An Analysis of the Curie Temperature obtained from the Ising Model using the Metropolis Algorithm

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The Ising Model was investigated by applying the Metropolis Algorithm. It was found that thermal equilibrium was established after a certain amount of sweeps were calculated, depending on the dimensions of the lattice used. It was observed that for 1 dimension, no phase transition is observed, while in 2 and 3 dimensions a phase transition is observed, agreeing with predictions hypothesised by Onsager in 1944. Various properties were calculated (such as the Curie Temperature) for different geometries of the lattice, such as 1D, 2D, 3D, BCC, FCC, triangular lattices etc. The size of the lattice used to calculate an accurate Curie Temperature was investigated and different boundary conditions were applied to investigate which boundary conditions provide us with an accurate result. Distance dependence was also investigated for the square lattice as well as how interactions between different amounts of neighbours.

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1. INTRODUCTION

First proposed by Lenz in 1925, the Ising Model is a mathematical model used to describe various physical phenomena such as magnetization, the behaviour of alloys, lattice gasses and more recently Bacterial Vortexes. Ernst Ising, Lenz's PhD student first solved the one dimensional Ising Model in 1924, concluding that no phase transition was observed and proposed this was the case for all dimensions. Contradicting this result, in 1944 Lars Onsager, proved that for a two dimensional lattice, a phase transition is observed. It is now accepted that for dimensions greater than two, a phase transition is observed for the Ising Model. Recent investigations of the Ising Model include analysing the Ising Model with different geometries, disordered coupling, distance dependency and impurities in the lattice.

2. AIMS

The aims of this computational project were the following:

1. To solve the Ising Model in one, two and three dimensions and analysis the behaviour of the critical temperature if one exists
2. To compare the Curie Temperatures and properties (such as Heat Capacity) of the triangular and square lattice
3. To investigate the behaviour of the Ising Model with both periodic, cylindrical and non periodic conditions and what size lattice must be used for periodic boundary conditions to obtain similar results to the non periodic boundary conditions under the same conditions
4. To investigate the dependence of the interaction term in the Hamiltonian by increasing the number of interactions between neighbours i.e. adding more neighbours to each lattice point.
5. To investigate the Curie Temperature of the Base Centred Cubic Lattice
6. To investigate the relationship between the size of the lattice and the Curie Temperature
7. To analyse the dependence on distance between adjacent atoms
8. To investigate the distance dependency between neighbouring atoms and the Curie Temperature

3. THEORY

The Ising Model is a mathematical model, commonly used in statistical physics, to describe the behaviour of certain materials and their phenomena, such as ferromagnetic materials. This is a material that can form a permanent magnet, or be attracted to one, by the alignment of electron spins in the material (i.e. they demonstrate spontaneous magnetisation in the absence of a magnetic field, when the temperature is lower than the Curie Temperature of the material). Examples of such materials include Iron, Cobalt and Nickel. The Ising Model can be used to

analyse phenomena such as phase transitions, magnetic susceptibility and the Curie Temperature of these various materials and alloys containing these materials.

To investigate various properties of ferromagnetic materials, we shall construct a N dimensional lattice, with a discrete value σ_i of ± 1 assigned to each point. To create a model for a magnetic material using the above lattice, each point of the lattice corresponds to an electron, with the value of the point corresponding to spin up $(+1)$ or down (-1).

An exact solution for the free energy f, to the $2D$ lattice was found by Onsager in 1944, and is described using the following equation:

$$-\beta f = \ln 2 + \frac{1}{8\pi^2}\int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln[\cosh(2\beta J)\cosh(2\beta J)$$

$$-\sinh(2\beta J)\cos(\theta_1) - \sinh(2\beta J)\cos(\theta_2)].$$

where $\beta = k_b T^{-1}$ and J is the interaction term between each lattice site. Onsager determined the Critical Temperature for the 2D lattice (defined later in this report) to be:

$$T_c = \frac{2J}{k\ln(1+\sqrt{2})}$$

Throughout this report, we will use several approximations to arrive at a similar formula to Onsager's solution.

We first assume the Hamiltonian of the lattice can be described by the following equation:

$$H = -\sum_{(i,j)} J_{ij}\sigma_i\sigma_j + \sum_i h_i\sigma_i$$

where J_{ij} is the interaction term between the ith and jth electron, σ represents the value assigned to a given point, h_i represents the external magnetic field.

Each atom is interacting with all other atoms in the given lattice, and each pair will therefore have an interaction energy.

However, this would take a sufficient amount of time to calculate the all the interaction energies for a given N dimensional lattice.

Instead we simplify the Hamiltonian, taking the sum over the nearest neighbours of a given point, which simplifies the Hamiltonian and allows us to calculate the approximate energy of the system in a relatively short space of time. The minus sign of the Hamiltonian is chosen by convention.

We can therefore rewrite the Hamiltonian as:

$$H = -\frac{1}{2}J\sigma_i\sum_{(i,j)}\sigma_j + h\sum_i\sigma_i$$

in which the first sum is over the lattice sites nearest neighbours. Here J and h are assumed to be equal for all lattice points. Using these assumptions and approximations, we can calculate an approximate solution for Onsager's equation. The half is introduced as the sum contains every pair of neighbouring lattice sites or atoms twice.

If the spin of one of the lattice points is flipped the change of energy is given by:

$$\Delta H_j = 2J\sigma_j\sum_i\sigma_i + 2h\sigma_i$$

or rewriting it as:

$$\Delta H_j = 2H_{eff}\sigma_i$$

where $H_{eff} = J\sum_i\sigma_i + h$. Here H_{eff} is known as the effective Hamiltonian and reduces to $H_{eff} = J\sum_i\sigma_i$ when no external field is applied.

The principle of minimum energy determines whether the spin of the atom flips. It states that for a closed system, with constant external parameters and entropy, the internal energy will decrease and approach a minimum value at equilibrium. Thus if $J_{ij} > 0$, the Hamiltonian or energy of the system will be lowered is favoured. Hence the system is ferromagnetic and the spins will align. If $J_{ij} < 0$, the change in energy is positive, and hence the system will be anti ferromagnetic.

Similarly, if $h < 0$, the spins will desire to be aligned in the negative direction, due to a negative component contributing to the energy, and if $h > 0$, the system will tend to align in the positive direction.

