of temperature. The relationships found here agreed with theory and were used to determine the Curie Temperature, T_C, to be at a value of $2.45 \pm 0.15(J/k_B)$. A phase transition was confirmed to occur at this point, which can be clearly seen in the plots made. Plots for the average energy and magnetisation show two continuous functions, while plots for the heat capacity and magnetic susceptibility show two discontinuous functions. These functions were expected, with the discontinuities occurring at a temperature equal to that of the Curie Temperature, representing a phase change of the second order. Finally, the magnetisation per site changed from a value of +1 to 0 when T_C was reached, agreeing with theory once again.

1 Introduction & Theory

The Ising Model is a mathematical model used in statistical mechanics to help describe interacting systems. A very good example of such an interacting system would be the electrons inside a magnetic material. Depending on certain properties of the magnetic material, the electrons tend to either align or anti-align with the neighbouring electrons in the material. We can think of these electrons as an infinite array of N lattice sites. This lattice can be of many different dimensions and/or geometries [**1**]. Each site contains exactly one spin that is defined by the spin state σ_i. This can be either spin-up (+1) or spin-down (-1), hence $\sigma_i = \pm 1$. Making the assumption that the lattice spins only interact with its nearest neighbours through a coupling strength J, and that the spins are subjected to a uniform external magnetic field h, the overall energy of a state $s = \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ can be represented as the sum of two terms:

$$E[s] = -J_{ij} \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \, . \tag{1}$$

The first term is a coupling term which is a sum over all nearest neighbour pairs in the lattice. The second term is known as a field term which is a summation over all the lattice sites. The simplest case of the Ising Model is the non-interacting one, where the coupling constant, J, is equal to zero. For interacting systems, the sign of J determines whether the spins prefer to align or anti-align with their neighbours. This gives us two possible states for the system to settle into:

Ferromagnetic State: In this low energy state, the spins tend to align with their neighbours so that they are parallel with each other. This occurs when the coupling strength is greater than zero.

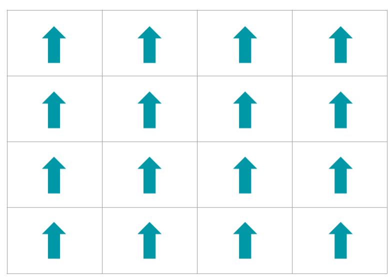


Figure 1: Spin orientation for a ferromagnetic material where $J > 0$.

Paramagnetic State: An anti-ferromagnetic or paramagnetic state is one in which the spins tend to dis-align with their neighbours. This occurs when the coupling strength is less than zero.

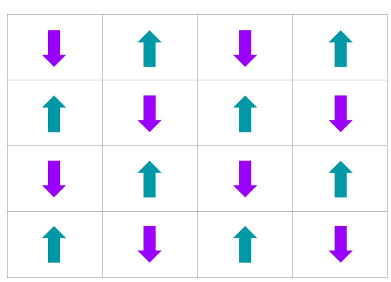


Figure 2: Spin orientation for a paramagnetic material where $J < 0$.

Paramagnetic materials differ to ferromagnetic ones in that their magnetism disappears when the external magnetic field they are subjected to is removed. In contrast, ferromagnetic materials are able to retain their magnetic properties whether the magnetic field is present or not [**2**]. Materials can go from one state to the other as the temperature of the system is changed. It is found that above a certain temperature, known as the **Curie** or **Critical Temperature**, certain ferromagnetic materials make a transition into a paramagnetic state, hence, losing their permanent magnetic field [**3**]. The increase in thermal energy as the temperature increases excites the atoms within the material, causing the electrons to change their spin alignment and anti-align with one another.

For this experiment, a number of starting simplifications were made. Firstly, for the 2D case, the lattice is considered to be square and can be represented by a matrix of size $N \times N$ with periodic boundary conditions. We assume that long range interactions between each site is very weak and so can be neglected. Hence, only the nearest neighbour interactions are deemed relevant. Finally, the energy exchange is made constant ($J_{ij} = J$) and the external magnetic field is also removed ($h = 0$) to reduce 1 to:

$$E[s] = -J_{ij} \sum_{\langle i,j \rangle} \sigma_i \sigma_j \,. \tag{2}$$

1.1 System Observables

The Ising Model can be used to capture important changes regarding some of the physical quantities of a system. The model allows us to investigate how some properties react when the temperature of the system is changed and, in particular, whether or not the system undergoes a phase transition. The observables investigated in this experiment include the **average energy**, **magnetisation**, **specific heat capacity** and the **magnetic susceptibility** of the system. The average energy, $\langle E \rangle$, refers to the expected value per spin of the system. This can be expressed using 2 as:

