The Ising Spin Model

Amir El-Hamdy
&
Magnus Hall

School of Physics and Astronomy
The University of Manchester

2nd Year Theory Computing Report

May 2016

Abstract

An investigation into the properties of the Ising model produced estimates of critical temperatures of 0 J/K_B for 1D, 2.301$\pm$0.038 J/K_B for 2D, and 4.543$\pm$0.035 J/K_B for 3D. A further study into the effects of lattice shape on critical temperature prompted speculation that it was linked to the long distance relations between points, as shown by the correlation function. A conclusion was made that a minimum side length of 4 was required to produce an accurate approximation to an infinite lattice for square and cubic lattices.

1 Introduction

The Ising model, the brainchild of Wilhelm Lenz, was given to its namesake, Ernst Ising, as a thesis project in 1928. Ironically, after having thought that he'd proved its uselessness as a physical model, Ising gave up research in physics. It wasn't until 20 years later that the model rose up out of obscurity, becoming one of the most studied models in modern physics. This was partly due to to its demonstration of spontaneous symmetry breaking (a phase transition between disorder and order), and the fact that its 2D form is simple enough to yield to an exact treatment in statistical mechanics. Its structure, although crude, offers important insights into domain formation in ferromagnets. [1] [2] [3]

This report details the findings of an investigation into the basic properties of the Ising model with further analysis on the effect of shape and size on results obtained.

2 Background Theory

2.1 The Ising Model

The Ising spin model (ISM) is made up of a lattice of N spin-$\frac{1}{2}$ objects, each with a magnetic momentum μ. The intrinsic lattice energy is determined by the interactions of the objects with their adjacent counterparts in the lattice. This is known as 'nearest neighbour' interaction. Each spin is also able to interact individually with an external magnetic field, B, with this energy given by the the standard equation for magnetic dipole interaction [4]

$$U = -\underline{\mu} \cdot \underline{B} \tag{1}$$

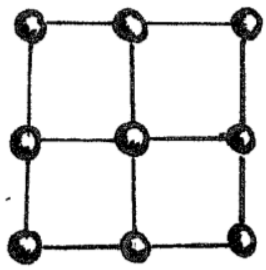


Figure 1: Diagram showing all nearest neighbour interactions for a 3x3 lattice

Hence, the total energy is given by

$$E(s) = \sum_{\langle ij \rangle} \varepsilon_{ij} s_i s_j - \mu B \sum_i s_i \tag{2}$$

where s_i is the z-component of the spin of the i^{th} object, (given as ± 1 for spin-$\frac{1}{2}$ objects), the notation $\langle ij \rangle$ indicates nearest neighbour interaction, and ε_{ij} is the magnetic interaction between adjacent objects i and j. If $\varepsilon_{ij} < 0$ and $B = 0$, the point of lowest energy will occur when all the spins are aligned. This implies that this is the model for ferromagnetic materials.

If $\varepsilon_{ij} > 0$, lowest energy occurs when the spins are all misaligned. This is the model for antiferromagnetic materials. The magnetisation of the system is simply the sum of the spins.

$$M(s) = \sum_{i}^{N} s_i \tag{3}$$

As in all statistical mechanical systems, the behaviour of the lattice is governed by a partition function, which in this case is

$$Z_N(T) = \sum e^{-E/K_B T} \tag{4}$$

where E refers to Equation 2, T is the temperature, K_B is the Boltzmann constant, and the sum is over all possible combinations of spins in the lattice (2^N). It is at this point that the temperature dependence of the system becomes clear. $K_B T$, sometimes denoted by β^{-1}, gives the thermal energy of the system. [4]

Whilst magnetic interactions are inclined to make the system more ordered, thermal energy has the opposite effect, creating higher levels of disorder. The 'order - disorder phase transition', as mentioned in the introduction, occurs as a result of these two opposing factors. At low temperature the system will be in a more ordered state, whereas with high temperature, disorder becomes more probable. At some point between the two temperature ranges, there is a point where disorder gives way to order. This is the critical temperature (T_c) at which the phase transition occurs.

