Analysing the Phase Transition of a material using the Ising Model

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Abstract

The aim of this project was to assess the effectiveness of an Ising model simulation when modelling the behaviour of an arbitrary material undergoing a phase transition. Comparing the model to its mean field and exact solution counterparts shows that the simulation is more effective at modelling the material when undergoing paramagnetic behaviour. However, analysing the error in the simulation shows that large amounts of processing power are needed to obtain a greater understanding of the material during its phase transition.

1. Introduction

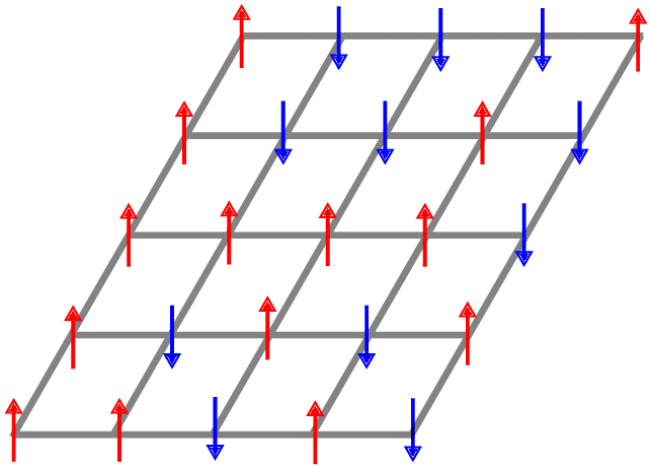

Figure 1. The Ising model setup for a two-dimensional square lattice grid (Wald, 2017).

In the fields of condensed matter physics and statistical mechanics, a large amount of research has been conducted on materials with regular crystalline atomic structures. Within these structures, the spin of each atom will tend to align with its neighbours and an external magnetic field if present. If the field is pointing in a fixed direction, the spins will roughly point in that direction as well and magnetise the material. When aligned, two distinct types of behaviour can be found in the atoms when slowly decreasing the intensity of this external field. The structure could exhibit paramagnetic behaviour, where the orientation of the spins is increasingly lost as the field strength decreases. The direction is entirely lost when the field strength decreases to zero, meaning that the material has no magnetic properties. Another is ferromagnetic behaviour, which is when the general direction of the spins is lost but maintains a magnetised behaviour due to the interactions between the spins. This magnetised behaviour can be maintained even without the presence of an external magnetic field.

When analysing these behaviours, Pierre Curie observed that crystalline structure materials can exhibit both paramagnetic and ferromagnetic behaviour depending on its temperature T (Mould, 2007). When the temperature is increased past a particular value, the behaviour can suddenly change from ferromagnetic to paramagnetic. This value is known as the Curie temperature T_c of the material corresponds to a sudden change in magnetisation called the phase transition. Consequently, the Ising model was introduced to understand these phase transitions from ferromagnetic to paramagnetic behaviour. This model was the first to determine if phase transitions could be described using statistical mechanics as a framework (Friedli, 2018). Using this model allows for a quantitative analysis of the magnetic behaviour of a material (Ikeda and Hirakawa, 1974). The regular crystalline structure of the material is modelled corresponding to a two-dimensional, unoriented square grid lattice of atoms. The atoms in this grid, as well as their corresponding spin state, can be found at every vertex. The spins are initially restricted to one direction at a low temperature T, where they point either “up” or “down”. Consequently, the two states will have a spin value of either +1 or -1 for up and down states respectively.

Once the external field strength reaches zero, some of the spin up particles in the grid will occasionally flip to spin down. When $T < T_c$, the grid is almost entirely populated by one of the two states, usually spin up ($s_i = 1$), with fluctuations of the other spin occurring as isolated clusters. As T increases, the size of these spin clusters and the number of their occurrences will increase but is still dominated by the one spin state value. At $T = T_c$ there is suddenly no clear dominance of either spin and the size and frequency of these clusters will begin to greatly fluctuate. As T increases into the $T > T_c$ region the state of each spin fluctuates even further, meaning that no discernible patterns can be observed in the grid.

