Numerical Solutions to the Ising Model using the Metropolis Method

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November 23, 2018

1 Abstract

Solutions to a variety of cases of the Ising Model were obtained using the metropolis algorithm. Initially solving for the 2D square lattice case, once the metropolis algorithm was successfully execute it was determined the number of sweeps through the lattice until it was brought to equilibrium. Following successfully bringing the system to equilibrium the average magnetization per site, Average energy per site, heat capacity and magnetic susceptibility were graphed as functions of temperature analysis its properties. From these plots ground energy was determined to be $-2J$ and the Curie temperature, $T_c = 2.28 \pm 0.02 J/k_b$. The affects of varying an applied magnetic field on ferromagnetic and anti-ferromagnetic substances were then investigated which agreed with theory showing a clear hysteresis loop and a first order phase transition where expected in the graphs. The 2D triangular lattice was then investigated, the ground energy was determined to be $-3J$ and the Curie temperature, $T_c = 4.2 \pm 0.02 J/k_b$. The 3D cubic lattice was then investigated the ground energy was determined to be $-3J$ and the Curie temperature, $T_c = 4.6 \pm 0.02 J/k_b$. Following successful application of the methods they were used to investigate the properties a 2D lattice of nickel oxide. The ground state of this system was determined to be $-42 \pm 1 meV$ and the substance was determined to be anti-ferromagnetic.

Contents

2 Introduction and Theory

2.1 Ising Model

The Ising model is a mathematical model used in statistical mechanics to model the behaviour of magnetic systems. The model consists of a number of atomic sites with discrete values, σ ={ -1,1} representing the up or down atomic spin at each site. The Hamiltonian representing such a mathematical model is given by equation 2.1.

$$H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j \tag{2.1}$$

with $\langle i, j\rangle$ representing all combinations of adjacent sites, J_{ij} representing the interactions, μ = magnetic moments due to spin, h_i= external magnetic field applied at each site
If $J_{ij} > 0$ the atomic spins at neighbouring sites will tend to align implying the material being modelled is ferromagnetic whilst if $J_{ij} < 0$ the atomic spins at neighbouring sites will tend to oppose alignment and be a anti-ferromagnetic.

2.2 Partition Function

The partition function is a function that describes a number of the statistical properties of a system in thermodynamic equilibrium. For the systems that we intend to investigate the partition function is given by.

$$Z = \sum_i e^{-\beta E_i} \tag{2.2}$$

with E_i = the energy of microstate i and $\beta = (k_bT)^{-1}$, and k_b = boltzman's constant
Following directly from the this the probability of a particular micro-state occurring is given by

$$P_i = \frac{e^{-\beta E_i}}{Z} \tag{2.3}$$

Then hence taking equation 2.3 the probability that a particular atomic sites spin will flip is given by

$$\begin{aligned} P_{flip} &= \frac{P_x}{P_y} \\ &= \frac{e^{-\beta E_x}/Z}{e^{-\beta E_y}/} \\ &= e^{-\beta(E_x - E_y)} \\ &= e^{-\beta\Delta E} \end{aligned} \tag{2.4}$$

where ΔE = the change in energy from the spin flip

2.3 Calculating Observables

Once the system has been successfully modelled it becomes necessary to calculate a number of observables in order to analysis the properties of our material. The average magnetization per site is given by

$$\langle M \rangle = \frac{1}{\text{No. of sites}} \sum_{i,j} \sigma_{ij} \tag{2.5}$$

where in the case of an NxN lattice, (No. of sites) = N^2.

Then the average energy per site is given by

$$\langle E \rangle = \langle \sum_{\langle ij \rangle} H_{ij} \rangle = \frac{1}{2} \langle \sum_{ij} H_{ij} \rangle \tag{2.6}$$

The specific heat is given by

$$\begin{aligned} C_v &= \frac{\partial \langle E \rangle}{\partial T} \\ &= \frac{\partial}{\partial}(-\frac{1}{Z}\frac{\partial Z}{\partial \beta}) \\ &= \frac{\beta}{T}\frac{\partial^2 lnZ}{\partial \beta^2} \\ &= \frac{\beta}{T}(\langle E^2 \rangle - \langle E \rangle^2) \end{aligned}$$

Similarly the Magnetic susceptibility is given by

$$\begin{aligned} \chi &= \frac{\partial \langle M \rangle}{\partial H} \\ &= \beta(\langle M^2 \rangle - M \rangle^2) \end{aligned}$$

2.4 Curie Temperature

The Curie temperature is the temperature above which materials lose there permanent magnetic properties only to be influenced by magnetization from external magnetic fields(paramagentic) in other words it makes the phase transition from a ferromagnetic/antiferromagnetic material to a paramagnetic material.
The Curie temperature of a ferromagnetic material can be determined by plotting the average magnetization per site of the material as a function of temperature then determining where the magnetization dramatically drops as seen in figure 2.1.

