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PYU33C01 Project: Computational Simulation of the Ising Model

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Abstract

In this computational project, the Metropolis-Hastings algorithm was implemented to obtain solutions to the Ising model. Variations to the model were also carried out and their solutions computed. In varying the temperature of the system, thermodynamic properties such as average energy & magnetisation per spin, susceptibility and heat capacity were obtained and then plotted as functions of the temperature. The Curie temperature of $T_c = 2.3 \pm 0.1$ was determined from the magnetisation, while the ground state energy was determined to be $-2J$ for the 2-D square lattice. For the Triangular Lattice and Hexagonal Lattice, the ground state energies were determined to be $-3J$ and $-1.5J$ respectively. The Curie temperature of both lattices were also determined to be $T_c = 1.6 \pm 0.1$ and $T_c = 3.4 \pm 0.1$ respectively. For the 1-D lattice, it was found that no phase transition occurred for the Nearest Neighbour interaction for a sufficiently strong J. For the long-range $\frac{1}{r^\alpha}$ decay interaction it was found for $1 < \alpha \leq 2$ that a phase transition did in fact occur, but for $\alpha > 2$ there was none.

1 Introduction & Theory

1.1 The Ising Model

In in the field of statistical mechanics, the *Ising model* is an idealised model of magnetic systems. A specialised version of the more general *Z N spin model* or *Clock Model*, the *Ising model* consists of a lattice of discrete variables representing magnetic "spin" σ_j and assigned the values $\sigma_j \in \pm 1$. The assignment of values to each site on the lattice is called the spin configuration. Allowing each spin to interact in the lattice, the energy of a spin configuration is therefore given by the Hamiltonian

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

The notation $\langle ij \rangle$ indicates that i, j are nearest neighbours, J_{ij} is the interaction exchange energy between sites i, j and h_j is the external magnetic field strength at site j. By convention, the signs in the Hamiltonian are negative, which then means that if $J_{ij} > 0$, then the interaction is ferromagnetic. If $J_{ij} < 0$ then the interaction is anti-ferromagnetic.
For the purposes of this project (unless stated otherwise), simplifications to the model were made. Firstly, assuming no external magnetic field , we set$h_j = 0$. We also assume, for the nearest neighbours $\langle ij \rangle$, that J_{ij} remains constant and so $J_{ij} = J$. Therefore, the Hamiltonian simplifies down to

$$H(\sigma) = -J\sum_{\langle ij \rangle} \sigma_i\sigma_j \tag{2}$$

For the 2-D case, which is a simple $N \times N$ matrix with entries of $\pm$1m employing periodic boundary conditions gives a toroidal topology. In the isotropic case $J_{ij} = J$, we can then compare the numerically obtained results from the analytic solution provided by Osengar in 1944 [1] and thus obtain the validity of the results.

1.1.1 Curie Temperature

In certain materials, magnetic properties are observed in the absence of a magnetic field below a certain temperature called the Curie temperature T_c. These are called *ferromagnetic* materials. Prior to the establishment of ferromagnetic properties in these materials, domains are formed. These are microscopic regions that exhibit a strong magnetic field due to the alignment of spins. In the collection of all domains, the spins are typically randomly aligned and so will be non-magnetic. By applying a magnetic field, the domains become 'saturated' and thus align with the magnetic field. In removing the magnetic field, the domains will remain aligned. Therefore, in ferromagnetic materials, spontaneous magnetisation (also referred to as *remanence*) can be observed.
If the material's temperature is raised to above it's *Curie Temperature*, it undergoes a second order phase transition and loses it's spontaneous magnetisation. The material is then said to be paramagnetic, where applying an external magnetic field induces a magnetic field by aligning spins.