To model how the spins in the grid change with temperature, computational adaptions of the Ising Model utilise Monte Carlo simulations to randomly change the individual spins. In recent models these Monte Carlo simulations now use the Metropolis algorithm, which will change the spins such that the

average probability of a certain configuration occurring follows a Boltzmann distribution. Using this method, the total magnetisation of the grid is then

$$M = \frac{1}{N}\sum_i s_i \qquad (1)$$

where s_i is the state of spin i and N is the number of atoms in the grid. Since the spins either equal +1 or -1, the value of M will equal a value between -1 and +1. Due to the average configuration probability following a Boltzmann distribution, there should be an equal likelihood that a spin state is either in an up or down state at high temperatures. Consequently, this will mean that the average magnetisation at high temperatures will be approximately equal to zero. Considering the total energy of the system, the Hamiltonian of the Ising model is defined by

$$H = -J\sum_{\langle ij\rangle} s_i\, s_j - h\sum_j s_j \qquad (2)$$

where h is the field strength of an external magnetic field applied to the system. As it is assumed there is no external field applied to the grid, the energy will only be dependent on the spin interactions of its nearest neighbours. This means that the total energy of the grid is now

$$E = -J\sum_{\langle ij\rangle} s_i\, s_j \qquad (3)$$

where J is the strength of these interactions and the $\langle ij\rangle$ notation denotes the sum runs over all the pairs of each nearest neighbour. Following these equations, the values for specific heat capacity c and magnetic susceptibility χ can then be calculated using the equations

$$c = \frac{\partial}{\partial T}\langle E/N\rangle = \frac{1}{Nk_bT^2}Var(E) \qquad (4)$$

and

$$\chi = \frac{\partial}{\partial h}\langle M\rangle = \frac{N}{k_bT}Var(M) \qquad (5)$$

where h is an external magnetic field applied to the system and Var is the variance of a given variable. As a simplification, another model was created that used a mean field approximation (MFA) of the Ising model. This MFA model assumes that each spin i behaves like a single isolated spin with an applied average magnetic field. This oversimplifies the system to a large degree, but still displays a phase transition when $T = T_c$. In addition to MFA, an exact solution to M in the $T \le T_c$ interval equals (Onsager, 1944)

$$m = \pm\left[1 - \frac{1}{\left(sinh\left(\frac{T}{T_c}ln\left(1+\sqrt{2}\right)\right)\right)^4}\right]^{\frac{1}{8}} \qquad (6)$$

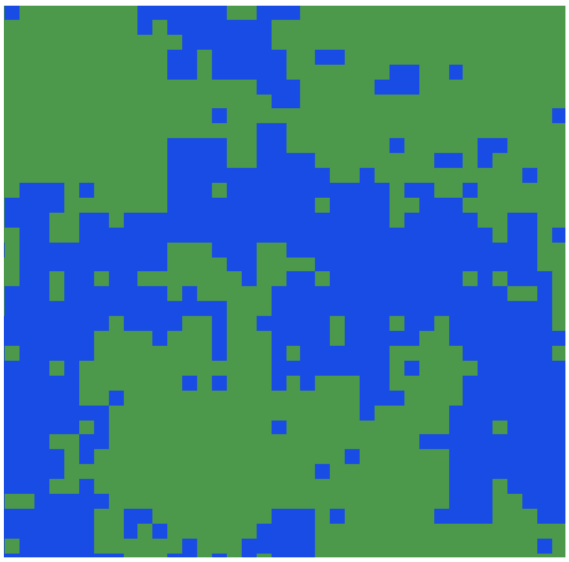

Figure 2. Still shot of the Ising model used when temperature T_0=2.27.

As such, this project focuses on comparing the computational simulations of the Ising model with its MFA and exact solution counterparts. By investigating how variables M, E, c and χ behave as temperature increases, Both the simulation and MFA can be compared to determine the behaviour of materials undergoing a phase transition. This involves analysing the initial transitions of the computational model, comparing the average values gathered from the simulations and MFA respectively, then to determine how these spin interactions change with temperature T.