A. Solving the Ising Model

It is often tedious to obtain the exact solution to the Ising Model, as the number of different type of configurations of the lattice is given by 2^n (n being the number of sites on a given lattice), which is often a huge number. Instead, to solve the Ising Model, the Canonical Ensemble is used, where we characterise a large system by its microstates. The canonical ensemble is used to investigate properties of systems which can exhange energy with its surroundings. This is appropriate for the Ising Model as the system can lose energy to its surroundings and thus reach equilbrium. To do so, we use the partition function, Z, which tells us the probability of the system to be in a given state for a given temperature and energy.Using the partition function reduces the number of microstates, by ignoring configurations with a low probability and therefore very unlikely to occur. For the Canonical Ensemble, the system to be in a certain configuration at thermal equilibrium is given by the Boltzmann Factor:

$$p_s = e^{-\beta\Delta E}$$

To normalize the probabilities we introduce the partition sum/function over all energies $Z = \sum_i e^{-\beta\Delta E}$ (Z being the partition function), and rewrite the probability as:

$$p_s = \frac{1}{Z}e^{-\beta\Delta E}$$

This solution requires the sum over all configurations which can often be quite tedious. To simplify the solution, we make a further approximation, *the Mean Field Approximation*, replaces the sum of the neighbouring sites with the average spin/magnetisation obtained per lattice site $\bar{\sigma}$. Substituting this into the partition function we obtain:

$$Z = \sum_i e^{-\beta 2dJ\sigma_i\bar{\sigma}}$$

where d is the dimensions of the lattice (the 2d is introduced as each site has 2d nearest neighbours). The product of the spins can only be two values ± 1 and hence this sum can be simplified and reduced to

$$Z = 2\cosh 2dJ\beta$$

Using this we conclude that the energy of a lattice site is

$$E = -\tanh\beta(J2d\bar{\sigma} + h)$$

Applying the same method above, we can derive the average spin/magnetisation is

$$M = -\tanh\beta(2d\bar{\sigma} + h)$$

where d is the dimensions the lattice. The average spin of one atom is multiplied by $2d$ as each atom in z dimensions will have $2d$ neighbours, and the sum simplifies to $2d\bar{\sigma}$.

The energy can then be solved using the following formula:

$$H = \sum H_{ij} = NH_{eff}\bar{\sigma} = NH_{eff} \tanh \beta(J2d\bar{\sigma} + h)$$

with N being the number of sites in the lattice.

First we assume that no external field is applied, ie $h = 0$, and use the change of variable $y = \beta 2dJ\bar{\sigma}$ to obtain the following formula:

$$\frac{yT}{2dkJ} = \tanh(y)$$

One can solve this equation by plotting both the left (LHS) and right (RHS) equations and investigating the intersection between the two functions, which can be seen in Figure 1.

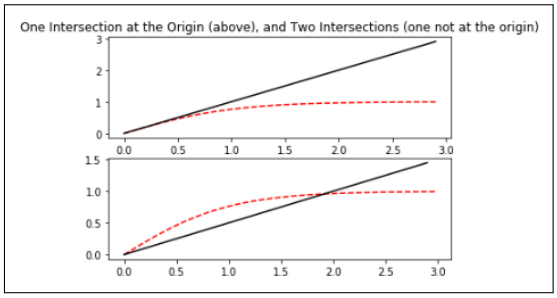

Fig. 1. $\frac{yT}{2dkJ}$ and $\tanh(y)$ plotted. The intersection between the two is the solution to the equation above.

It is clear that for large temperatures, both functions intersect once at the origin, which implies that the average energy of the lattice is approximately zero. Decreasing the value of T, the slope of the LHS equation decreases, and will eventually become tangent to RHS equation. Decreasing the temperature any further will lead to the equation obtaining two solutions, which can be observed in Figure 1 This implies that the average energy will reach a constant non zero value and all the spins will become aligned. The material has undergone a phase transition, and is said to be ferromagnetic.

The temperature at which the LHS of the equation is a tangent to the RHS is known as the Curie Temperature, and is the temperature at which the phase transition occurs, or when the number of intersections between the two functions increases and there are thus two solutions to the equation above. The LHS is at a tangent when its slope is equal to one. This implies that the Curie Temperature is defined by the following equation

$$T_c = 2dJ$$

which gives us a crude approximation for the Curie Temperature of the d dimensional lattice.

From this equation, one can see that as the dimension of the lattice increases, the Curie Temperature will also increase.

Comparing this with Onsager's exact solution, we can indeed see that both formulas imply that the critical temperature is also proportional to the exchange energy J.

When an external field is applied, one can see from the equation describing the energy of the lattice, that the intersection with the x axis will translate along the x axis, which can be seen in Figure ... This will result in no intersection between the LHS and RHS equation at the origin, but will instead have an intersection elsewhere along the function $tanh(x)$, which implies that the spins or magnetisation of each lattice site will align in a certain direction. This is as one would expect when an external magnetic field is applied to a magnetic material, as all the spins tend to align in a certain direction.

4. METHODS

To computationally solve the Ising Model, the Metropolis Algorithm was used which involved carrying out the following tasks:

1. An N dimensional lattice was constructed, with each point randomly assigned a value of $\sigma_i = \pm 1$, which represents the spin of the atom at that given point.

2. Periodic boundary condition were then applied to the lattice, effectively transforming the lattice to a torus, in order for each atom on the lattice to have an equal amount of nearest neighbours. This was achieved using the Modulo operator.

3. The energy of the lattice is calculated. The change of energy of each lattice point is then calculated if the spin is flipped. If the $\Delta E > 0$, the change is favoured and thus the lattice point will flip spins. If $\Delta E < 0$, the spin is only flipped when the value of $e^{\frac{\Delta E}{KT}}$ is greater than a random integer between zero and one.

4. This process is repeated for each site, and the whole process is known as a sweep. Each sweep then contributes a time step. A new lattice grid is returned after every sweep, and the lattice is said to be updated.

A flow chart of one sweep can be seen in the appendix.

5. INVESTIGATION OF THE ISING MODEL

A. Thermal Equilibrium of the Ising Model

For a system to reach thermal equilibrium, the entropy of the system must be at a maximum, or the Gibbs Free Energy described by the equation $F = U - TS$ (where U is internal energy, T is temperature and S is the Entropy) must be at a minimum. At constant temperature, one can see that the free energy and energy are proportional to one another, therefore we can interchange the two energies). As the lattice is updated throughout each sweep, one can see from the Hamiltonian that the energy of the system will favour a lower energy (if J is positive), and thus will eventually reach thermal equilibrium, in which the free energy of the system will reach a minimum and remain approximately constant throughout each sweep.

A randomised 10×10 lattice and 100×100 lattice is initialised where periodic boundary conditions are applied. A large number of sweeps was then carried out for the 100×100, with the energy after each sweep being stored. A graph of the average energy vs the number of sweeps for each can be seen in Fig 4 and 5.