1.2 Observables & Thermodynamic Properties

By employing the Metropolis-Hastings algorithm over the lattice, the various thermodynamic observables of the Ising model are then investigated and their properties are explored. Most importantly, the dependence of the observables as a function of temperature are explored. The average magnetisation per unit spin is given by (in the 2-d case)

$$\langle M \rangle = \frac{1}{N^2} \sum_{(i,j)} \sigma_{ij} \tag{3}$$

By iterating over the lattice at a constant temperature and calculating $\langle M \rangle$ for each iteration, we can then compute the number of iterations it takes for the system to 'thermalize' and reach a constant value of $\langle M \rangle$. Plotting $\langle M \rangle$ as a function of temperature, we can also numerically determine when a phase transition has occurred in the lattice and thus calculate the approximate Curie Temperature T_c.
In the case of the isotropic 2-D square lattice with boundary conditions, if the lattice is above the Curie Temperature, the spins are aligned randomly and we expect $\langle M \rangle = 0$. Below this temperature, the symmetry is spontaneously broken and is analytically described by [1,2]

$$M = \left[1 - \sinh^4\left(\frac{2J}{T}\right)\right]^{\frac{1}{8}} \tag{4}$$

from which we can compute the analytical result of $T_c = XXX$. We can therefore compare the obtained results.
The average energy per spin is given by

$$\langle E \rangle = \langle \sum_{\langle ij \rangle} H_{ij} \rangle = \frac{1}{2} \langle \sum_{i,j} H_{ij} \rangle \tag{5}$$

the $\frac{1}{2}$ is included as summing over $\langle ij \rangle$ includes each interacting pair twice. In the ground state (where by $\mathbb{Z}_2$ symmetry either all spins are either ± 1), the value of $langleE\rangle$ is expected to be $-2J$ for a 2-D square lattice using the Nearest-Neighbours interaction model. In evaluating $\langle E(T) \rangle$, we should observe an inflection point at T_c, which signifies that a phase transition occurred. Using these observables, we can derive extra thermodynamic properties of the system, such as the specific heat capacity C_v.

$$\begin{aligned} C_v &= \frac{\partial \langle E \rangle}{\partial T} \\ &= \frac{1}{T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \end{aligned} \tag{6}$$

Similarly, for magnetic susceptibility χ

$$\begin{aligned}\chi &= \frac{\partial \langle M \rangle}{\partial H} \\ &= \frac{1}{T}\left(\langle M^2 \rangle - \langle M \rangle^2\right)\end{aligned} \tag{7}$$

1.3 Lattice Configurations & Dimensionality

1.3.1 2-D Lattice Types

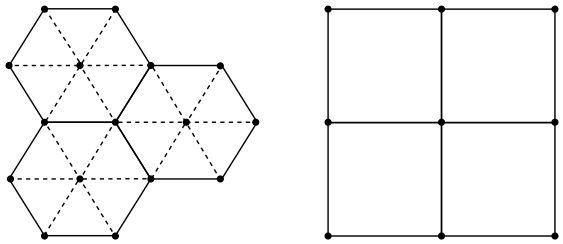


Figure 1: Lattice configurations for the 2-D case. The triangular lattice is the dashed lines, while the hexagonal sublattice is the solid lines

In this report, the underlying lattice structure of the model was changed and the appropriate observables were also calculated. Two other lattices were utilised, the honeycomb/hexagonal lattice and the triangular lattice. In the case of the Nearest Neighbours interaction, the lattice property that affects the observables is the lattice connectivity (ie. how many neighbours each lattice point is connected to). Thus, the ground state energies are expected to be $\langle E \rangle = 1.5, 3$ respectively. The analytical results of the Curie temperatures can be obtained using Dual Lattice methods to get $T_c = XXX$ and $T_c = YYY$ for the hexagonal and triangular lattices respectively

1.3.2 1-D Chain

For the 1-D case, two interaction decay types were considered, that of Nearest-Neighbour (where long-range interactions are considered negligible) and one of long-range decay $\frac{1}{r^\alpha}$, $r > 0, \alpha > 1$. For $1 < \alpha \leq 2$, it was proven in [3,4] that if $J_{ij}\ |i-j|^{-\alpha}$ there is a phase transition at a small enough temperature, there is a phase transition. According to [3], for any $\alpha > 2$, the Free Energy of the system is analytic (which means that the derivatives admit Taylor expansions around a critical point, and so are not discontinuous as is needed for phase transitions) and so no phase transition occurs at finite T.
In Ising's exact solution of the 1-D case with Nearest-Neighbour interaction [6], At any positive temperature the free energy is analytic in the thermodynamics parameters, but a second order phase transition occurs at $T = 0$. An argument is also given by Landau in [7] using Landau Theory. Using this, we get

$$F = E - TS = n\varepsilon - nT\ln(\frac{n}{N} - 1)$$

with F minimised in the limit of $n- > L$. However, since this argument is only useful in the large-scale thermodynamic limit (the reason Landau theory was developed for analyticity in the free energy), in computational results a phase transition may be observed for small values of J.