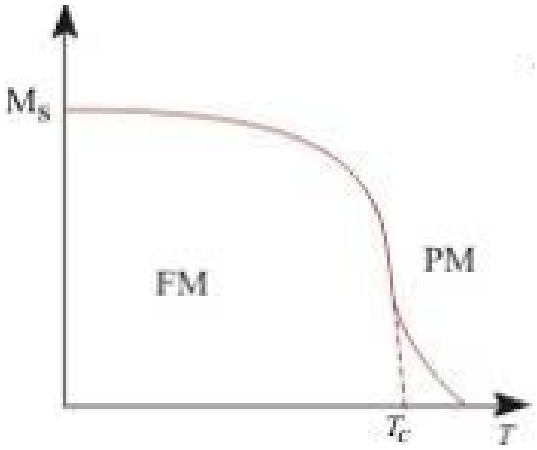

Figure 2.1: sketch plot of average magnetization per site as a function of temperature illustrating Curie's temperature

2.5 Hysteresis Loop

When a magnetic field is applied to a ferromagnetic material they exhibit hysteresis loop which is the pattern traced out by the the magnetization as a function of magnetic field it is irreversible and follows a definite path as seen in figure 2.2. We should be able simulate this effect in our Ising model by varying the value of h_j in equation 2.1.

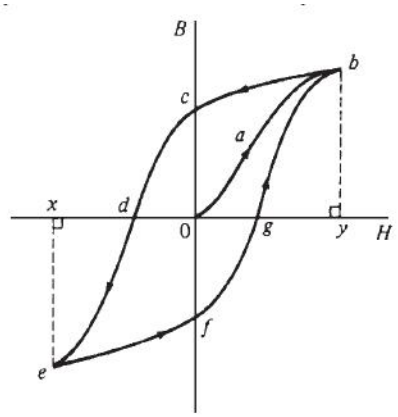

Figure 2.2: Hysteresis loop for a ferromagnetic material

2.6 Phase Transitions

The phase transition is a phenomenon that occurs frequently in the nature it is known as the point at which the free energy density of a substance is no longer analytic this can be seen as a discontinuity in the change of the energy or magnetization(1st order phase transition) or a discontinuity in the slope in the slope(2nd order phase transition when it is graph as a function of a chosen parameter. In the case of magnetic materials this

can occur when the temperature of a material reaches the curie temperature or when the direction of an applied magnetic field changes both of these cases will be analyzed.

2.7 Triangular Lattice

By making alterations to the metropolis algorithm it is possible to apply the algorithm to a 2D-triangular lattice. It has a very similar form to that of the 2D-square lattice except each 2nd row being horizontally off set resulting in each atomic site having 6 nearest neighbours and forming a hexagonal shape as seen in figure 2.3.

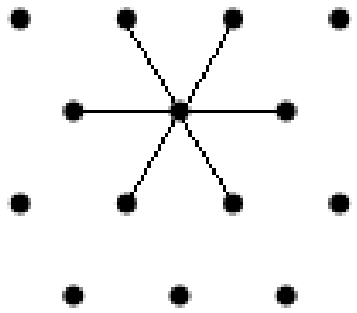

Figure 2.3: Triangular lattice denoting nearest neighbours

3 Experimental Method

3.1 The Metropolis Algorithm

- Set values for parameters, the desired temperature, applied magnetic field, etc.
- Determine a starting configuration by randomly assigning σ= -1 or 1 at each lattice site.
- Sweep through all lattice sites calculating P_{flip} from equation 2.4, then if:
  - $\Delta E \leq 0$, flip spin of lattice site.
  - $\Delta E > 0$ flip spin with a probablilty of P_{flip} by randomly generating a number, $n \in [0, 1]$ and flip if $n < P_{flip}$.
- Sweep through lattice several times until equilibrium is reached.
- Collect statistical information from resulting lattice.

3.2 Periodic Boundary

For an accurate representation of any NxN square lattice we would need a sufficiently large matrix which would require N$\rightarrow \infty$. This is very expensive computationally and there for in order to avoid this and achieve similar results we apply a periodic boundary. A periodic boundary is easily achieved by using the modulo function such that an element at boundary point j's nearest neighbour is (J+1)mod(N)= 0, hence the element at the opposite side of the boundary are treat as neighbouring sites.

3.3 Statistically Approximating Observable

Due to the random nature of the initial state there is fluctuation in the resulting lattice created it was there for necessary to repeat the metropolis algorithm a number of times for each value of temperature, applied magnetic field, etc., calculating the observables outlined in section 2.3 and storing this information. Then having created a sufficiently large data set for each observable calculate the average over each data set. Repeat this for a number of values for temperature, applied magnetic field, etc. to determine how your calculable valuables act as a function of these quantities.

3.3.1 Effects of Applied Magnetic Field

The effects of varying magnetic field on ferromagnetic and anti ferromagnetic substances were then investigated creating an initial square lattice setting the necessary coupling constant. Following this I varied the magnetic field bringing the system to equilibrium and taking readings for average magnetization and energy per unit spin at regular intervals. Then graphed my findings for both ferromagnetic and anti-ferromagnetic cases.

3.4 Triangular Lattice

In the case of applying the Metropolis Algorithm applied to a triangular lattice it will exhibit all the same properties and characteristics as a square lattice except when calculating the sum of nearest neighbours spin which for NxN model used is given by

$$\begin{aligned} nb_{ij} = M[(i+1)\%\ N, j] + M[(i-1)\%\ N, j] + M[(i+(j+1)\%\ 2-(j)\%\ 2)\%\ N, (j+1)\%\ N] \\ + M[i, (j+1)\%\ N] + M[i, (j-1)\%\ N] + M[(i+(j+1)\%\ 2(j)\%\ 2)\%\ N, (j-1)\%\ N] \end{aligned} \tag{3.1}$$

with M=triangular lattice represented as a square matrix; % = mod function
The reason for this can be seen in figure 3.1:

3.5 2D Model of Nickel Oxide

In the proceeding parts the 2D Metropolis algorithm and ising model as outlined earlier is used to simulate a simplified version of the Nickel Oxide as a 2D square a lattice.