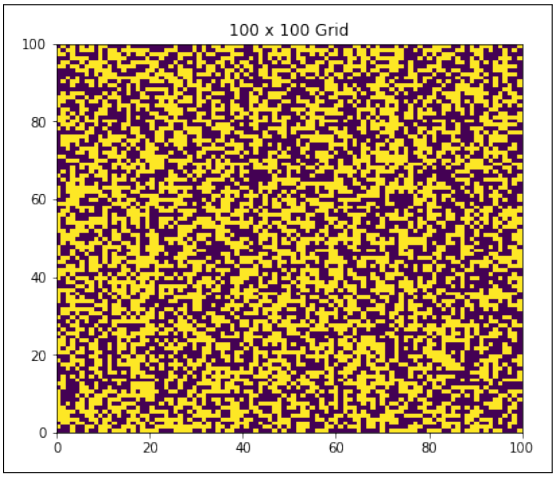

Fig. 2. 100 × 100 grid before equilibrium

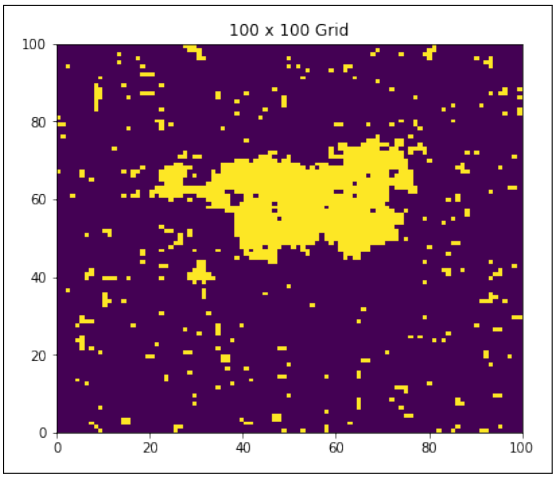

Fig. 3. The Average Energy vs The Number of Sweeps Required for the 100 × 100 lattice

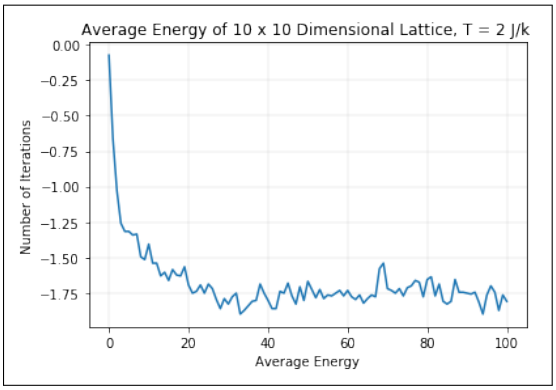

Fig. 4. Average Energy vs Number of Sweeps for the 25 × 25 lattice

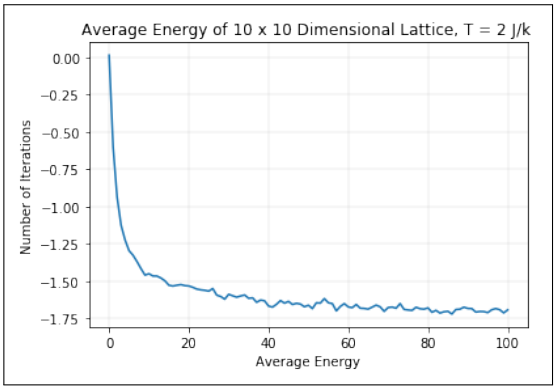

Fig. 5. 100 × 100 grid when equilibrium has been achieved. Notice that domains have begin to form, where all the spins are aligned in certain areas.

It is clear from both Graphs that as the number of iterations increases, the average energy and average magnetisation reach a constant value, implying that the system is indeed in thermal equilibrium and the Gibbs Free Energy is minimised. For the larger lattice, one can see that the number of steps to reach equilibrium is approximately 500 which is considerably larger than the amount of steps required for the smaller lattice to reach equilibrium, approximately 25. This is due to the number larger amount of sites in the larger lattice. Larger magnetic domains must be formed, which will require a longer amount of time.

From the grid figures (Fig 2 and 3) one see that the lattice sites are originally randomised and there is no order for the spin sites in the lattice. However, when the system reaches equilibrium, it is clear that magnetic domains begin to form, and area of the lattice at which all the magnetic spins are aligned.

Above, periodic boundary conditions have been used. This implies that a lattice site could have 2, 3 or 4 neighbours. The energy of each lattice site can range from -8 to +8 if J = 1. One can see that the average energy approaches a constant value of approximately -1.75 at equilibrium. This agrees with intuition, as the number of sites, as each site can have approximately 2, 3 or 4 neighbours. As the energy contains half the value of the sum of the spins of its neighbours, the average energy should be around -2 when all spins are aligned in the negative direction, as the majority of sites have four neighbours.

Ferromagnetic materials contain a large number of atoms. Therefore when using the Ising Model to investigate the properties of ferromagnetic materials, N should be large.

B. Convergence at Different Temperatures of the Ising Model

Next, the energy and magnetisation of the lattice vs sweeps is plotted over various different temperatures.

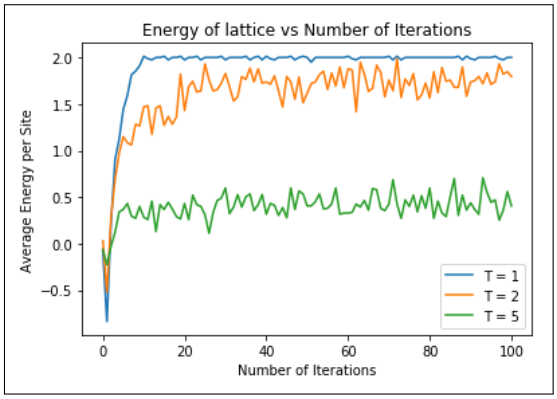

Fig. 6. Thermal Equilibrium reached over various different temperatures of the Ising Model

One can indeed see that convergence does indeed depend of the temperature used. From the graph, one can see that as the temperature increases, the lattice requires a longer amount of time to reach equilibrium. This is seen for T = 1, 2. However for T = 5, the magnetisation does not converge. Instead it remains approximately zero, implying that all the lattice sites remain randomly aligned.

Computationally this makes sense, as we use the Boltzmann probability in our algorithm to determine whether a lattice site flips values or not. As the temperature increases, the probability of the lattice point flipping increases and the probability converges to a value of 1, implying that the lattice site will change value. This can be seen for the large temperature in the graph shown as it doesn't seem to converge, implying that each lattice site has a large probability of flipping, and the majority of lattice sites flip throughout each sweep.

This also makes sense intuitively. As the temperature of the lattice is larger, the slope of the straight line in figure 1 is greater than one, and the two lines will thus only have one intersection at zero for the overall magnetisation, implying that the spins remain randomly aligned regardless of the number of sweeps/time.

Overall we can conclude that in order for a system to reach equilibrium, the temperature must be at a low value. Throughout the remainder of the reports, the temperature T = 1, which demonstrates convergence for both magnetisation and energy as seen above.

C. Measuring Various Observable of the System

To calculate the average value per site for an observable O such as energy or heat capacity, one must use the following equation:

$$\bar{O} = \sum \frac{O}{n}$$

where the sum is over all n observables O.