2. Methodology

Using a programme written in C++, the magnetisation M and energy per particle E were calculated in the functions 'CalcMagValue' and 'CalcEnergyValue' respectively. As shown in Appendix A, these functions used equations (1) and (3) to calculate the magnetisation and energy of the system. After these values are calculated, the programme then uses the Metropolis algorithm to update the spins in the system by 'flipping' them. For any spin in the system, an energy change ΔE needed to flip a spin state to the opposite direction is calculated. If this change is negative and the energy of the system decreases that means the change is accepted, thus the spin is flipped. Alternatively, increasing the energy of the system means that the flip is accepted with a probability following the Boltzmann distribution

$$p = exp\left[-\frac{\Delta E}{k_bT}\right] \qquad (7)$$

If the change is still not accepted, the change is rejected and the spin remains in its original state. When recording the values, a dimensionless temperature T_0 was implemented to obtain the general behaviour of the system. The M and E values were then logged to separate text files, as well as the temperature of the system and the number of MC sweeps needed to produce the M and E values. This process was then repeated in a for loop using 100 T_0 values between 1.0 and 4.0. The text files were then analysed using the pandas and matplotlib libraries in Python.

The average magnetisation $\langle M \rangle$ and $\langle E \rangle$ were calculated for each sweep number, then plotted using matplotlib to determine where the results stabilised. To ensure that the data points were effectively independent from each other, the sweep numbers used were separated by a value of 10 sweeps. Once found, $\langle M \rangle$ and $\langle E \rangle$ were calculated again for each sweep number of 10 and for each value of T_0. These data points and average values were then used to calculate the variance of M and E, meaning that the values of c and χ could then be calculated using equations (4) and (5) respectively. To analyse the change in error across multiple values of T_0, the standard error of $\langle M \rangle$ and $\langle E \rangle$ were also calculated using the pandas library with the M and E values. After calculating these values, the data for $\langle M \rangle$, $\langle E \rangle$, c and χ were plotted in matplotlib against the data gathered using the Mean Field Approximation so the two methods could be compared both quantitatively and qualitatively. As the temperature in the MFA data is given as a ratio of T_c, the temperature scale of the simulation results were adjusted to fit the same units as the MFA data. To do this, the temperature values were divided a value given by the approximation

$$T_c = \frac{2J}{k_b ln\left(1+\sqrt{2}\right)} \approx 2.27J/kB \qquad (8)$$

where k_b is the Boltzmann constant. To measure the effect temperature had on the spin interaction between particles, the correlation function G_{ij} was recorded between a particle at the centre of the grid and 3 particles a set distance from the centre as shown in Appendix B. The values calculated for G_{ij} follow the equation

$$G_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \qquad (9)$$

Which considers both short and long distance interactions between two spin states. The G_{ij} values at these distances were then logged to a data file for 10 simulations of 500 sweeps, repeating for values of T_0 between 1.0 and 4.0. G_{ij} will equal 1 if the two spins directly interact with each other, so a G_{ij} value of 0 means the spins do not interact. The average values of G_{ij} were then plotted against T_0 for different distances from the centre.