$$\langle E \rangle = \frac{1}{2} \left\langle \sum_{i,j} E_{ij} \right\rangle , \tag{3}$$

where the factor 1/2 accounts for the fact that each spin pair is counted twice in the summation. As this experiment only takes nearest neighbour interactions into account, it can be shown that for a ferromagnetic system the average energy for a 2D $N \times N$ lattice would be $\langle E \rangle = -J$. This energy will approach 0 as the state of the system changes to that of a paramagnetic one. This change will occur as the temperature reaches and surpasses the Curie Temperature, T_c, which also represents a point of inflection when displayed on a phase diagram or graph of some quantity against the temperature of the system. The average magnetisation $\langle M \rangle$ per unit spin of the overall lattice also refers to the expected value of M per unit spin of the system. This can be expressed as the sum of the whole system's spin divided by the number of sites in that system:

$$\langle M \rangle = \frac{1}{N^2} \sum_{i,j} \sigma_{ij} \,. \tag{4}$$

Finding a value for the magnetisation can be useful in determining whether or not the system has undergone a phase transition. As the system is initially in a ferromagnetic state, the magnetisation of the overall system should be ± 1. However, once the temperature exceeds that of the Curie Temperature, the magnetisation will tend to zero and the system will settle into a paramagnetic state.

Finding a value for the magnetisation also helps in determining the amount of time it would take for the system to equilibrate. When equilibrium is reached, the system converges to ± 1 and each value for the magnetisation is equal to that of $\langle M \rangle$. This allows us to find the minimum number of iterations needed to bring the system into equilibrium, meaning that the efficiency of the algorithm can be increased.

Using equations 3 and 4 to find values for $\langle E \rangle$ and $\langle M \rangle$, other important quantities can then be found. The specific heat, C, refers to the amount of heat per unit mass needed to increase the temperature of the system by 1°C [**3**]. Using the partition function, Z, and the Boltzmann distribution, the specific heat can be found as follows:

$$
\begin{aligned}
C &= \frac{\partial \langle E \rangle}{\partial T} \\
&= -\frac{\beta}{T} \cdot \frac{\partial \langle E \rangle}{\partial \beta} \\
&= \frac{\beta}{T} \cdot \frac{\partial^2 ln(Z)}{\partial \beta^2} \\
&= \left(\frac{\beta}{T} \cdot \frac{\partial}{\partial \beta} \right) \left(\frac{1}{Z} \cdot \frac{\partial Z}{\partial \beta} \right) \\
&= \frac{\beta}{T} \Big(\langle E^2 \rangle - \langle E \rangle^2 \Big) ,
\end{aligned}
\tag{5}
$$

where $\beta = 1/(k_B \cdot T)$ encodes the inverse temperature (with k_B being the Boltzmann constant). In a similar fashion, the magnetic susceptibility can also be expressed:

$$
\begin{aligned}
X &= \frac{\partial \langle M \rangle}{\partial E} \\
&= \beta \Big(\langle M^2 \rangle - \langle M \rangle^2 \Big) .
\end{aligned}
\tag{6}
$$

Although the average energy and magnetisation are continuous functions of temperature, the specific heat and the magnetic susceptibility do not follow this trend. When graphed against the temperature these quantities show a discontinuity at the Curie temperature. This represents a phase transition of the second order as both C and X are second order derivatives (of the free energy) [**6**].

2 Methodology

This experiment was carried out using the programming language Python. The main component that was implemented into the Python script is called the **Metropolis-Hastings** algorithm, a Markov Chain Monte Carlo method used for producing samples from distributions that are generally hard to obtain samples from [**4**]. Monte Carlo operations refer to the wide range of numerical methods which use repeated random sampling to reach the results needed [**5**]. Markov chains are used to model random processes in a statistical way. This chain refers to a sequence of states that are used to average over whose distribution approximates the canonical distribution [**5**]. The Metropolis-Hastings algorithm incorporates these processes through the following steps:

1. A 2D square lattice is generated and filled with random spin sites of value ± 1, representing spin-up and spin-down.
2. A 'sweep' is made throughout the lattice, flipping the spin of a randomly chosen site over the entire lattice.
3. The energy change, ΔE of this flip is calculated:
   - If $\Delta E < 0 \longrightarrow$ accept the flip and do (5).
   - If $\Delta E > 0 \longrightarrow$ is the probability $< e^{-\beta \Delta E}$? If yes, accept the flip and do (5). If no, do not accept the flip and do (5).
4. This process is then repeated for each lattice site until the system reaches equilibrium.
5. Finally, the lattice is returned and system observables are measured and the results collected.