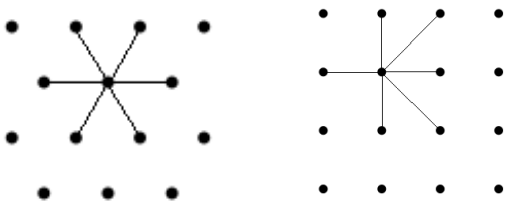

Figure 3.1: Visible representation of triangular lattice nearest neighbours when stored as a square lattice

Nickel Oxide can be effectively described by 2D square lattice with two sets of nearest neighbours, directly next to with interacting energy, J=2.3meV and diagonally next to with interacting energy J=$-21meV$. The Oxygen atoms present have spin zero and there for can be neglected and treated as spin zero sites in the matrix model used. The expected ground state from the system should be, $E_0 \approx 42meV$. As in its ground state energy the first set of neighbours for each atoms will be completely misaligned summing a total energy of zero and then the only contribution to the ground state energy is from the second set of neighbours giving a total interaction energy of $84meV$ then dividing this by 2 to avoid double counting of interactions gives an estimated ground energy of $42meV$.

4 Results and Analysis

4.1 Error Analysis

Due to the statistical nature of the results created and the lack of computational power to create a large enough data set such that outliers become negligible. It there becomes more efficient to calculate the standard deviation of your data set and neglect all values outside of 1 standard deviation of this set before calculating the average and insert error bars to the size of one standard deviation into my plot. By doing so it becomes more clear the nature of the observables in a shorter number of iterations.

4.2 Results

The Metropolis algorithm as outlined in section 3.1 was successfully applied as can be seen from figure 4.1 where black represents spin down and white represents spin up.

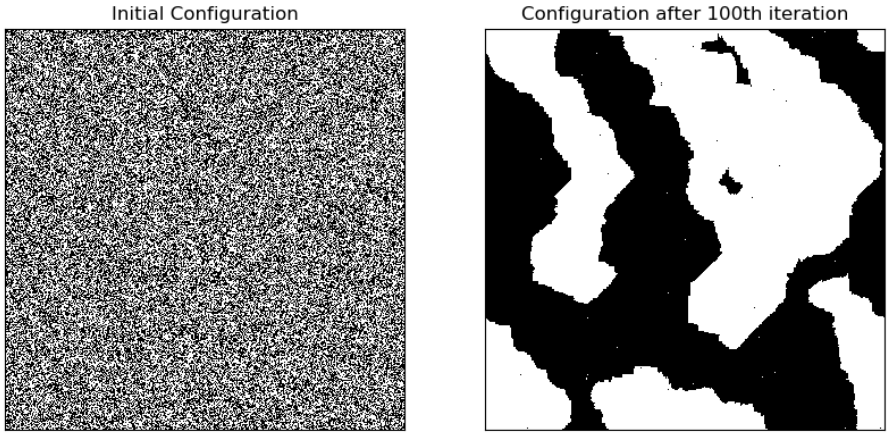

Figure 4.1: Example of Metropolis Algorithm applied 100 times to a 500x500 square lattice

4.2.1 Equilibrium

To determine the number of iterations required for our square lattice to reach equilibrium I plotted the average magnetization per site as a function of number of sweeps this can be seen in figure 4.1.

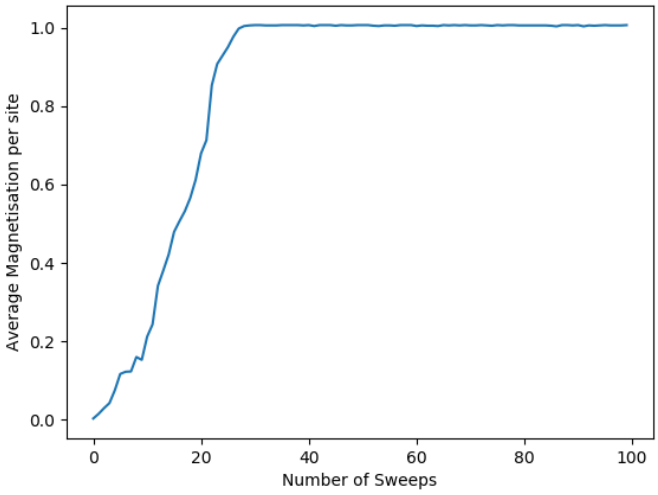

Figure 4.2: Average Magnetization per site as a function of number of sweeps for 50x50 square lattice at T=1J/k_b

As seen from figure 4.2 it takes approximately 30 sweeps for the 50x50 square lattice to

reach equilibrium. Alternatively the number of sweeps required for a 10x10 lattice takes only approximately 25 sweeps were required to reach equilibrium the applying this with the periodic boundary outlined in section 3.2.

Whilst at higher temperatures as seen in figure 4.3 the lattice exhibits a sort of chaotic behaviour(non convergent) in its average magnetization per site suggesting a lack of equilibrium position at higher temperatures.