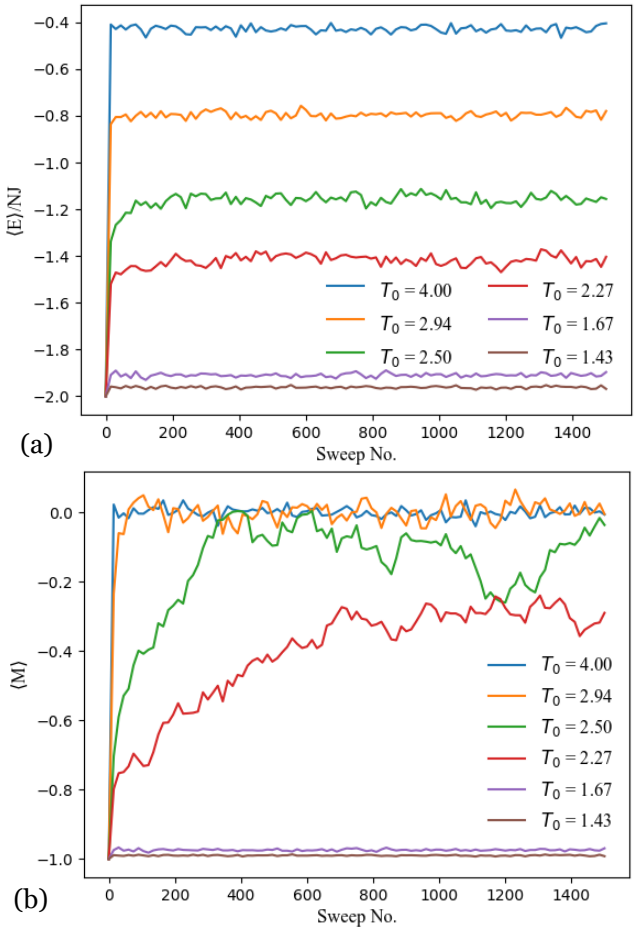

Figure 3. Change in $\langle M \rangle$ (a) and $\langle E \rangle$ (b) against the number of MC sweeps for a given temperature T_0.

3.1 Initial transients

For figure 2(a) where $T < T_c$, the $\langle M \rangle$ plots all stabilise around where M = -1.0 and stabilise at larger M values as T increases. The $\langle M \rangle$ values in this region also become stable very quickly and need less than 100 MC sweeps to stabilise. This indicates the system is magnetised at low values of T and shows a dominance of down spins described by ferromagnetic behaviour. However, when $T \approx T_c$, the system does not reach a stable value of M and instead stabilises around the M=0 region. This instability between M=-1 and M=0 indicates that there is no clear dominance of any one spin during the phase transition. Consequently, it is likely the $\langle M \rangle$ values at this temperature do not stabilise for any given amount of MC sweeps. For temperatures where $T > T_c$, the plots show a similar behaviour to when $T < T_c$ but now quickly stabilise around M=0. In addition, the M values fluctuate much more after reaching the M=0 region than the M values around the M=-1 region. By fluctuating around the M=0 axis, it can be implied that the spins in the systems are not pointing in any one direction for a long period of time. As such, the system can be described as paramagnetic when $M \approx 0$, indicating that no dominance of either spin state.