A **flow-chart** for the algorithm was also made to clarify each step. This can be seen in the figure made below:

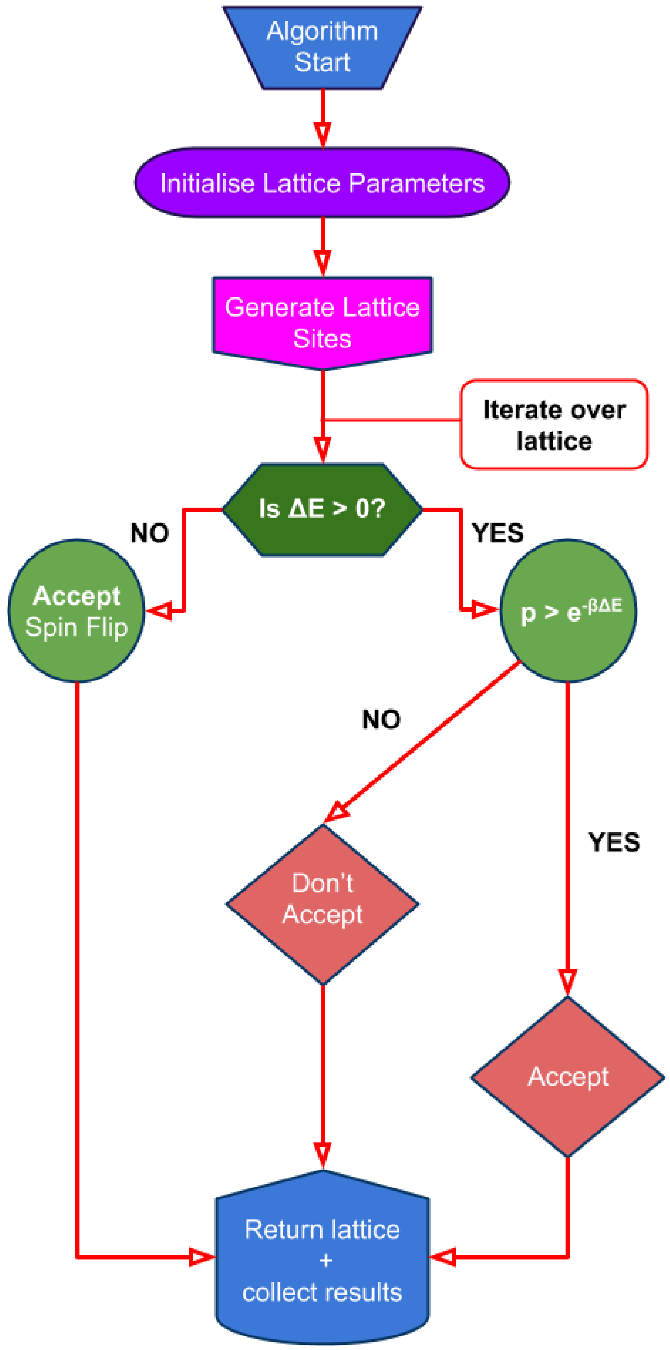


Figure 3: The Metropolis-Hastings algorithm illustrated using a flow-chart.

3 Results & Analysis

The results for each lattice state as it evolved over time was represented using a mesh-grid, with each colour representing either spin-up (+1) or spin-down (-1). The initial state of the lattice consists of disordered, randomly aligned spins. This can be seen in the figure made below:

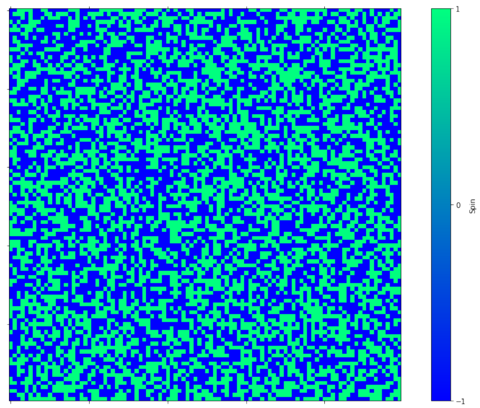


Figure 4: The initial lattice configuration. This example uses a 100×100 lattice size.