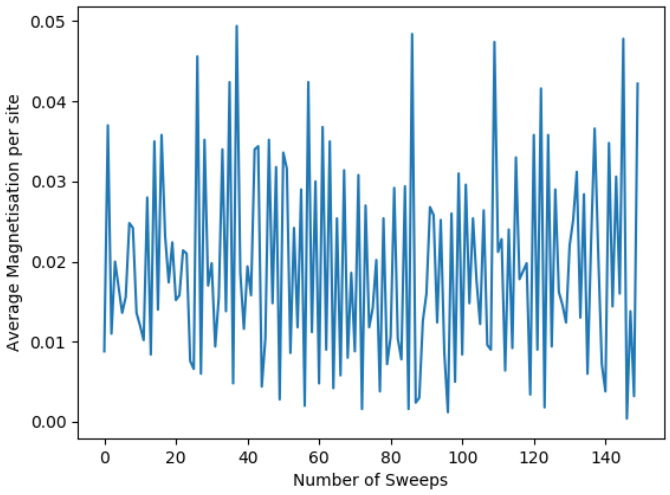

Figure 4.3: Average Magnetization per site as a function of number of sweeps for 50x50 square lattice at T=$10J/k_b$

4.2.2 Calculating Observables

The Figure 4.4 it can be observed that the metropolis algorithm was successfully applied to a number of initial configurations of a 10x10 square lattice and averaged at a number of different temperatures.

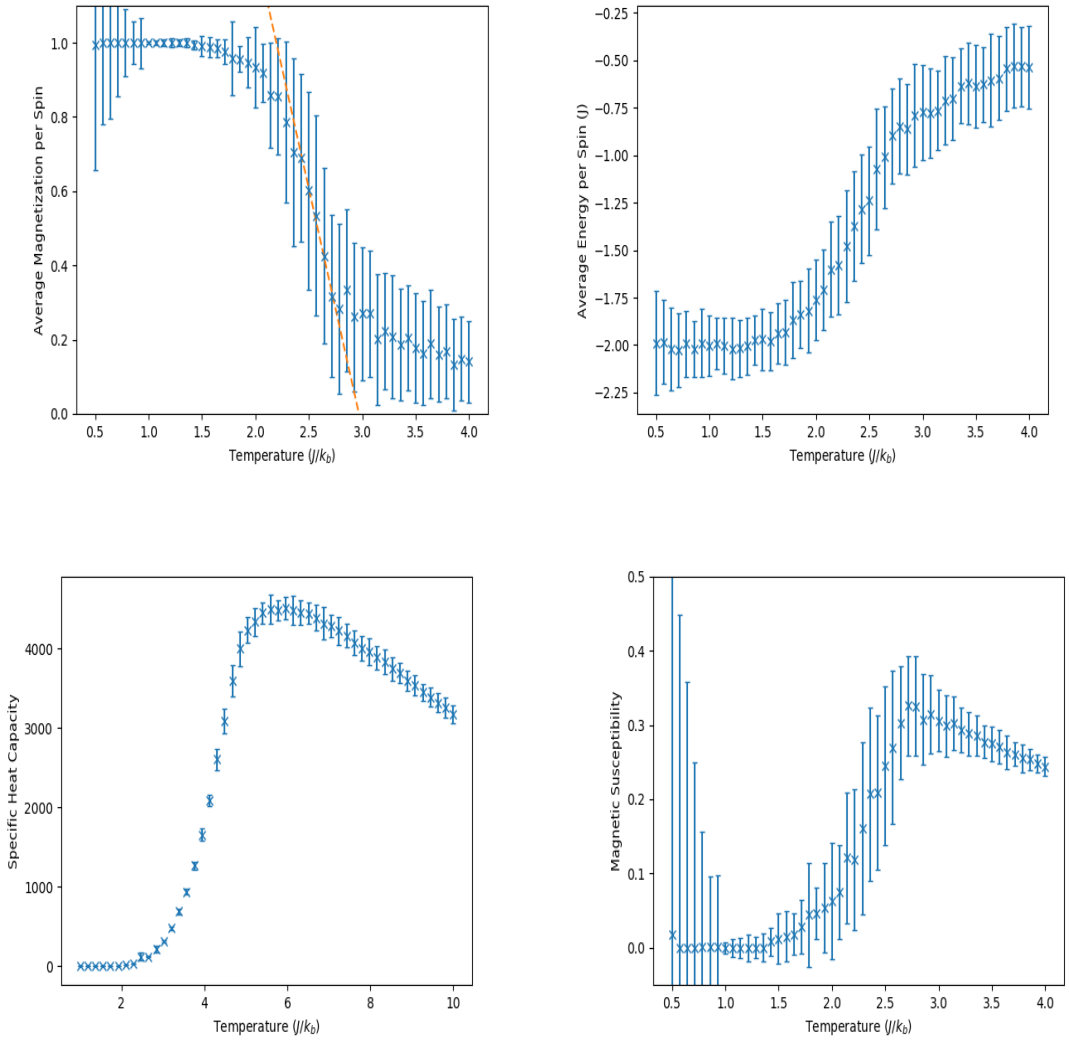

Figure 4.4: Calculatable observable as a function of temperature for a 10x10 square lattice, J¿1

From analysis of the plot of the average Magnetic field per spin it is clear that the lattice spins tends to be magnetized a low temperatures implying a ferromagnetic material which aggrees with theory. Once it passes the Curie temperature the average magnetization per site dramatically drops(discontinuity in slope). From this drop I was able to approximate the Curie Temperature to be $T_c = 2.28 \pm 0.02 J/k_b$ the points at which there is a second order phase change.
Similarly from analysis of the graph of the average energy per site it is clear from initial plateau of the curve that the ground state energy is -2 J.
Finally from analysis of the heat capacity as a function of temperature there exists a singularity at the Curie temperature which is what we would expect from theory due to the discontinuity in the energy.