2.2 The Computational Ising Model

2.2.1 The Monte Carlo algorithm

When studying the Ising model numerically, it is impractical to calculate the partition function for each temperature. Instead the equilibrium states of the system are found via the Monte Carlo algorithm. In this method, once the lattice is set up as a matrix of randomly assigned 1s and -1s, a 'sweep' is performed. This consists of randomly picking out individual sites and looking at their interaction energy given by

$$w(s_i) = -\varepsilon s_i \sum_{nn} s_{nn} - B s_i \tag{5}$$

where ε is the same as in Equation 2 and nn refers to nearest neighbour interactions.

As can be seen, if the spin, s_i, were to be flipped, w would change sign from + to - or vice versa. The Metropolis algorithm governs the likelihood of this spin flipping.

If $w > 0$ flip s_i
If $w < 0$ flip s_i with probability $e^{-2\beta w}$

This algorithm is repeated many times per sweep and produces the same situation as in the original statistical model. Magnetic interaction energy still encourages order whilst thermal energy promotes disorder. [5]

This process results in the system, after many sweeps, tending toward a series of equilibrium states in which the energy of the lattice remains roughly constant. Once the system is at equilibrium, the average lattice energy and magnetism over several sweeps are found and given as being the values at that temperature. After every temperature change, a period in which no measurements are taken is needed to allow the system to achieve its new equilibrium.

2.2.2 Periodic Boundaries

In the statistical model, critical temperature is found by taking $\lim_{N\to\infty}$. This is impossible to do numerically as it would take an infinite amount of time to perform just one sweep. Instead a compromise is reached in the form of 'periodic boundaries'. Under these conditions, the missing nearest neighbour for a site on the edge of the lattice is defined as its mirror either horizontally or vertically across the lattice. This allows matrices to be fairly small whilst still simulating an infinite lattice.

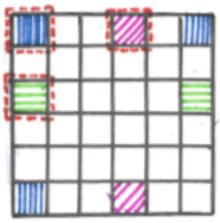


Figure 2: Diagram displaying how boundary conditions map nearest neighbour interactions for points on the edge to the far side of the lattice.

2.3 Measurements Taken

Temperature, magnetisation and energy were recorded for each lattice. These values were used to find heat capacity

$$C = \frac{1}{K_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{6}$$

and magnetic susceptibility

$$\chi = \frac{1}{K_B T}\left(\langle M^2\rangle - \langle M\rangle^2\right) \tag{7}$$

where $\langle\rangle$ denotes the average of a value.

Another property that was observed was the relationship between spins at varying distances. this observation was done via the correlation function

$$C(r) = \langle s_1(r)\cdot s_2(r+R)\rangle - \langle s_1(r)\rangle\langle s_2(r+R)\rangle \tag{8}$$

where spins s_1 and s_2 are distance R apart. The output of this function gives an indication of how strong the relation between s_1 and s_2 is with a strong relation resulting in a correlation value closer to 1.

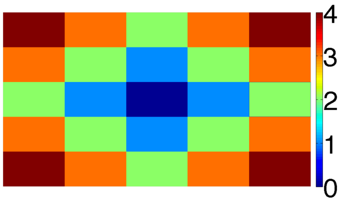


Figure 3: Diagram to show how distance R is specified for the correlation function. Squares of the same colour are the same distance from the centre point.

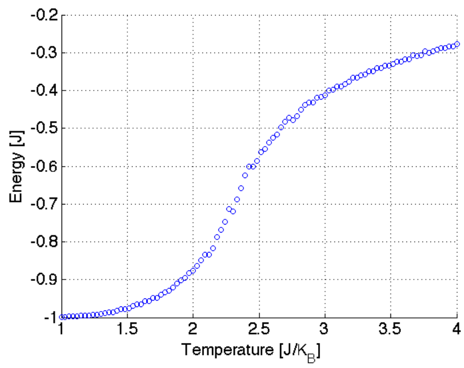
2.4 Phase transitions

As mentioned before, one of the main features of the ISM is its ability to exhibit a phase transition. Phase transitions are characterised by the behaviour of an ‘order parameter’ around the critical temperature. Generally the order parameter ranges from non-zero at temperatures lower than T_c to zero for temperatures greater than T_c. In the case of the ISM, the order parameter is the net magnetisation. At T_c, the susceptibility of the order parameter diverges (goes to infinity) producing a recognisable peak. Therefore when looking for T_c in the ISM it is easiest to find the temperature at which the highest value of magnetic susceptibility occurs.