Once the system has reach thermal equilibrium, observables of the system at a given temperature can be obtained. The average energy per atom of the system can be calculated using the equation:

$$\bar{E} = \sum \frac{E}{n}$$

where n is the number of lattice sites.

Similarly the average magnetisation per spin can be found using:

$$\bar{M} = \sum \frac{\sigma}{n}$$

To calculate the heat capacity of a system at given temperature the following formula was used

$$C_v = \frac{\beta}{T}\sigma_E^2$$

and for the magnetic susceptibility:

$$\chi = \beta\sigma_m^2$$

where σ_E and σ_M are the standard deviations of the energy and magnetisation of the lattice respectively. Derivations of these two formulas can be seen in the appendix.

Using the average magnetisation per spin and average energy per spin, we can calculate the amount of sweeps required to reach equilibrium, by observing when both values reach a constant value. For the 10×10 dimensional lattice, this require approximately 25 sweeps. To calculate the different observables, a randomised lattice is swept 25 times before any measurements of observables are carried out. This increases the accuracy of the measurements performed, as the observables tend to fluctuate before equilibrium is reached.

We can determine the Curie Temperature of the lattice by observing what value the energy of the system is for a given temperature. For a randomised lattice, the average energy should be approximately zero, due to the randomised spin states cancelling each other in the summation of all values appointed to each lattice site. As the system becomes ferromagnetic the spins tend to align and thus the energy should reach a constant value, which depend on the dimensionality and the number of nearest neighbours for a given point. Two formulas for the Curie Temperature are given in the theory section above, the approximate solution we derived and Onsager's exact solution.

The 10×10 lattice was updated until equilibrium was reached, and different observables were measured for various temperatures and can be seen below.

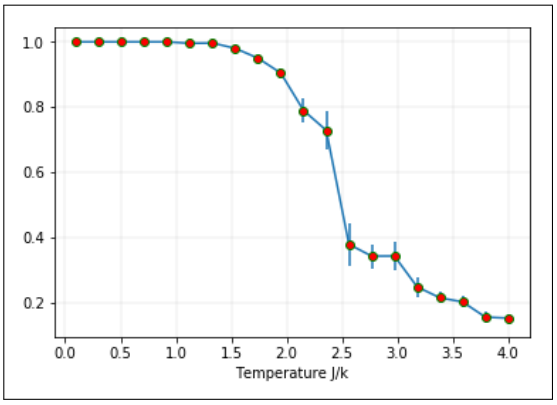

Fig. 7. 25×25 Average Energy for a variety of different temperatures

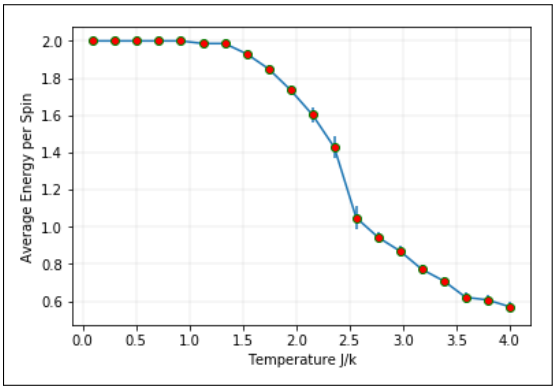

Fig. 8. 25 × 25 Average Spin per atom for a variety of different temperatures

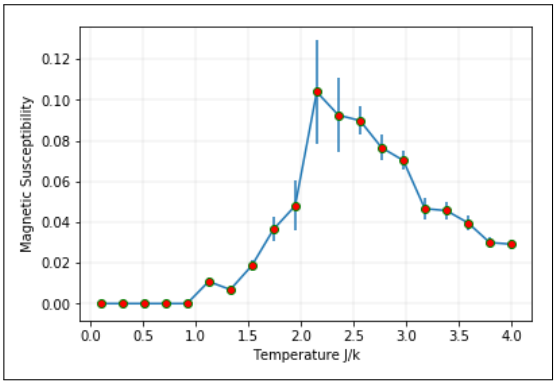

Fig. 10. 25 × 25 Magnetic Susceptibility for a variety of different temperatures

Firstly one can see that a phase transition does occur for the 2D Ising Model, where the lattices properties change and different phenomena are observed.

This is firstly clear in the average magnetisation per spin. Initially for larger temperatures, the average magnetisation remains approximately zero, which corresponds to the spins of each lattice being randomly aligned, and the sum of all the spins is therefore approximately zero. However at a certain temperature (the Curie/Critical Temperature), the spins begin to align, and the average magnetisation per spin reaches the value of one (the spins are aligned). For the 25 × 25 lattice, the Curie temperature observed is approximately $2.5 \pm 0.3 J/k_B$ which agrees with the value obtained from P.A Slothe (1982), which is a value of 2.7 J/k. The reason our solution may deviate from the exact solution is due to the number of approximations made throughout the report, such as the mean field approximation and N = 10. To obtain a more accurate result, we should increase the value of N.

The average temperature vs spin is also plotted below and the value of the energy reaches a constant value of -2 J for low temperatures. This agrees with equation derived for the energy in the theory section, which implies that after a the curie temperature, a non zero solution is obtained for the equation, and the energy will tend towards that value.

The heat capacity and magnetic susceptibility is also investigated and can be seen in the graphs below. The heat capacity reaches a maximum value at approximately 2.2 J/k, which again corresponds to the Curie Temperature.

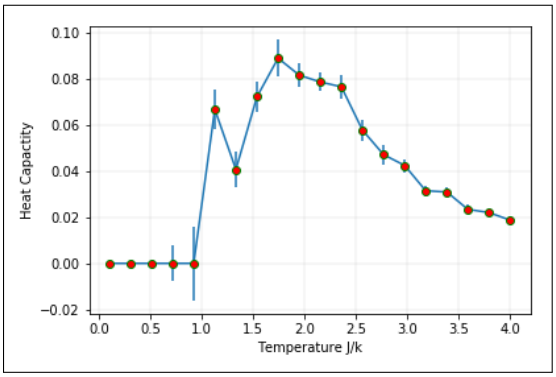

Fig. 9. 25 × 25 Heat Capacity for a variety of different temperatures

The heat capacity can also be described by the equation: $C_v = \frac{dE}{dT}$. At the Curie temperature the energy changes almost instantaneously, leading to a discontinuity for C_v at the Curie Temperature. One can see that there is indeed a discontinuity in the Heat Capacity at the Curie Temperature, which again corresponds to a phase transition occurring at approximately $2.4 \pm 0.3 J/k_b$.

The result obtained for the Curie Temperature above agrees with the exact solution obtained from Onsager and P. A Sloethe (see references), which predict that a phase transition will occur at approximately 2.7 J/k. This differs from our results due to the approximations made throughout the report, which included using the Mean Field Approximation, using a small lattice size as well as using periodic boundary conditions.