4.2.3 Effects of Applied Magnetic Field

Initial I studied the effects on a ferromagnetic lattice(J¿0) which can be seen in figures 4.5, 4.6. From figure 4.5 it can be seen that a clear hysteresis loop was generated agreeing with theory. From figure 4.6 is can be seen that there is a discontinuity in the energy

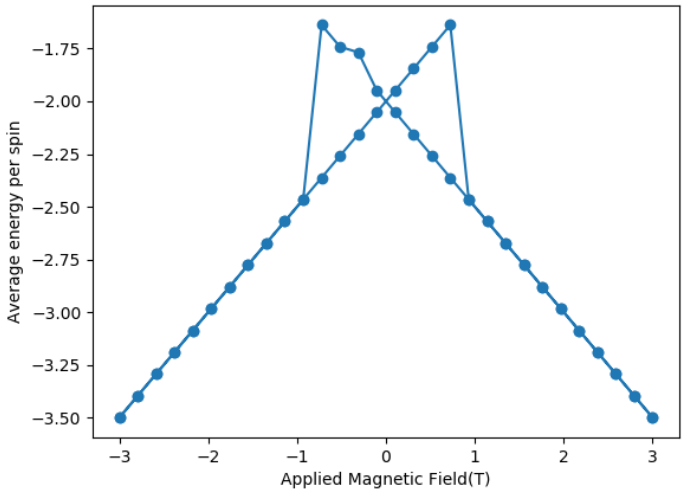

Figure 4.5: Plot of energy as your vary the applied magnetic field

at the point that the direction of the applied magnetic field is flipped(first order phase transition).

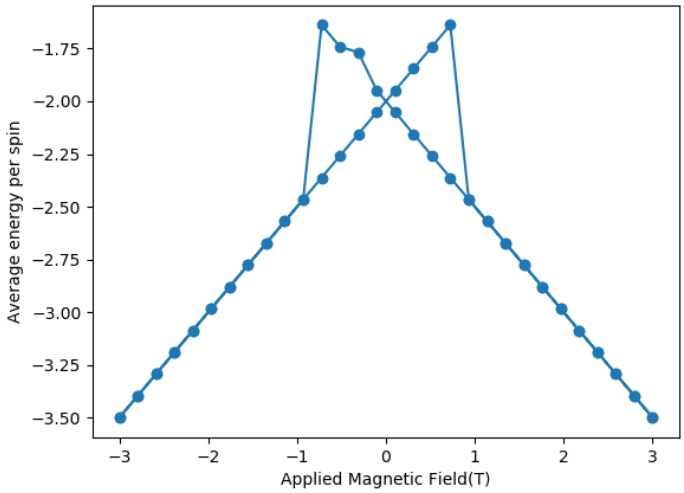

Figure 4.6: Plot of energy as your vary the applied magnetic field

Following this I studied the effects on an anti-ferromagnetic lattice(J¡0)

From figure 4.7 it can seen a plateauing of the slope which would imply and a second order phase transition is occurring.