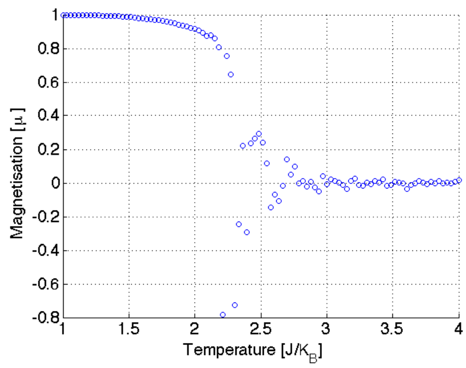
3 Results and Discussion

For the entirety of the investigation, the main subject of research was nearest neighbour interactions. Magnetic field was left at 0 throughout and so it can be assumed in all graphs that $B = 0$.

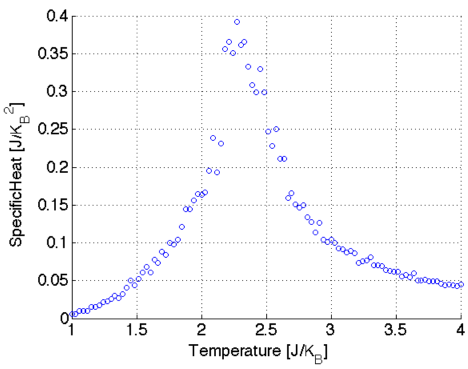
3.1 Phase changes in a square lattice



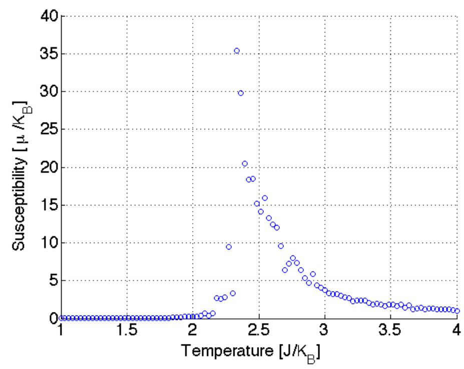
(a) Energy vs. temperature



(b) Average magnetisation vs. temperature



(c) Specific heat capacity vs. temperature



(d) Magnetic susceptibility vs. temperature

Figure 4: Graphs showing how the energy, magnetisation, heat capacity and magnetic susceptibility of a 14x14 lattice change with temperature.

In Figure 4b, spontaneous symmetry breaking can be seen around $T = 2.5$ J/K$_B$. Above a certain temperature, the total magnetism lies around 0 with the lattice exhibiting high levels of disorder. As it cools, there is a certain temperature at which the lattice suddenly gains an overall magnetisation with average spin going to $+1$. Figure 5 demonstrates that this spontaneous symmetry breaking can just as easily go in the other direction, resulting in all spins at -1.