The Magnetic Susceptibility also appears to have a discontinuity at approximately $2.5 \pm 0.3 J/K$, also at the Curie Temperature. Again this implies that a phase transition has occurred as the Magnetic Susceptibility can also be described by the following equation: $\frac{d\langle\sigma\rangle}{dT}$, which implies that a discontinuity will be observed due to the almost instantaneous change of the average magnetism per site of the given lattice at the Curie temperature.

In conclusion, several arguments are produced to demonstrate that a phase transition occurs for the 2D lattice. This is observed from the discontinuities in the heat capacity and magnetic susceptibility at a given temperature as well as the change in the average energy and magnetisation/spin per atom of the lattice, suggesting that a second order phase transition occurs.

We can therefore reject Ising's Hypothesis that no phase transition occurs for the Ising Model, and approximate the Curie Temperature of the 10 × 10 lattice used to be approximately between the values obtained for the Curie temperature using each properties. We can therefore conclude that the Curie temperature for the Square lattice is approximately $2.5 \pm 0.2 J/k$, which agrees with Onsager's exact solution, within an error of 0.2 J/k. Errors are discussed at the end of this report.

D. The Ising Model in Other Dimensions

After investigating the one dimensional Ising Model, Ising concluded that no phase transition would occur, and hypothesised this was the same for higher dimensions.

In this computational report, the Ising Model was investigated for one, two and three dimensions for a square lattice. An investigation into Ising's result was then carried out, in which the average magnetisation and energy per spin were calculated for various temperatures in order to investigate whether a phase

transition was observed, and if so, what the Curie Temperature is and how this depends on the dimensionality of the lattice.

To investigate whether a phase transition occurs the average magnetisation was observed for the three lattices after reaching equilibrium for each dimension. Results can be seen in the graph below.

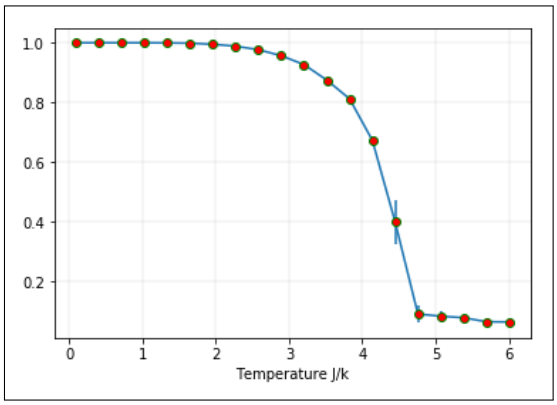

Fig. 11. Average Magnetisation (y axis) of the 3D Ising Model for Various Temperatures (x axis)

Firstly, when comparing the 3D results to the 2D results obtained above, one can see that both the 2D and 3D lattices experiences a phase transition as the magnetism switches from 0 to 1 at a temperature of 2.5 ± 0.2 and 4.1 ± 0.1 respectively, which again agrees with Sloethe's predicted value, which can be seen in the references. It is clear that the 3D lattice undergoes a phase transition at a higher temperature. This is mainly due to the greater number of neighbours each lattice point has, which implies magnetic domains will form much faster.

An error in our analytic result arises mainly due to the small number of sites used for the lattice (for a 25×25 Matrix 100 sites were analysed), the number of approximations used such as the Mean Field Theory, as well as periodic boundary conditions being applied. Regardless, we can conclude from our results, that the critical temperature is dependant on the dimensionality of the lattice used and will increase for larger dimensions as the amount of nearest neighbours increases.

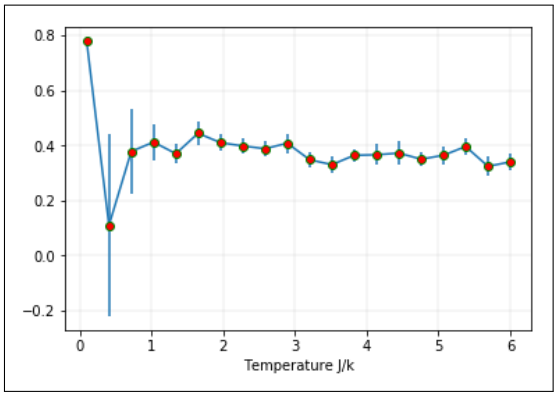

Fig. 12. 1D Ising Model:Average Magnetisation over various Temperature. One can see that it no phase transition occurs

However, one can see from the graph above that no phase transition is observed for the 1D lattice, as the average magnetisation remains at an approximately constant value and no Curie Temperature is observed. This agrees with Ising's initial solution, first proposed in 1924, that no phase transition is observed for a 1D Ising Model, and no ferromagnetic phenomena are observed.

E. Size Dependency of the Lattice

The Curie Temperature was calculated for three square N x N lattices, where N = 3, 10 and 25 for the 2 dimensional. The results of the magnetisation can be seen in Figure 13.

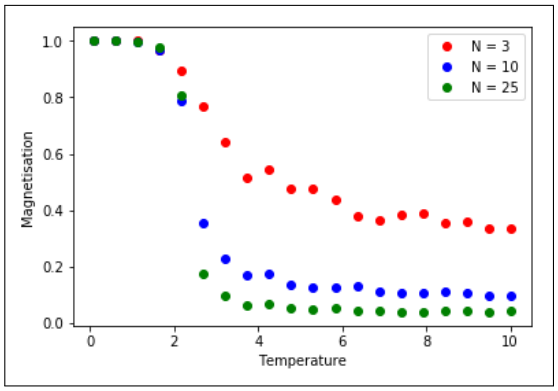

Fig. 13. The average magnetisation of each lattice site for a Lattices of different sizes.

One can see that the Curie Temperature for each was approximately equal for each lattice, 2.1 ± 0.2. This agrees with the exact solution obtained by Onsager with an error of 2.27 J/K.

It is observed that for a smaller lattice size, the phase transition occurs more gradually than high temperatures and it is therefore more difficult to obtain the Curie Temperature, as a larger error is observed. One can also see that as the temperature approaches infinity, the average magnetisation of the lattice gets closer to zero as the lattice size increases, which is what is expected in Onsager's exact solution (where the canonical ensemble is used, which implies a large system is used). We can therefore conclude that to obtain an accurate value for the Curie Temperature obtained from the exact solution obtained by Onsager and a good model for the Ising Model, one must use a large square lattice. Due to larger lattice sizes requiring a longer computational time, N = 25 was used for the remainder of the report.

F. Different Geometries of the Lattice

The square and hexagonal two dimensional lattices were investigated throughout this report in order to investigate how the geometry of the lattice effect the curie temperature and the phase transition. To create the triangular matrix, the square matrix was adjusted and an additional two neighbours were added. A visualisation can be seen in Figures 14 and 15.