'Snap-shots' of the system were recorded as the lattice evolved from its initial state with changing temperatures. This can be seen below:

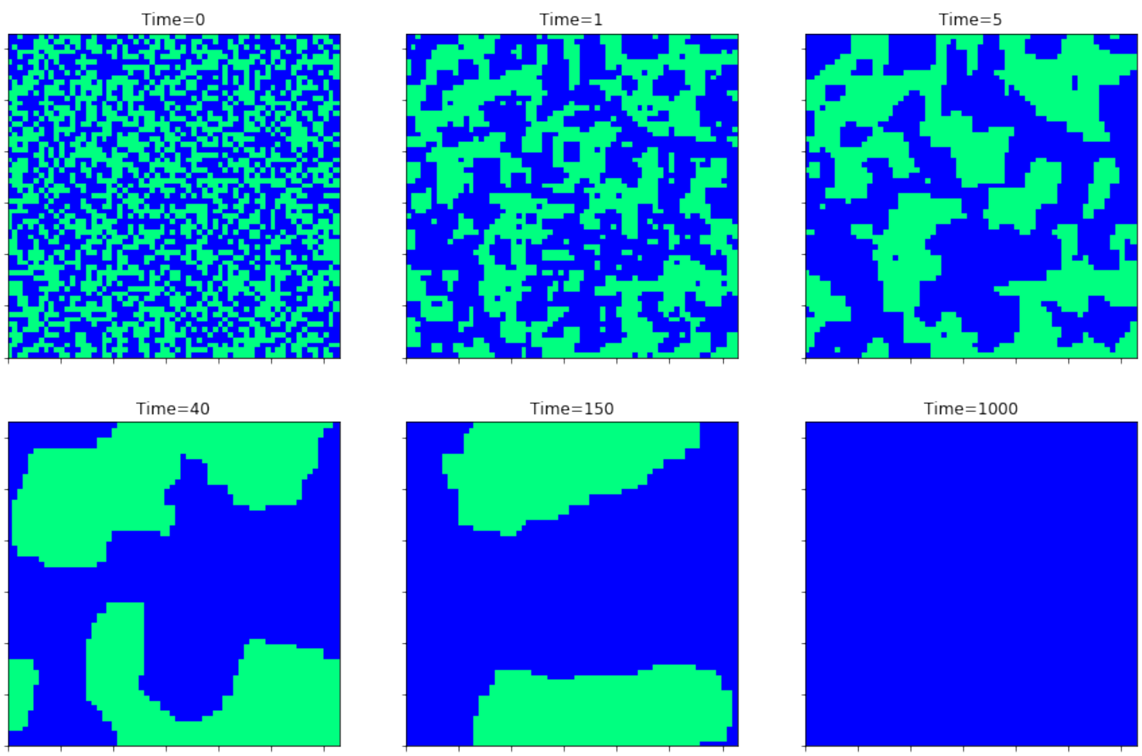
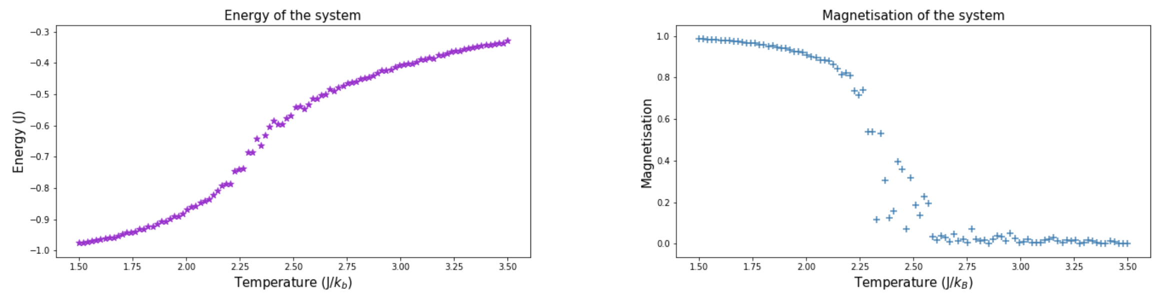


Figure 5: This simulation used a 64×64 lattice system to carry out the algorithm with.