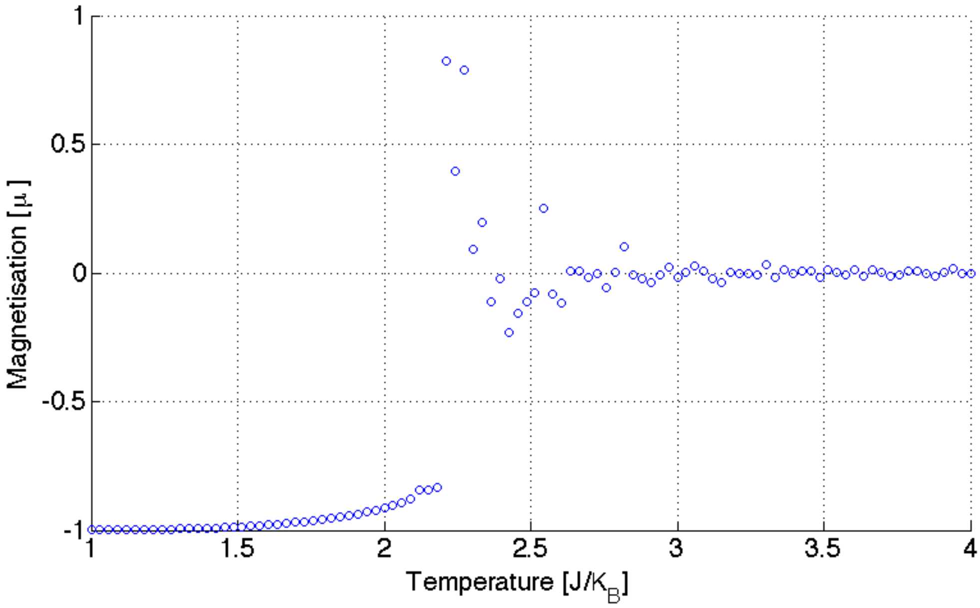


Figure 5: Average magnetisation vs. temperature for a 14x14 lattice. Symmetry breaking in this graph goes the other way from in Figure 4b despite the lattices being essentially identical.

In each of the graphs of Figure 4, one of the most prominent features is the phase transition, seen most clearly as a discontinuity in magnetic susceptibility (4d) between 2 and 3 on the temperature scale.

The temperature at which this phase transition occurs is shown to converge on a single point with increasing lattice size by Figure 6. The statistical model for the 2D lattice yields an exact value of $T_c = 2.269$ J/K$_B$. Since the y intercept of Figure 6 is 2.301 ± 0.038 J/K$_B$, it can be deduced that this convergence is towards the exact value for an infinite lattice.

Figure 7 helps provide a reason for this convergence. It shows the correlation between spins as calculated by Equation 8. It can be seen that although correlation rapidly decreases with increasing R, it takes quite a large R for C to become 0. The shape of the graph suggests that it is asymptotic at 0. This means that with periodic boundary conditions, each site has some degree of interaction with itself. In a similar vein, sites on opposite sides of the lattice will have influences from one another affecting them from both sides. With increasing lattice size, these effects are reduced and hence the behaviour more resembles that of an infinite lattice.

Figure 8 shows how temperature affects correlation curves. The reason for such high correlation at $T < T_c$ is fairly self evident as almost all spins are aligned at this point, so from the perspective of the function there is a high correlation. In truth this is not so much an indicator of how much one spin affects another as it is that all the spins are in a fixed orientation. The curve for $T = T_c$ is much the same in that it shows that there are some