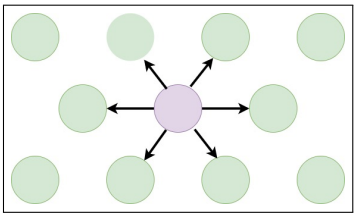

Fig. 14. 25×25 Heat Capacity for a variety of different temperatures

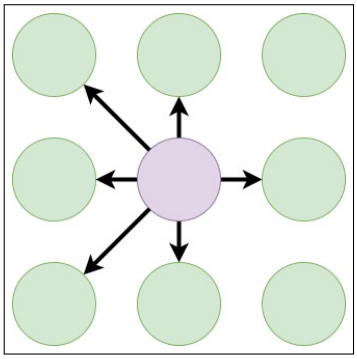

Fig. 15. 25 × 25 Heat Capacity for a variety of different temperatures

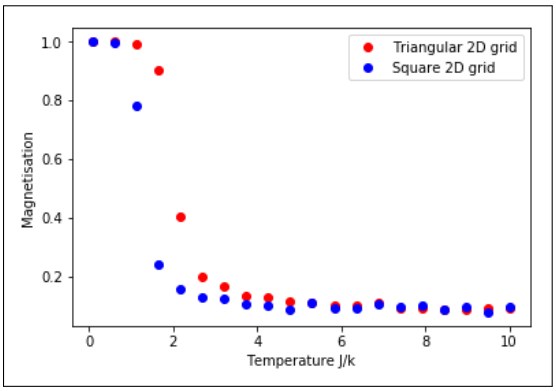

Fig. 16. The average magnetisation vs temperature for the square and triangular lattices

The number of nearest neighbours was also increased, and the diagonal neighbours of each lattice point were also included in the Hamiltonian, to see how this would effect the phase transition.

Results of the average magnetisation for a variety of different temperatures is seen below for both geometries. The initial 10×10 lattice is also plotted for comparison at a temperature of 0.1. One can see that the Curie Temperature indeed increases for the different geometries, with the Curie Temperature for the Triangular Lattice being 2 ± 0.1 J/K. Again this is mainly due to the amount of nearest neighbours increased, with six being for both the triangular while there is only four nearest neighbours for the square lattice. An increase in neighbours implies information travels between neighbouring lattice sites (i.e. their spin) and magnetic domains can form much faster.

The Curie Temperature obtained for the triangular lattice was $4 \pm 0.4 J/k_b$ which agrees with with previous literature, comparing this with the obtained value from P.A Sloethe (1982), which predicts the triangular 2D lattice to have a Curie Temperature of 4.3 J/k. An error arises in our result and exact solution mainly due to the number of approximations used throughout this report, such as the mean field theory approximation as well as periodic boundary conditions and a small lattice size used.

Comparing for the value of the Curie temperature obtained for the square lattice (2.3 J/K), it appears that for the triangular lattice, a phase transition occurs at a larger temperature. This is mainly due to the extra two neighbours each point on the lattice has for the triangular matrix, which will ultimately lead to domains being formed at a faster rate, as information can travel much faster between neighbouring atoms due to additional connections between sites.

From this we can conclude that the Curie Temperature depends on the geometry of the lattice and the number of nearest neighbours for each given point.

This is important when trying to determine the Curie Temperature for various material. Different crystal structures will have different lattices and geometries such as simple cubic or hexagonal structures. To computationally solve there Curie Temperature, it is therefore vital that we use the same geometry of the physical crystal in order to calculate a correct solution.

G. Periodic (PBC), Cylindrical (CBC) and Non Periodic Boundary Conditions (NBC)

An investigation into how periodic boundary conditions and cylindrical periodic conditions of the lattice affects the value determined for the Curie Temperature. Unlike periodic boundary conditions, where each lattice site has the same amount of nearest neighbours, in the NPBC and CBC the surface atoms of the lattice have either two or three neighbours.

To investigate further, a plot of the systems energy and the number of sweeps was plotted in the Graph below.

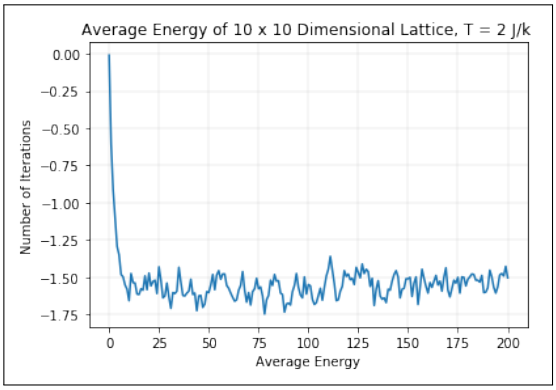

Fig. 17. Energy of the Ising Model with NPBC reaching equilibrium

One can see that unlike the PBC, which reaches a constant value of -2 J, NPBC reach a constant value of approximately -1.75 J. This can be described using the same logic for the square lattice and triangular lattice, as seen above. The energy of each site is dependant on the amount of nearest neighbours when all the sites are aligned in a certain direction. Therefore as the average value of neighbours per site decreases, due to the non periodic boundary conditions, the overall average energy per site will also decrease.

These boundary conditions were applied to a square lattice, and the average magnetisation over a range of temperatures was plotted.

One can see that a phase transition is observed regardless whether PBC, NPBC or CBC is applied. From the table above it appears that the Curie Temperature remains approximately equal for PBC and NPBC for the 25×25 lattice.

The values obtained for the Curie Temperature for the periodic, non periodic and cylindrical boundary's were 2.4 ± 0.2, $2.1 \pm 0.1$and $2.2 \pm 0.2 J/k$ respectively. One can see that for different values of the Curie Temperature was calculated for each boundary condition, with CBC being closer to NPBC than PBC, with an error of approximately 0.3 and 0.1 respectively. We can

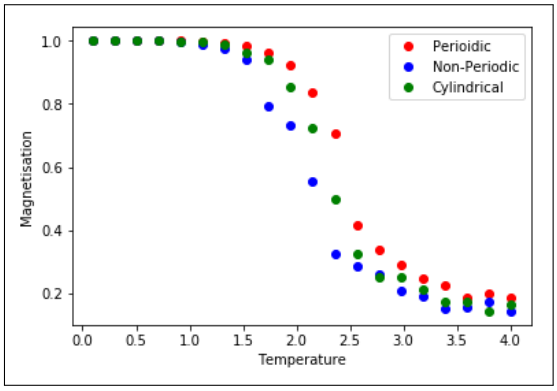

Fig. 18. The average magnetisation vs temperature for lattices with different boundary conditions

therefore conclude that the PBC provide an accurate approximation for the Curie Temperature of the Ising Model with NPBC.