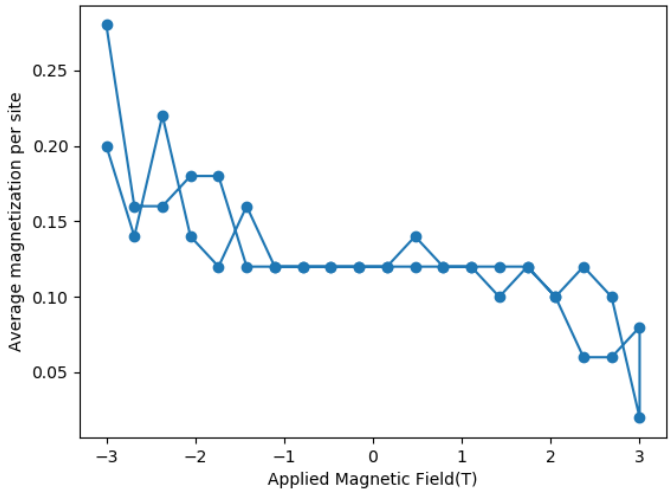

Figure 4.7: Plot of energy as your vary the applied magnetic field

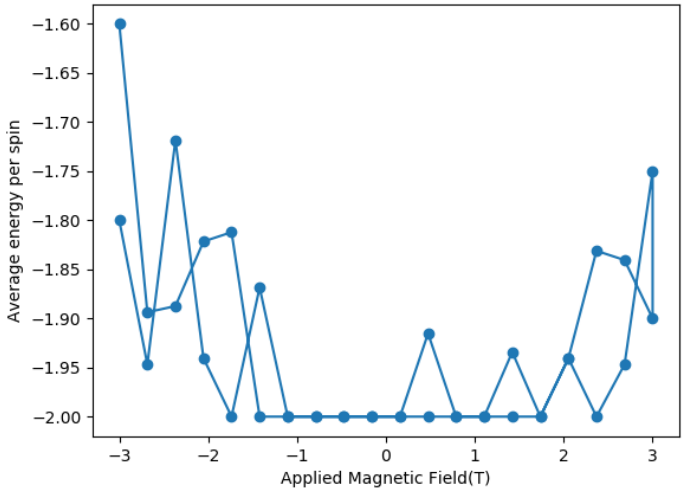

Figure 4.8: Plot of energy as your vary the applied magnetic field

4.3 3D Cubic Lattice

The metropolis method was then successfully applied to the cubic lattice for a number of different temperature an example of two temperatures can be seen in figure 4.9 where yellow and black represent up and down spin respectively.

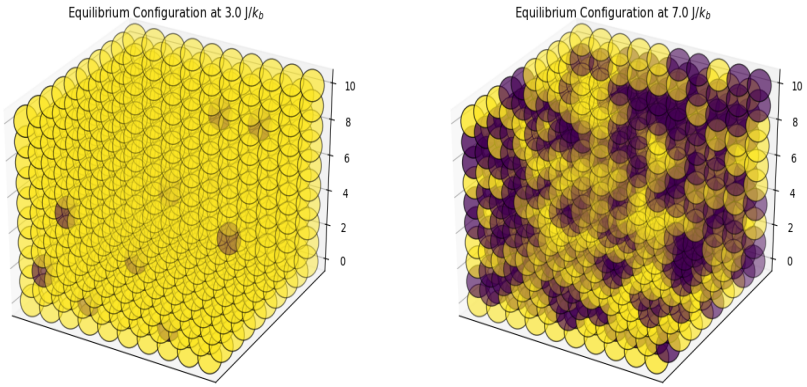

Figure 4.9: 3D cubic lattice being brought to equilibrium using Metropolis method at two different temperatures

4.3.1 Calculating Observables

From analysis of the graphs in figure 4.10 of average magnetization per site vs. temperature we were able to approximate the curie temperature to be $T_c = 4.3 \pm 0.2 J/k_b$. Which is higher than that of the 2D square which from theory is due to the fact that there is a higher number of nearest neighbour interactions in in the case of 3D which would require greater energy to over come.
Similarly from analysis of the graph of the average energy per site it is clear from initial plateau of the curve that the ground state energy is -3 J.

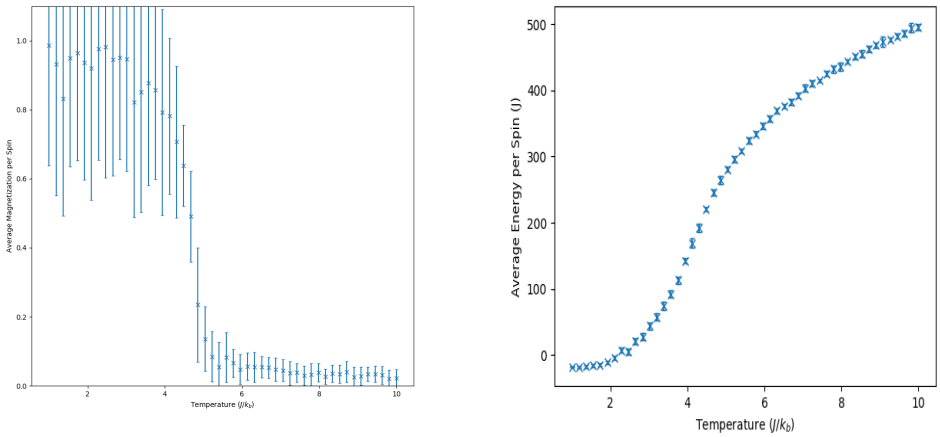

Figure 4.10: Calculatable observables as a function of temperature for a 10x10x10 3D lattice

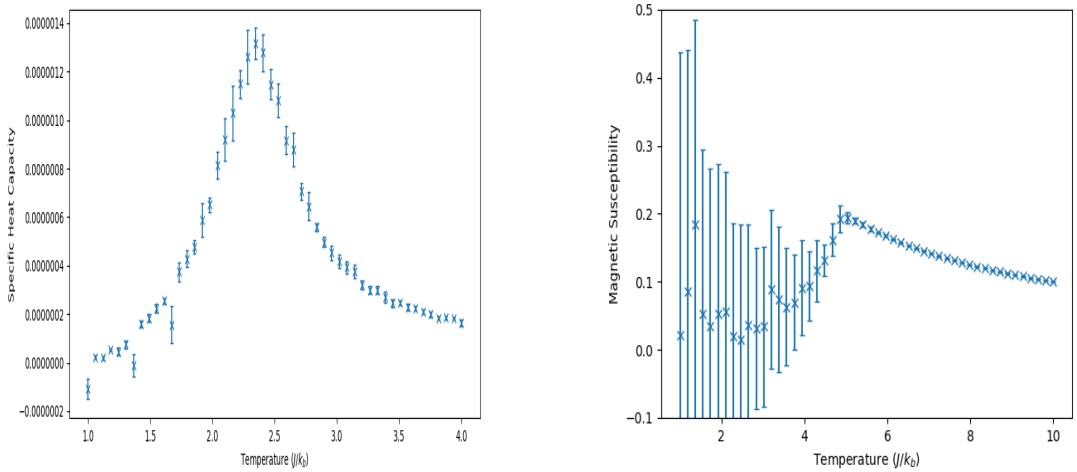

Figure 4.11: Calculatable observables as a function of temperature for a 10x10x10 3D lattice

4.4 Triangular Lattice

A 2D triangular lattice was then investigated where the metropolis method was applied in a similar fashion for a number of different temperatures, two examples of which can be seen below.