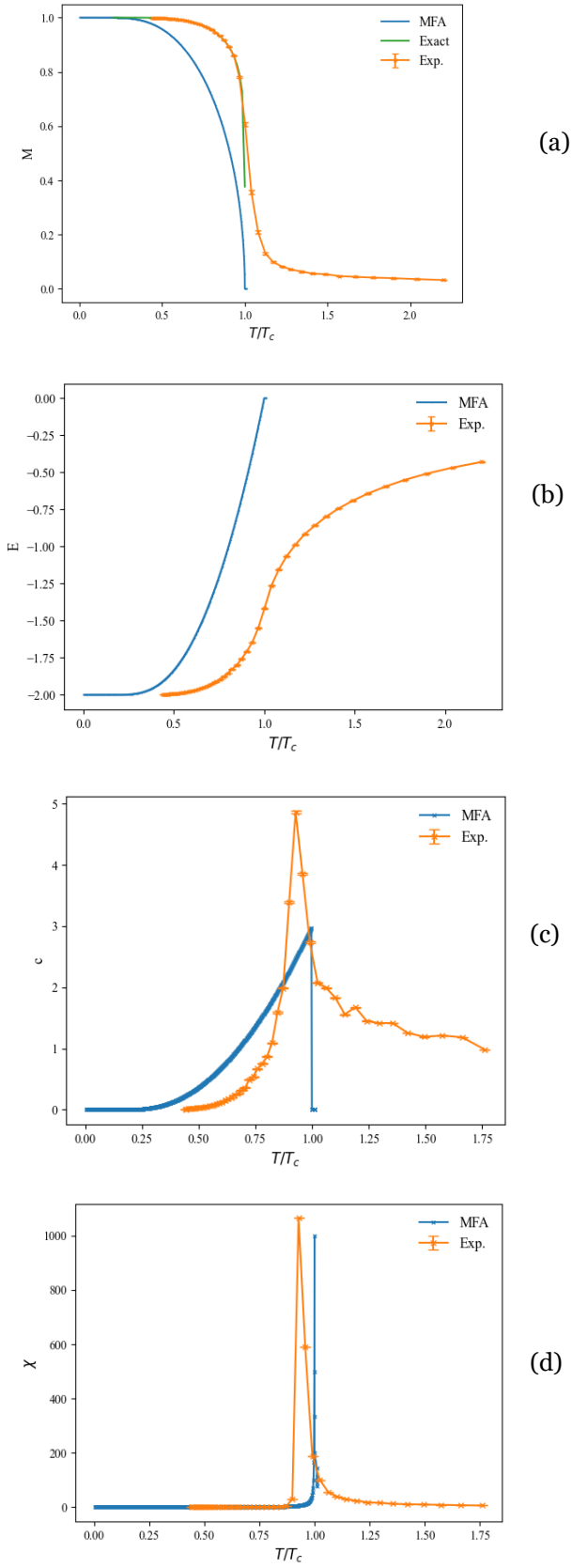

Figure 4. Comparisons of the MFA and Ising simulations for M (a), E (b), c (c) and χ (d).

Despite these variations in M after reaching stability, the E values at these temperatures will stabilise to a certain value of E after a small number of MC sweeps and will rarely deviate from this value as the sweep number increases. This is due to how the Hamiltonian is constructed for the Ising model. There is no external field introducing energy to the system as shown by equation (2), meaning that all the changes in energy after each MC sweep is due to the spin interactions in the grid.

3.2 Comparing Simulations to MFA

The MFA data in figure 3(a) remains fixed at M=1 for low values of T but starts to sharply decreases around $T = T_c$ to a value of 0 and stays at this value for $T \geq T_c$. Experimental data also shows a similar behaviour to MFA when $T < T_c$, except that it starts to decrease at a larger T value and does not decrease to a value of 0 at the $T = T_c$ point. Instead, it decays exponentially and tends towards zero as T increases for $T \geq T_c$. This inaccuracy in the MFA data will be due to the assumption that the spins in the MFA model are isolated and do not interact. As such, the only quantitative similarity that can be shared between the simulation data and the MFA data is the sharp decrease at $T = T_c$. The decrease in M also happens at a value of T greater than T_c, while the decrease in the MFA data happens at a T value less than T_c.

The trend shown in the exact solution of 3(a) shows the positive section of equation (6). The trend for this plot matches the data gathered from the simulation until reaching $T = T_c$, where the two plots start to diverge. The exact solutions also stop at $T = T_c$, meaning that both the MFA data and exact solutions cannot measure the values of M in the $T > T_c$ interval. In figure 3(b), the MFA data increases sharply at T=0.3T_c point, before reaching E=0 at $T = T_c$ and staying at that value for T>T_c. Contrastingly, the experimental data slowly increases until reaching T=0.6T_c, where it then sharply increases. The experimental data doesn't increase to E=0 like the MFA data and instead begins to plateau when T>T_c. The experimental plot tends towards E=0 as T increases, as there is an additional amount of thermal energy that is introduced to the system by increasing its temperature.

Both c and χ, in figures 3(c) and 3(d) respectively, show an exponential increase towards their peak value at T_c. While the value of c is meant to be a real number in theory, the value of χ theoretically tends towards infinity at T_c. Both the experimental values of c and χ peak at a higher value than the MFA data. However, both the simulated peak values of c and χ occur at 0.927T_c, suggesting that the simulation can be inaccurate when measuring the T_c of a material. MFA predicts that χ almost immediately decreases to zero