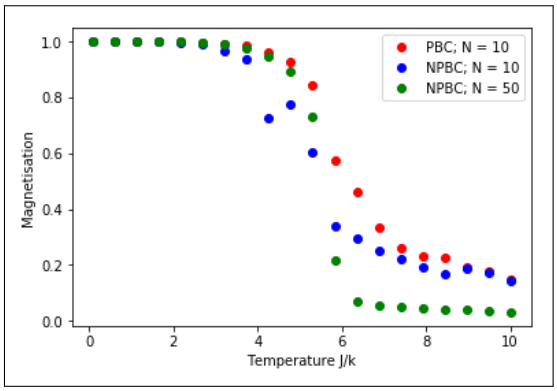

Fig. 19. PBC and NPBC of different sized lattices

The size of the PBC lattice was increased to N = 50 and plotted with the NPBC with N = 10 as seen below. One can see that as the size of the PBC lattice is increased (N = 50), it approaches the same Curie Temperature as the NPBC, implying that in order to reach an small error in the Curie Temperature using PBC, a larger value of N should be used to obtain the same value as the NPBC.

From these results, we can therefore that while the differences between PBC and NPBC may not be immediately obvious, there is indeed a slight change in Curie Temperature and average grid energy. This implies that the PBC applied throughout this report is indeed a good approximation for the Ising Model for the 2D model as the difference between the Curie Temperature for PBC and NPBC is 0.3 J/K for the 10×10 lattice.

H. Addition of the second nearest neighbours interaction

Below, the average magnetisation for various temperatures is plotted for two lattices, each with a different number of neighbours, which can be seen below in the visualisation.

In the second lattice, we also included interactions with next nearest neighbours, taking the distance dependency into account by dividing by $\sqrt{(2)}$. From the graph below, the Curie Temperature is 2.5 ± 0.2, with a difference of 0.5 when compared to the model only using the nearest neighbours. We can see that as one increases the number of lattice sites each site is interacting with the Curie Temperature increases.

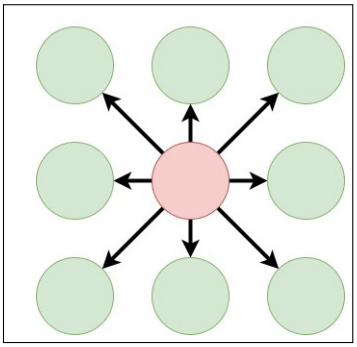

Fig. 20. Visualisation of lattice with nearest neighbour interactions

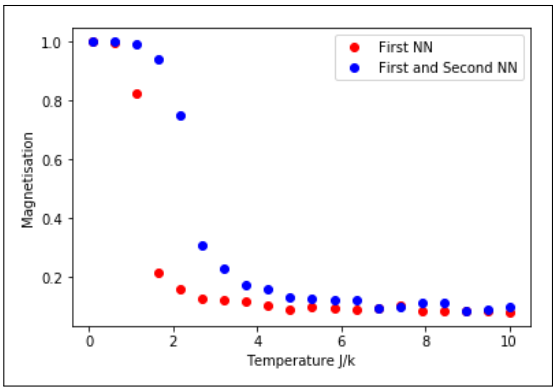

Fig. 21. Average Magnetisation of different lattices for first and fecond nearest neighbours taking into account for each lattice

Because each lattice site actually interacts with all other lattice sites in the Ising Model, we can conclude from above, that the value obtained for the Curie Temperature will be smaller than the actual value, due to the approximation that each lattice site only interacts with nearest neighbours. However, due to the interaction energy being inversely proportional to the distance between each atom, we can see that the Curie Temperature obtained provides us with a close approximation to the actual Curie Temperature of the magnetic material.

Computationally, it would require a large amount of time to calculate all the interactions between each site. However, from above, we can see that using only the nearest neighbours, we can obtain an accurate value for the Curie Temperature, which implies that using only the nearest neighbours provide a good approximation for the Curie Temperature, with next nearest neighbours changing the Curie Temperature only by 0.5 J/k.

Comparing with results obtained from P.A. Sloette, we can see that our results do agree with his analysis and lie within the error obtained above.

I. Distance Dependency

Throughout the report I assume that the interaction between neighbouring atoms is due to the Coulomb force, and therefore the energy depends on the inverse of the distance between them squared. Thus, as the distance between the neighbouring atoms increases, the interaction energy between the neighbouring atoms decreases and we can thus expect a decrease in the Curie Temperature observed.

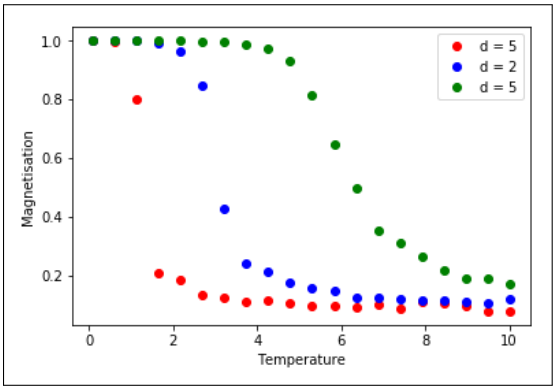

Fig. 22. Average Magnetisation of the Ising Lattice with different distances between neighbouring lattices

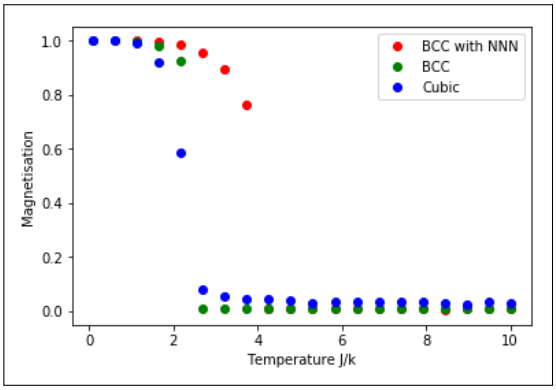

Fig. 23. Average Magnetisation for a cubic and BCC lattice over various temperatures

This also makes sense when referring to ferromagnetic materials. Again, looking at figure 1, one can see that the slope of the straight line will increase as the interaction energy increases, or distance decreases, which will imply a higher Curie Temperature, where there are two intersections between each line in Figure 1.

The average magnetisation of each lattice site is plotted for various different temperatures for d = 1, 2 and 5. From the graph, we can see that a Curie Temperature of 2.2 ± 0.2, 3 ± 0.3 and $6 \pm 1J/k$ was obtained respectively. From this we can conclude that the Curie Temperature is directly proportional to the distance between neighbouring atoms as previously hypothesised.