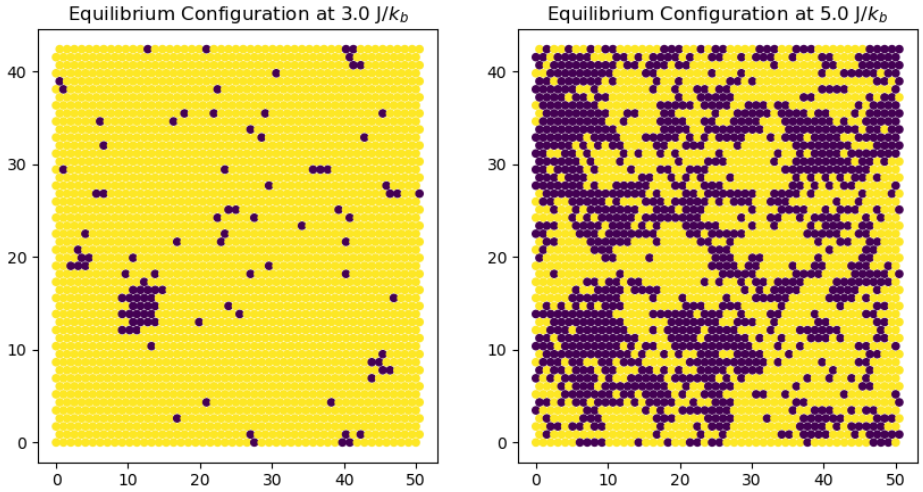

Figure 4.12: 2D triangular lattice being brought to equilibrium using Metropolis method at two different temperatures

From analysis of the graphs in figure 4.13 it is clear that it exhibits very similar properties to that of the 3D lattice. With its curie temperature coming out to be $T_c = 4.2 \pm 0.02 J/k_b$

and ground state energy of -3J which is very close to that of the 3D lattice. The reason for these similarities I believe is due to the fact that they both have the same number of nearest neighbours (6) for each spin site which would have a large effect on your calculations.

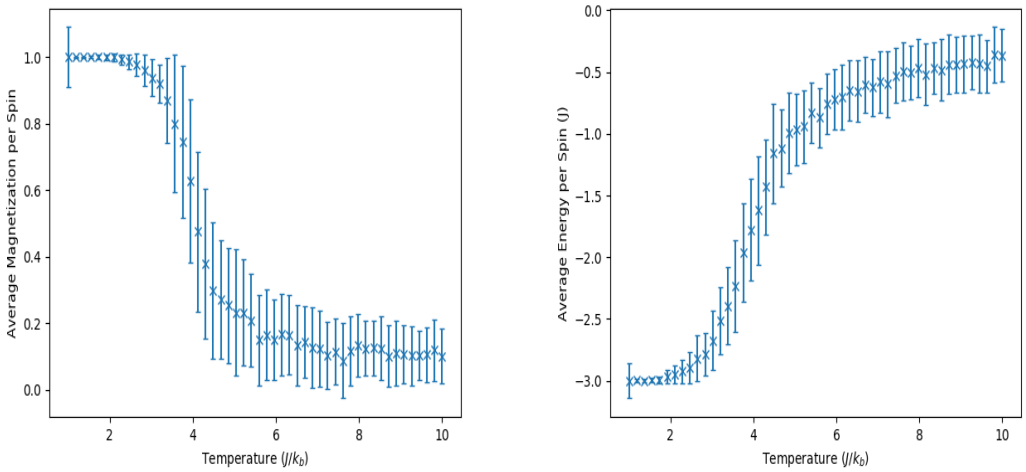

Figure 4.13: Calculatable observables as a function of temperature for a 10x10 triangular lattice

4.5 2D Modelling of Nickel Oxide

I simulated the simplified magnetic behaviour of the compound Nickel Oxide as discuss previously. Examples of the equilibrium states at two different temperatures can be seen below.

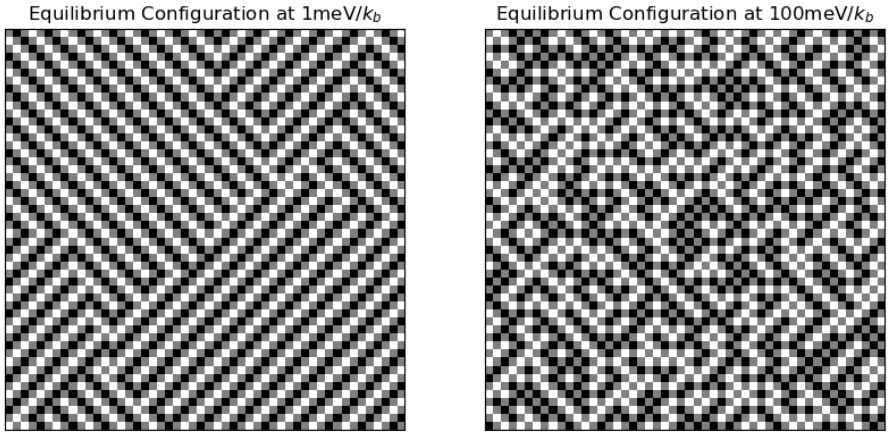

Figure 4.14: Plot of NiO spins at different temperatures black, white and gray representing spin down, up and zero respectively

Following successful simulation of the compound I analysised it properties by plotting some observables which can be seen below.