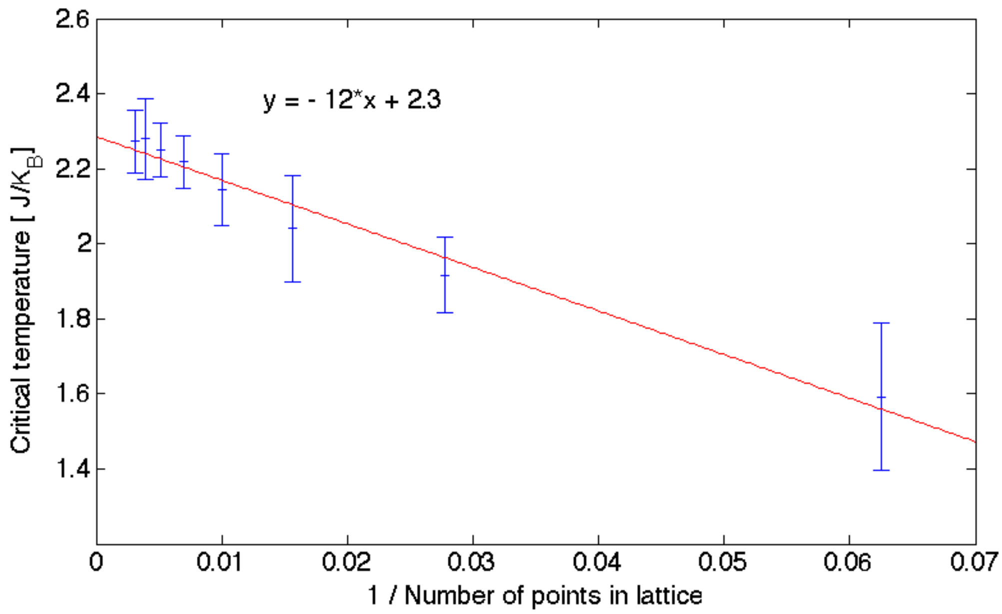


Figure 6: Graph displaying the convergence of the critical temperature with increasing 2D lattice size. An estimate for the critical temperature of an infinite 2D lattice, given by the y intercept, is $T_c = 2.301 \pm 0.038$ J/K$_\mathrm{B}$. $\chi^2 = 0.705$.

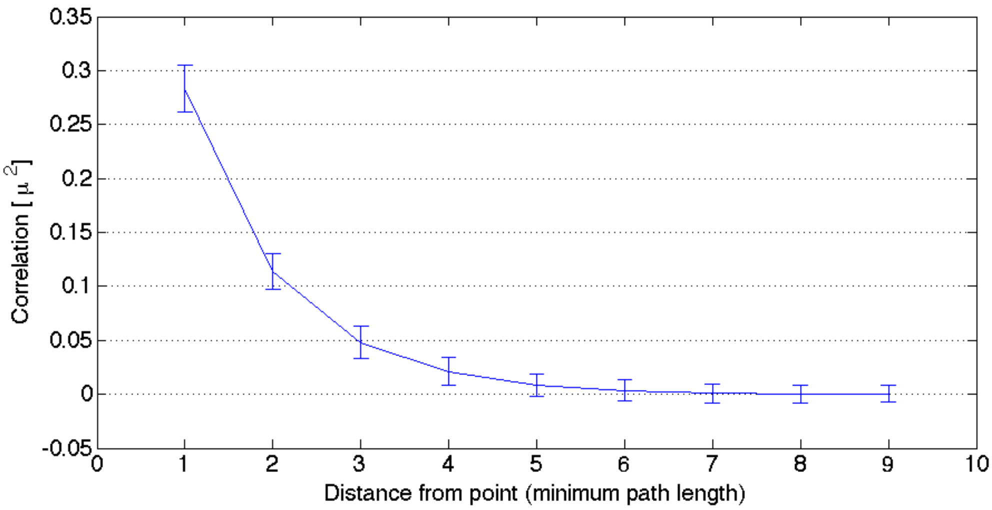


Figure 7: Graph to show how correlation between points changes with distance apart at a temperature greater than the critical temperature in a 2D lattice.

areas of alignment forming, resulting in a high correlation. The $T > T_c$ curve, shown more clearly in Figure 7, gives the best indication of the influence of one spin on another, as the spins are much more free to switch in the disordered state.

3.2 The 1D Lattice

Figure 9 shows clear evidence of a phase transition for 1D lattices at $T = 0$ J/K$_\mathrm{B}$. To explain this, one must consider nearest neighbour interactions in the lattice. As was mentioned before, the interaction energy encourages order in the system. In 1D there are just

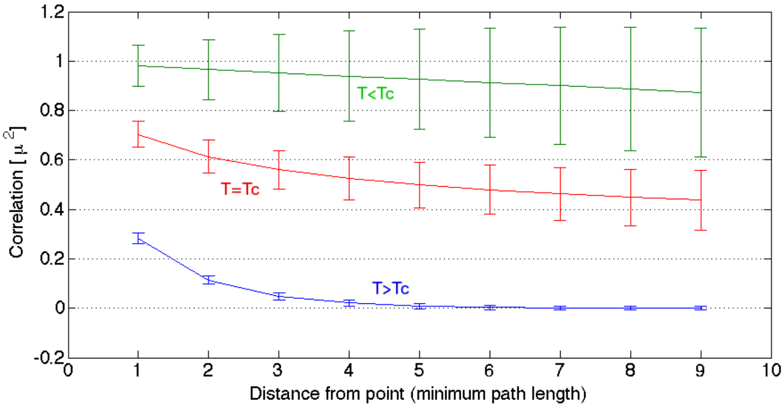


Figure 8: Graph to show how the correlation between points at varying distances changes with temperature for a 2D lattice.