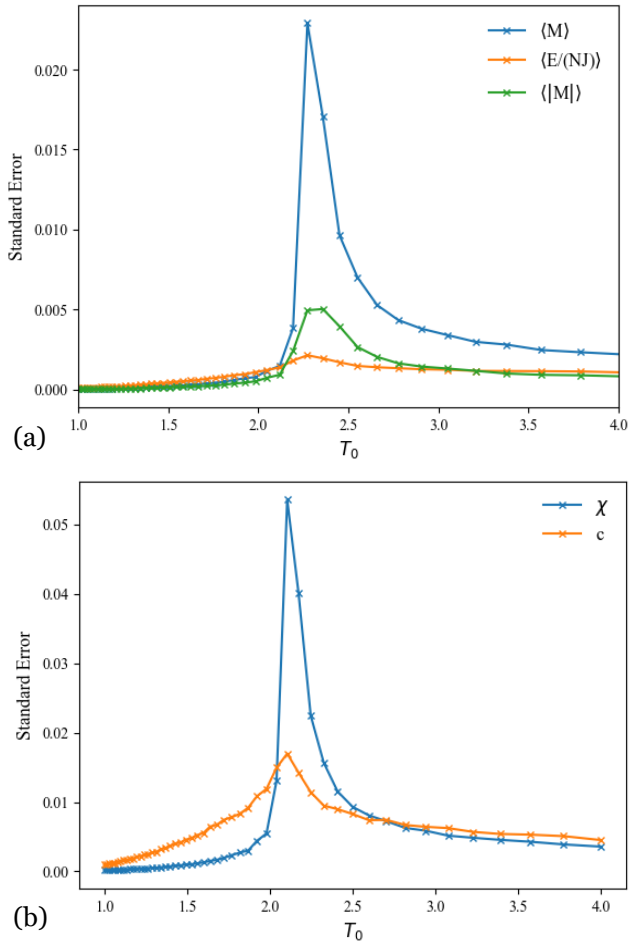

Figure 5. Trends showing the standard error of M and E against T_0 (a), as well as c and χ against T_0 (b).

after T_c, whereas the experimental values show χ tending towards zero as T increases. MFA also predicts that c immediately drops to zero at T_c, contrasting the experimental results which show c decreasing to a value greater than the c values in the T<T_c interval. This implies that, in a similar way to figures 4(a) and 4(b), the values of c and χ in the $T > T_c$ interval cannot be simulated using MFA.

3.4 Error Analysis

For both 5(a) and (b), the magnitude of the errors remains less than 0.02 for the $T < T_c$ interval. This corresponds to the stability of the system when exhibiting ferromagnetic behaviour, as the Boltzmann probability shown in equation (7) suggests that it is very unlikely for a spin state to flip at low temperatures. At $T = T_c$, the errors sharply increase for M and χ to values of 0.025 and 0.054 respectively. This is due to the behaviour of the spin states during the phase transition. As there is no dominance of either spin, the spin states will rapidly fluctuate between up and down, consequently resulting in a greatly fluctuating value for M. As χ is defined as the change in magnetisation with respect to the external field strength, this will also result in a rapidly fluctuating value for χ.

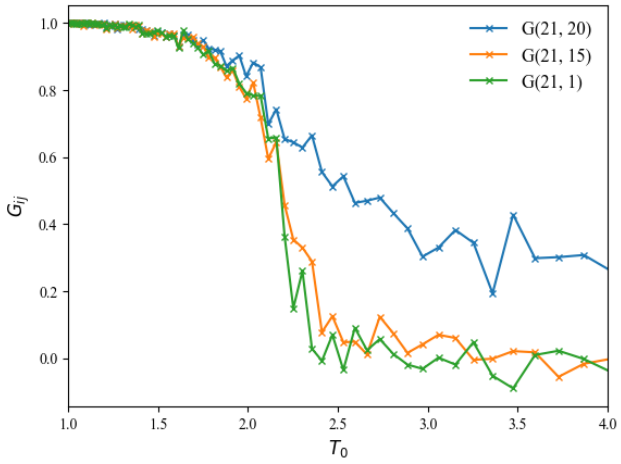

Figure 6. Trends showing the correlation function G_{ij} against T_0 for interactions between a particle at (20,20) 3 other particles at (21,20), (21,15) and (21,1).

Despite the large errors in M and χ, the error in E peaks at a value of 0.002. This is again due to how energy is conserved in the grid, as the only changes in energy occur when a spin flips in a MC sweep. This also explains why the error would be so low for ferromagnetic behaviour as very few spin flips can occur to change the energy of the system. In addition, the error will naturally be higher for paramagnetic behaviour as neither spin state dominates the grid at high temperatures, and as the spins frequently flip it results in a higher variance in the energy of the system.