From analysis of figure 4.15 it can be determined that the ground energy of Nickel

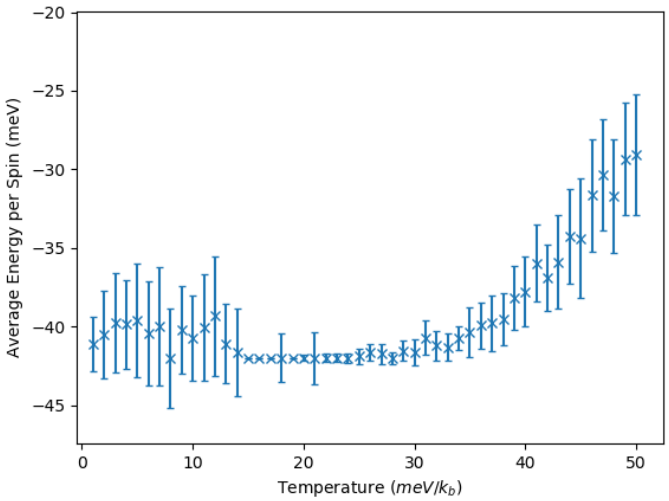

Figure 4.15: Plot Average energy per site of Nickel oxide as a function of temperature

Oxide is $-42 \pm 1 meV$ which agrees with theory within acceptable degree of error. From figure 4.16 it can be seen that the average magnetization per site is continuously zero indicating that it is a anti-ferromagnetic substance at sufficiently low temperatures.

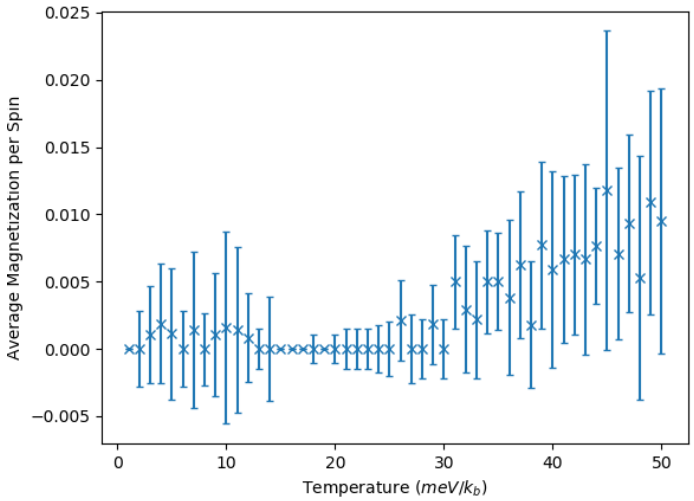

Figure 4.16: Plot Average Magnetization per site of Nickel oxide as a function of temperature

5 Discussion and Conclusion

The Metropolis algorithm was successfully applied to a number of different lattice types. The time taken to reach equilibrium was determined for a number of different lattice sizes. It was determined that it would be more efficient to use smaller lattice sizes due to limited computational power and instead find values for a number different initial configuration to get an average value and determine approximate error.

A 2D ferromagnetic spin sites were simulated by the Ising model for a number of different temperatures. Following this statistical values for the calculable observables were determined and successfully graphed. From analysis of the plots created I was able to determine the ground state to be -2 J and the curie temperature to be $T_c = 2.28 \pm 0.02 J/k_b$ at which point there was a clear second order phase transition which compares well with theory which approximates this number to be $T_c \approx 2.269 J/k_b$.
Similarly I analyzed the properties of the lattice with varying magnetic field for ferromagnetic and anti-ferromagnetic lattices. In the case of the ferromagnetic lattice a clear hysteresis loop in the average magnetization per site and first order phase transition in the average energy per site were simulated. In the case of the anti-ferromagnetic lattice a clear plateauing of the slope of the average magnetization per site was seen and hence a a second order phase transition was simulated.

The 3D cubic and Triangular lattice's were then investigated both of these lattices showing very similar properties with all curves taking approximately the same shape and the curie temperature's were determined to be $T_c = 4.3 \pm 0.2 J/k_b$ and $T_c = 4.2 \pm 0.2 J/k_b$ respectively and have the same ground state energy of -3J. The reason for these simi-

larities I believe is due to the fact that both lattices have the same number of nearest neighbours resulting in very similar interactions between spin sites.

A simplified model of nickel oxide was successfully simulated allowing us to analyze its properties. From a plot of the average energy per site I able to determine the ground state energy to be $-42 \pm 1meV$ which agrees within degree of error with theory which estimates this value to be 42meV. From analysis of the average magnetization per site I determined that the at low temperatures NiO behaves as a anti-ferromagnetic material.

6 References

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