To establish a ferromagnetic state within the lattice system, a sufficiently low temperature was used. The ferromagnetism can be seen in Figure 5 as the time passing increases, with like-spins beginning to assemble or collect together. It can also be seen here that the system equilibriates after enough time has passed. Below

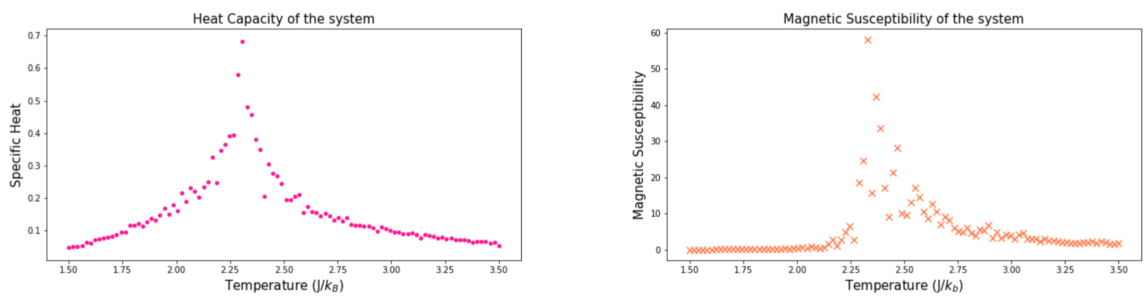
T_c, the system settles into that of an ensemble of a single spin - spin-down in this case. For investigating the observables of the system, a smaller lattice (25×25) was used to shorten the computation time. Plots of how these quantities develop as the temperature of the system changes can be seen below:



(a) Average energy $\langle E \rangle$.

(b) Average magnetisation $\langle M \rangle$.

Figure 6



(a) The heat capacity C.

(b) The magnetic susceptibility X.

Figure 7: N=25 lattice system.

These plots of the physical quantities show an expected relationship in regards to the temperature of the system. A clear point of inflection can be seen in Figure 6a displaying the average energy vs the temperature of the system. This represents a phase transition as the the Curie temperature is reached, which can be seen to be at around $2.3(J/k_B)$. This value for the Critical temperature concurs with the values observed in the plots made for the average magnetisation, heat capacity and magnetic susceptibility displayed in Figures 6b, 7a and 7b, respectively. Once again, the points of inflection found at this temperature in each plot of those observables represents the occurrence of a phase transition in the system. In actuality, T_c was found to be in the range of $2.30 - 2.60(J/k_B)$ between the four plots, giving us an approximation for T_c to be $2.45 \pm 0.15(J/k_B)$.

This transition is also evident in the plot for the average magnetisation vs temperature in Figure 6b as the magnetisation can be seen to jump from a value of +1 to 0, where the Curie temperature is the turning point for this jump. This coincides nicely with the theory, as this sort of jump in the magnetisation should represent a phase change. As expected, the plots for $\langle E \rangle$ vs T and $\langle M \rangle$ vs T show two **continuous** functions. In contrast, the plots for C vs T and X vs T show two **discontinuous** functions, which was also expected. The discontinuities for these two functions occur at a temperature around that of the value found for the Curie temperature, which can be seen in Figures 7a and 7b. This represents a phase transition of the second order, which agrees with theory once again.

4 Conclusions

The 2D Ising model for a square lattice was successfully carried out using Python. This was achieved by implementing the Metropolis-Hastings algorithm into the script to run a simulation of the system under changing conditions. Below T_c, the initial randomly aligned spins in the lattice settled into that of an aligned state as sufficient time passed, as expected. The overall results were found to agree with the theory also, confirming the success of the algorithm in simulating the model.

The plots produced for the system observables (average energy, average magnetisation, heat capacity and magnetic susceptibility) showed expected relationships with the changing temperature of the system. It was found that once equilibrium was reached, the average magnetisation oscillated between that of +1 and -1. However, this value was equal to zero when the temperature surpassed that of the Curie temperature. This occurred as the thermal energy became sufficiently large enough to disturb the 'atoms', causing a change in the alignment of the spins.

The Curie temperature found at the turning point in each plot agreed with one another, confirming this value to be around $2.45(J/k_B)$. This also confirms that a phase transition occurred at this point in the system. This value could be improved by increasing the size of the square lattice as well as the number of iterations made in the algorithm. However, this would require much more computational power to achieve this - or perhaps more concise and efficient code.

The plots conveying $\langle E\rangle$ and $\langle M\rangle$ showed continuous functions with temperature while those for C and X showed discontinuous functions with temperature. Once again this agreed with the theory, further confirming the algorithm's success.

References

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[4] Stephens, M. (2018). The Metropolis Hastings Algorithm. [online] Github. Available at: `https://stephens999.github.io/fiveMinuteStats/MH_intro.html`

[5] Power, S. (2019). Monte Carlo Methods.

[6] Jaeger, G. (1998). The Ehrenfest Classification of Phase Transitions: Introduction and Evolution. Archive for History of Exact Sciences, 53(1), pp.51-81.

Much of the code for this experiment was adapted from Professor Rajesh Singh's blog on the Ising Model. This can be found at `https://rajeshrinet.github.io/blog/2014/ising-model/`.