2 Methodology

The Ising model was implemented in `python` utilising a class structure containing a modular structure so that various parameters of the system could be extended and easily transformed for completing statistics. A `jupyter` notebook is included with a `README.md` to indicate was subroutines are included in the `isingsolver` class.

2.1 The Metropolis-Hastings Algorithm

- A random $N \times N$ matrix of entries with values ± 1 was created using the `np.random.choice()` routine in python, which corresponds to a system with $T \to \infty$. A 'Cold' spin configuration is also implemented, which is just an $N \times N$ matrix with every entry being 1. This corresponds to a system with $T = 0$.
- In order to bypass the thermodynamic limit $N- > \infty$ and increase the accuracy of the results, periodic boundary conditions on the lattice/matrix are utilised. This is done using the modulo operator on the neighbours of the lattice point (i, j) such as $((\mathtt{i}-1)\%\mathtt{N}, \mathtt{j})$
- The first site in the lattice was chosen (this is done so as make the spin magnetisation M converge to a value much faster and so use fewer lattice iterations, but the implementation then is not a true Monte-Carlo method. However, the thermodynamic variables remain unaffected) and the spin is flipped.
  - If $\Delta E > 0$, then the flipped spin was kept.
  - If $\Delta E < 0$, then a random number $n \in [0, 1]$ was computed. If $n > e^{\frac{-\Delta E}{k_b T}}$, then the flipped spin was kept. Otherwise, the flip was rejected.
- This process was repeated for each site on the lattice, called a 'sweep'. The new lattice was then returned for the next 'sweep'.
- Once the appropriate number of 'sweeps' were performed, the appropriate observables were then collected.

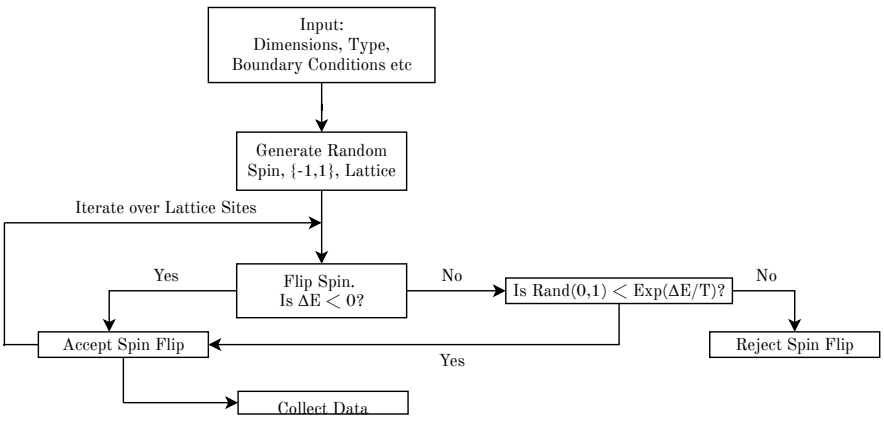


Figure 2

2.1.1 Calculating Thermodynamic Properties

At first, the algorithm was utilised to find the average number of iterations or 'sweeps' for the system to reach equilibrium. The average magnetisation per spin was recorded for each iteration and a graph comparing the value of the magnetisation versus iteration number was produced. This then allowed for an appropriate number of 'relaxation' sweeps, so that the system was 'thermalized' before the observables were gathered.
Functions were implemented in the class structure to enable the gathering of the observables. From those functions, the average magnetisation per spin, the average energy per spin, the specific heat capacity and magnetic susceptibility of the lattice were calculated. Each observable was then calculated over a temperature range (which was done by putting each run at a certain temperature inside a `for` loop indexed by a temperature array). For each property, several graphs were produced (as this is a Monte-Carlo process, so the observables contain some variation in their values) and an average was obtained. The standard deviation of each property was also calculated using the `np.std()` routine.