J. An analysis of different 3D Lattices

Rarely, do we observe materials with a simple cubic structure. Magnetic materials can take various other structures such as Face Centred Cubic (FCC), Body Centred Cubic (BCC) and Hexagonally Closed Packed (HCP). To investigate how the geometry of the lattice effects the Curie Temperature of the Ising Model, the average magnetisation of the BCC and square lattice for various temperatures of the three-dimensional Ising Model is plotted below. One can see that the Curie Temperature indeed differs, it being $2.1 \pm 0.1J/k$ for the BCC, and $2 \pm 0.2J/k$ for the square lattice when only nearest neighbour interactions are taking into account. Applying next nearest neighbours in the BCC, we obtain a Curie Temperature of 3.7 ± 0.3.

When comparing this result with Anders Rosengren's paper (seen in references), we can see that our results agree with previous analysis of a BCC ferromagnetic material and we can thus conclude that the Metropolis Algorithm is an accurate method to investigate ferromagnetic materials.

One can conclude from this that when determining the value of the Curie Temperature for various different materials, it is vital that one uses the correct crystal structure of the magnetic material, as it can can change the temperature as much as 0.2 J/K, which is observed in the obtained values for the BCC and Cubic Curie Temperatures, being $2.1 \pm 0.2J/K$ and $2.3 \pm 0.1J/K$ respectively. These results agree with previous results for the BCC lattice obtained by Rosengren in the references.

Intuitively this makes sense as the geometry of the structure determines the distance between adjacent neighbours as well as the amount of nearest neighbours, which will affect the Curie Temperature, as seen in the above investigation.

6. ERRORS THROUGHOUT THE COMPUTATIONAL REPORT

The Curie Temperature is defined as the temperature at which spontaneous magnetisation of a ferromagnetic material occurs. As this happens suddenly, a step function can be used to describe the magnetisation per lattice site, switching instantaneously from 0 to 1 at the Curie Temperature.

However, one can see that in each of the graphs representing magnetisation over a variety of temperatures, one can see that the change in magnetisation is not instantaneous but gradual, and it is thus difficult to determine the Curie Temperature.

Therefore, we can define the error of the Curie Temperature to be half the distance from when the magnetisation begins to change. This implies the more gradual the change of magnetisation, the larger the error of the Curie Temperature.

An error also arises due to the mean field approximation (described above) used, as well as a small lattice used throughout the investigation. Random fluctuations are more prominent in a smaller lattice as there is a smaller number of sites and therefore have a greater effect on the average properties of the lattice.

7. CONCLUSIONS

Overall we can conclude that the Metropolis Algorithm provides us with a statistical and probabilistic method to model and investigate the properties of the Ising Model. Firstly, we can conclude that the Ising Model does indeed reach thermal equilibrium, with the time required dependant on the size of the lattice used. Secondly, we can conclude that as the temperature of the lattice varies, one can see a phase transition, as all the atoms align after a certain temperature, the Curie Temperature when the dimension of the lattice used is greater than one. Thirdly we can conclude that this temperature is dependant on the Size, Boundary Conditions, Dimensions and Geometry of the lattice, which is again evident throughout the various investigations of the report.

8. REFERENCES

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Publications

The triangular Ising antiferromagnet with first- and second-neighbour interactions, P A Slotte and P C Hemmer

Curie temperature of the square Ising ferromagnet with first-, second- and third-neighbour interactions, P A Slotte

Curie Temperature for Small World Ising Systems of Different Dimensions, E.Z. Meilikhov, and R.M. Farzetdinova

The Ising model for the bcc, fcc and diamond lattices: A comparison by Anders Rosengren

9. APPENDIX

The flow chart of the Metropolis Algorithm can be seen below:

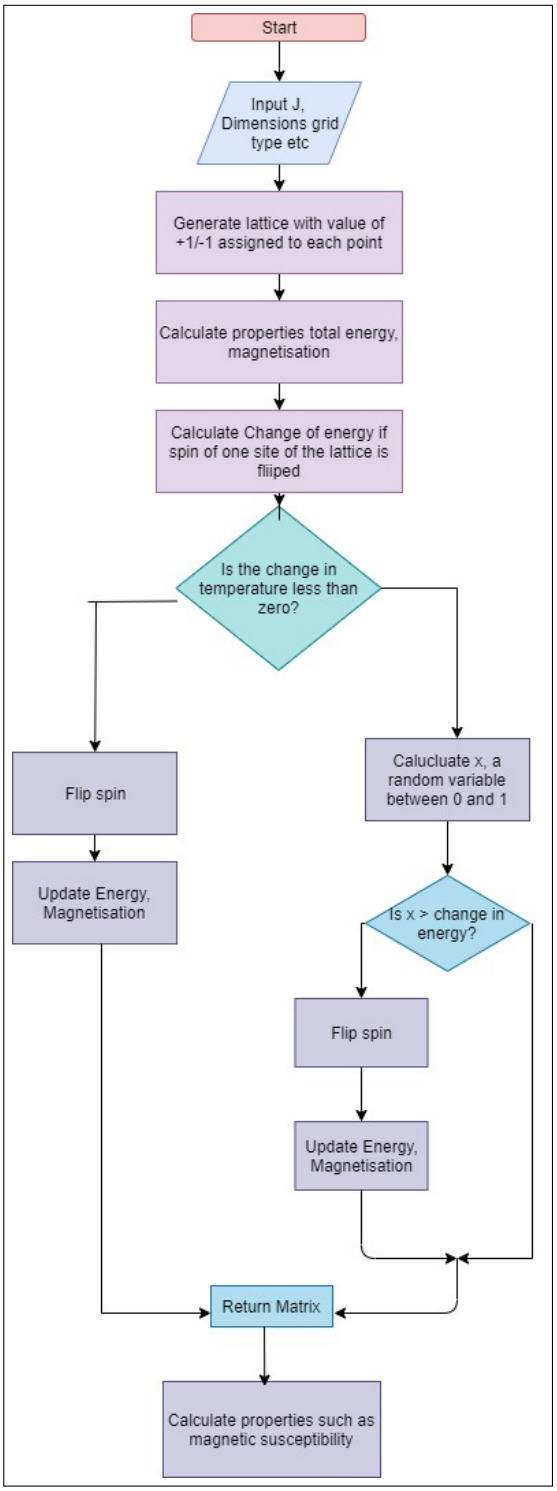

Fig. 24. Flow Chart of Metropolis Algorithm

Derivation of the Heat Capacity

$$C_v = \frac{d\bar{E}}{dT}$$

$$C_v = \frac{\beta}{T}\frac{d\bar{E}}{d\beta}$$

$$C_v = \frac{\beta}{T}\frac{d^2 lnZ}{d\beta^2}$$

$$C_v = \frac{\beta}{T}(E^2 - \bar{E}^2)$$

Derivation of teh Magnetic Susceptibility

$$\chi = \frac{d\bar{M}}{dh}$$

$$\chi = \beta(\bar{M^2} - \bar{M}^2)$$

We can rewrite these formulas in terms of the variance and thus obtain the formulas used in the report above.