3.5 G_{ij} Analysis

For the $T < T_c$ interval, the value for G_{ij} in figure 6 remains at an approximate value of 1 for all distances. However, when $T \geq T_c$, the value of G_{ij} starts to quickly decrease, tending towards zero for the short range interaction at (21, 20) and reaching an approximate value for zero at mid and long range interactions at (21,15) and (21,1) respectively. When comparing the plotted values to equation (9), it is apparent that G_{ij} can only equal zero when $\langle s_i s_j \rangle = \langle s_i \rangle \langle s_j \rangle$. As the right hand side of this equation represents the spin interaction between two independent states, this shows that at high temperatures the particles will only be affected by short distance spin interactions. Consequently, this also means that less computational processing power is needed for models of high temperature paramagnets and can be sufficiently modelled using smaller grid sizes. Additionally, this provides further evidence as to why energy only shows a large increase in variance for the $T \geq T_c$ interval. As the magnetism decreases and temperature increases, the changes in energy will be more due to temperature of the system and the nearest neighbours of the system and will be less effected by longer distance interactions.

4. Conclusion

The results shown in section 3.2 for MFA and the Onsager solution show a clear definitive behaviour at T_c, highlighting its effectiveness in modelling the general behaviour of a system during a phase transition. However, as the model cannot produce values for temperatures greater than T_c, it is more suitable to use the C++ simulation to model the material undergoing paramagnetic behaviour. Despite this, the error in the simulation show peaks for all values at the phase transition, implying that the data extracted from the simulation needs to be taken in very small data step sizes to properly analyse the grid. This is made more apparent when noting that only 6 data points out of 100 plot the behaviour of the variables during the phase transition, highlighting the need for small data steps during data analysis. This will also mean that larger amounts of processing power will be needed to run these smaller step sizes if further analysis on the phase transition is to be undertaken.

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Appendix / Appendices

Appendix A: C++ code used to calculate the magnetisation and energy of the system

```
196
197  float IsingSystem::CalcMagValue() {
198
199      //member variable equal to the sum of the spins in the grid
200      float SumSpin = 0;
201
202      for (int i = 0; i < gridSize; i++) {
203          for (int j = 0; j < gridSize; j++) {
204              int pos[2] = { i, j };
205
206              SumSpin += readGrid(pos);
207
208          }
209      }
210
211      MagTotal = SumSpin / (gridSize * gridSize); //Calculate total magnetisa
212
213      return MagTotal;
214  }
215
223  float IsingSystem::CalcEnergyValue() {
224      float NeighbourSpin = 0.0;
225      float SpinTotal = 0.0;
226      float EnergyTotal = 0.0;
227      int nborPos[2];
228
229      //Loop for every nearest neighbour pair in the grid
230      for (int i = 0; i < gridSize; i++) {
231          for (int j = 0; j < gridSize; j++) {
232
233              int pos[2] = { i, j };
234
235              for (int k = 0; k < 4; k++) {
236                  setPosNeighbour(nborPos, pos, k);
237                  NeighbourSpin += readGrid(nborPos);
238              }
239              SpinTotal += (-readGrid(pos) * NeighbourSpin);
240              NeighbourSpin = 0.0;
241          }
242      }
243
244      //Average energy per spin
245      EnergyTotal = SpinTotal / (2 * gridSize * gridSize);
246      return EnergyTotal;
247  }
248
```

Appendix B: C++ code used to calculate the magnetisation and energy of the system

```
253
254     float IsingSystem::CalcCorrFixed() {
255         int pos1[2] = { 20, 20 };
256         int pos2[2] = { 21, 20 };
257         float Spin = 0.0;
258         //float CorrelationF;
259
260         Spin += (readGrid(pos1) * readGrid(pos2));
261
262         //CorrelationF = Spin / (gridSize * gridSize);
263         return Spin;
264     }
265
266     int IsingSystem::Corr(int x1, int y1) {
267         float CorrValue = 0.0;
268
269         int fixPos[2] = { 20, 20 };
270         int VarPos[2] = { x1, y1 };
271
272         CorrValue += (readGrid(fixPos) * readGrid(VarPos));
273         return CorrValue;
274     }
```