Lattice Types & Dimensionality

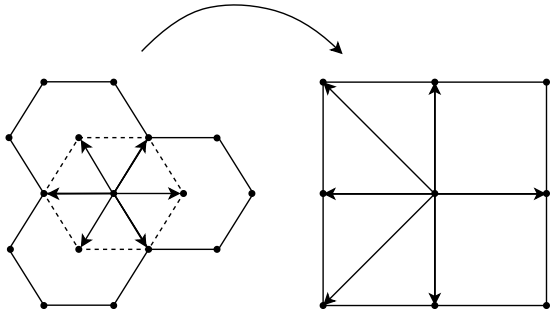


Figure 3: A diffeomorphism between the Triangular Lattice and Square lattice (Nearest Neighbours). This was utilised to reuse working code for the Square Lattice.

Since a natural diffeomorphism exists between every lattice in R^2 [8], it was straight-forward to add the extra nearest-neighbours (or in the case of the hexagonal lattice, remove) to the existing coded representation of the Square lattice.
In a similar manner, it was also straight forward to analyse the Ising model under a change of dimensions by extending the original code of the square lattice so that it works for a number of dimensions.

3 Results

A successful implementation of the Ising model was made. The code was able to sweep through the matrix and perform the correct calculations.

3.1 2-D Lattices

From Figure (3) and Figure (4), it is clear that ferromagnetic properties due to the interaction strength ($J = 1$) are displayed due to the formation of domains. The toroidal topology of the periodic boundary conditions are also clearly evident. However due to the excessive computation time to even do 10 iterations of a 200×200 lattice and accounting for the fact that it will take much longer and many more iterations for the system to reach equilibrium and sufficiently 'thermalize', a much smaller matrix (20×20) was used to complete the computations. This change will mostly affect the steepness and height of the gathered curves (such as the sharpness of the observed peak in the heat capacity), but the values obtained from those graphs, such at T_c should remain mostly unaffected.
In order to determine the number of iterations needed to have the system reach equilibrium, a graph of average magnetisation versus number of iterations was made. This means that from beyond a certain umber of iterations, the average magnetisation stays almost constant and the system was therefore appropriately thermalized. From the included graph (Figure (4)), it was found that the majority of runs for a 20×20 lattice reached equilibrium within 30 'sweeps'. However, it must be noted that it took some systems about 10 times longer to reach equilibrium. This was probably due to the initial random spin distributions being distributed in such a way that made the domain boundaries much stronger.

The thermodynamic observables were then calculated for the 2-D square lattice. For the observables that were dependent on another (ie: Susceptibility and Magnetisation), a small python script was produced, that enabled the calculations of the observables. Graphs were then produced, with a running average of the observables made over several runs of each calculation. The properties of average energy & magnetisation per spin, susceptibility and heat capacity were calculated and then plotted as functions of the temperature. These are included in Figures (5a-5d).
One can observe in Figure (5a) that a very steep inflection point occurs at around $T = 2.3 \pm 0.1$,

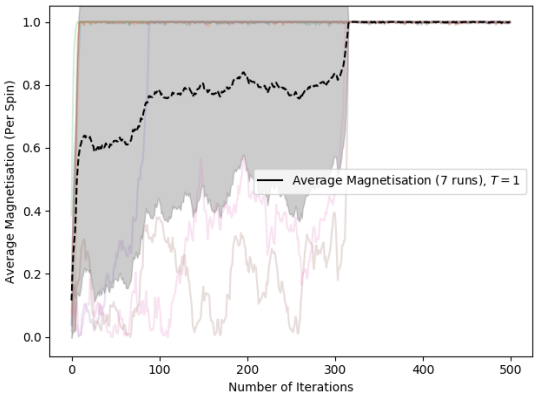
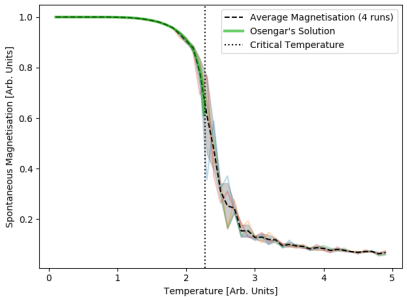
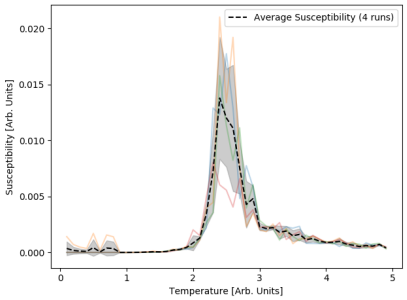


Figure 4: Iterations to reach equilibrium for 20×20 lattice.

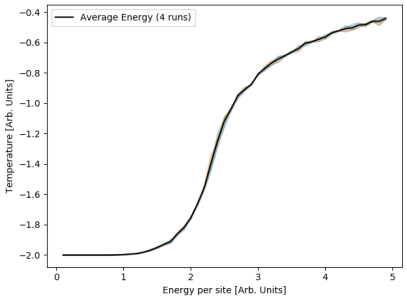
which compares favourably to the analytic results that can be obtained from Equation (4): $T_c = \frac{2}{\ln(\sqrt{2}+1}} \approx 2.269$. The average energy per spin (Figure (5c)) also agrees well with the established theory, as it approaches $-2J$ as T approaches 0. Discontinuities can be observed in Figures (5b) & (5d), but more-so in each individual run than in the running average (which makes perfect sense as taking average values 'smooths' out the discontinuities in the observables). Note that those discontinuities take place about the previously established T_c. This is indicative of a second order phase transition. We can therefore imply that this 2-D Ising model system is indeed ferromagnetic.



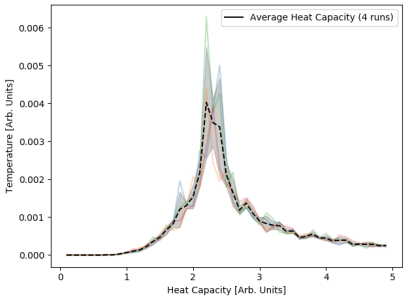
(a) Spontaneous Magnetisation vs. Temperature



(b) Susceptibility vs Temperature



(c) Average Energy vs Temperature

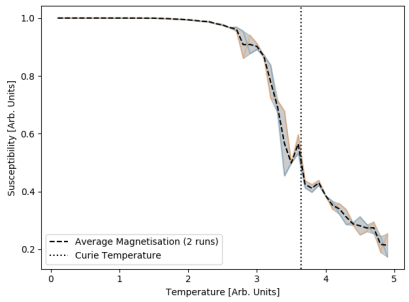


(d) Specific Heat Capacity vs. Temperature

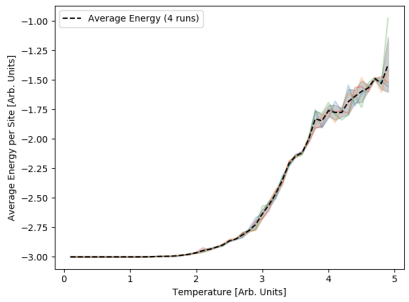
Figure 5: Thermodynamic Properties for a 20×20 2D Square Lattice. Each graph was iterated (for a single run) about 400 times and averaged over

3.1.1 Other Lattice Types

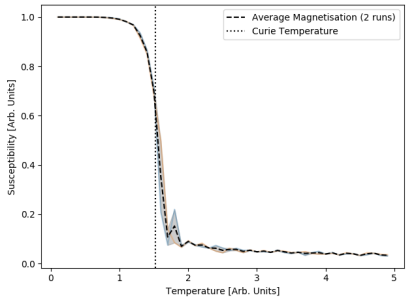
The Triangular and Hexagonal lattices were then investigated. Since connectivity of the two lattice configurations was the only difference, it was relatively straight forward to reuse the code that implemented the square lattice, only changing the Nearest Neighbours configuration. The average energy per spin and average magnetisation per spin are include in Figure (6) below for the two configurations. It can be immediately noted that the ground state energies for the two lattices are as expected: $-3J$ for the Triangular lattice and $-1.5J$ for the Hexagonal lattice. We can also determine the Curie Temperature of the lattices from Figures (6a) & (6c) respectively ($T_c = 3.4 \pm 0.1$ and $T_c = 1.6 \pm 0.1$) and therefore conclude that phase transitions occurred in the two lattices and thus, the two systems are ferromagnetic.



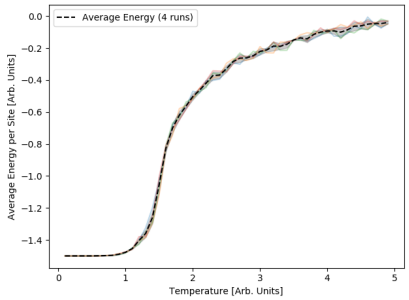
(a) Magnetisation vs. Temperature (Tri. Lattice)



(b) Energy vs Temperature (Tri. Lattice)



(c) Magnetisation vs Temperature (Hex. Lattice)



(d) Energy vs. Temperature (Hex. Lattice)

Figure 6: Thermodynamic Properties for 20×20 2D Triangular and Hexagonal lattice . Each graph was iterated (for a single run) about 400 times and averaged over

3.2 1-D Lattices

For the One dimensional lattice (ie: a chain), two interaction types were investigated

1. Nearest Neighbours
2. Long-range decay: $J_{ij} = |i-j|^{-\alpha}, \quad \alpha > 1, \quad i - j \neq 0$

In the case of the Nearest Neighbours interaction (Figure (7)), there appears to be a phase transition for $J = 1$, which is provably impossible [6,7]. This is because at low temperatures the Metropolis-Hastings algorithm fails to give a physical representation of the system. When $\Delta E < 0$ the spin is flipped (or not flipped) by comparing a random number to the Boltzmann factor $e^{\frac{-\Delta E}{k_b T}}$. But as $T \to 0$ and we have that $\lim_{T\to 0} e^{\frac{-\Delta E}{k_b T}} = 0$. So, in the low temperature regime, spins tend to stay aligned and rarely flip, so $\langle M \rangle \approx 1$. Increasing J to a suitably high strength removes this tendency and so the results stay as expected.
In the long-range decay, the results are as expected. For $1 < \alpha \leq 2$, a phase transition occurs for very low temps ($T \approx 0.1$ 0.2), while for $a > 2$ is is observed that no phase transition occurs. The results are included in Figures (8b)-(8d).

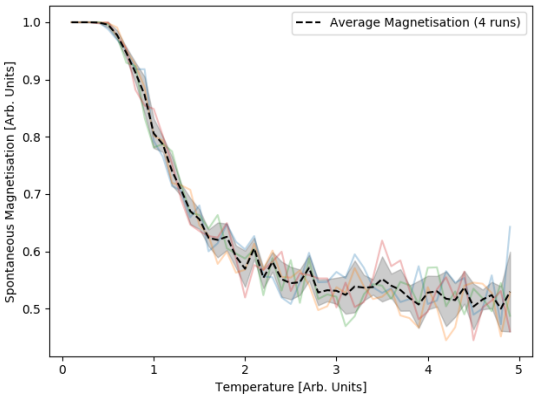


Figure 7: Nearest Neighbour Interaction for 1-D lattice, with $J = 1$

4 Discussion & Conclusion

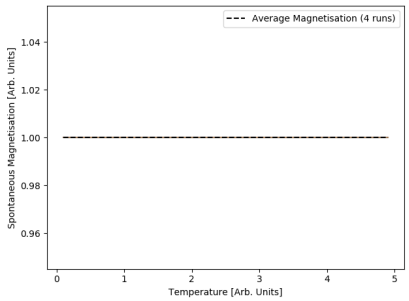
Table 1: Table of results. Not that for the Nearest-Neighbours case, the connectivity of the 2-D triangular and 3-D cubic are the same, thus the observables remain the same

Lattice	Connectivity (N.N)	$T_{c,\text{exact}}$	$T_{c,\text{observed}}$	$\langle E_{\text{ground}} \rangle$
Hexagonal	3	1.519	1.6 ± 0.1	$-1.5J$
Square	4	2.269	2.3 ± 0.1	$-2J$
Triangular	6	3.641	3.4 ± 0.1	$-3J$
Cubic (3-D)	6	3.641	3.4 ± 0.1	$-3J$

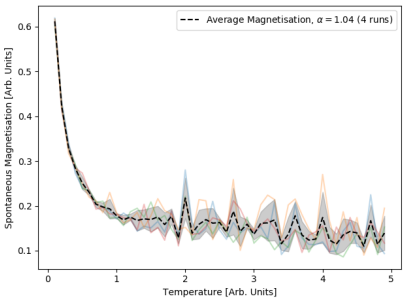
In conclusion, an implementation of the Metropolis-Hastings algorithm was successful, which was then used to simulate the Ising model for various system configurations. The number of iterations to reach equilibrium was determined for several lattice sizes. From this, it was determined that a 20×20 lattice was the most appropriate taking into account computational time versus accuracy of results.
In the case of the 2-D square lattice, it was determined that the system displayed ferromagnetic properties. Spontaneous symmetry breaking was observed when the temperature of the system was below it's Curie Temperature $T_c = 2.3 \pm 0.1$. This is consistent with the analytical results published in [1,2]. Plots of the average energy per spin also indicates that the ground energy state has an energy of $E = -2J$. A discontinuity in the Susceptibility and Specific Heat Capacity plots indicate that a second order phase transition had occurred in this specific version of the Ising model.
For the 2-D Triangular and Hexagonal Lattices, the ground state energies were observed to be $-3J$ and $-1.5J$ respectively. The Curie temperature of both lattices were also determined to be $T_c = 1.6 \pm 0.1$ and $T_c = 3.4 \pm 0.1$ respectively.
For the 1-D case, the computational results perfectly agreed with the published results. For the Nearest Neighbours, a sufficiently strong interaction strength ensured that there was no phase transition in the lattice (as discussed Section 3.2). For $1 < \alpha \leq 2$, a phase transition occurs for very low temps ($T \approx 0.1$ 0.2), while for $a > 2$ is is observed that no phase transition occurs.

4.1 Improvements

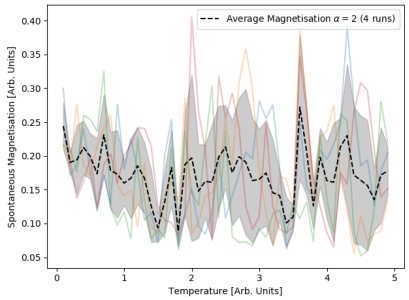
Overall, the results of the model were satisfactory. However, I would certainly would have liked to have made some improvements to the model implementation. The calculation of the results took an excessively long time to compute and using lists in the model would certainly have slowed down the computation by the magnitude of array access per run. A `cython` implementation would also have made the model orders of magnitude quicker.
It is also known that about the Curie Temperature, the Ising Model fails to describe the phase transition reasonably well. Rather than the phase transition being a sharp discontinuity, it



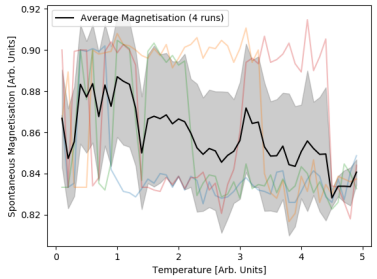
(a) Nearest Neighbour, $J = 20$



(b) Decay, $\alpha = 1.04$



(c) Decay, $\alpha = 2$



(d) Decay, $\alpha = 10$

Figure 8: Average Spin Magnetisation of a 1-D lattice for different interaction types & strengths

follows a steep continuous curve instead. Instead of using `np.arange()` or `np.linspace()` to create variables such as temperature, using a routine that accumulates more points around the Curie Temperature would make those results more accurate.

5 References

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