2 interactions per site. There are not enough nearest neighbours in this situation for the ordering effect of the interaction energy to become apparent when competing with the disorder encouraged by the thermal energy. Therefore it is only when $K_B T = 0$ that the system becomes ordered.

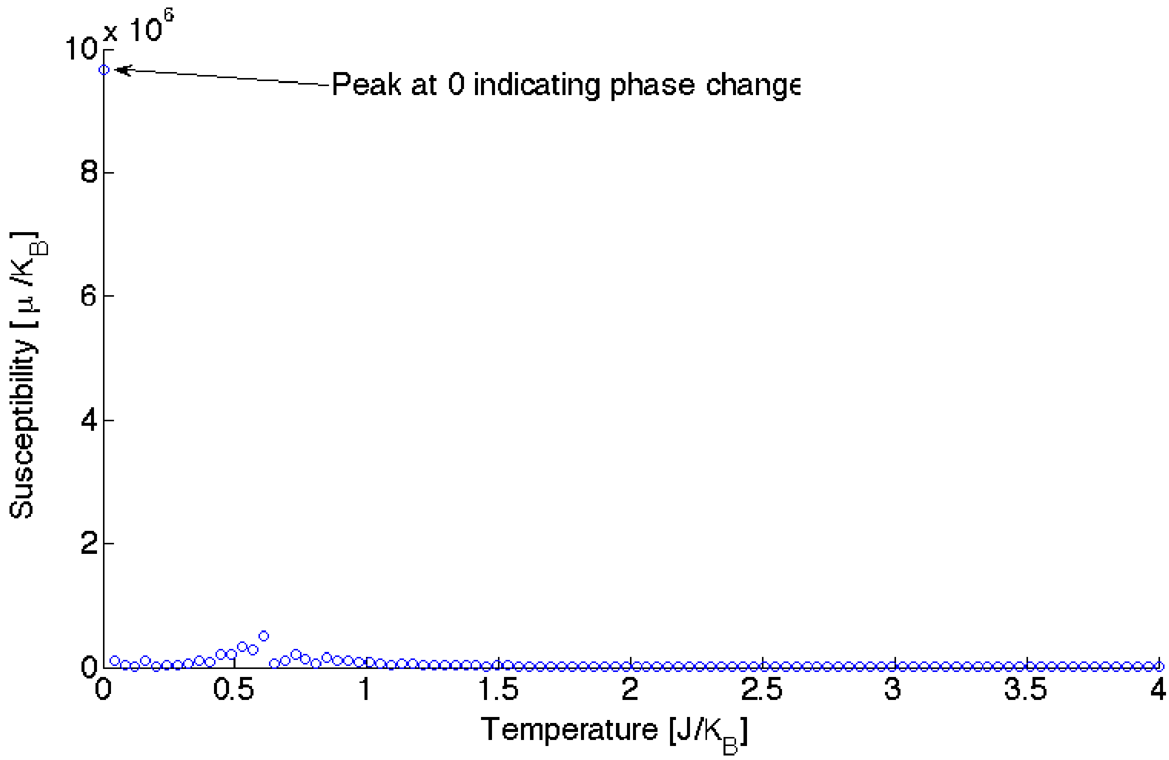


Figure 9: Graph of magnetic susceptibility against temperature showing evidence of a phase transition at 0 J/K$_B$ for a 1D lattice of length 10000.

Figure 10 shows what happened when the same method for finding T_c was carried out on results for smaller 1D lattices. Interestingly this graph shows no convergence as Figure 6 does. This anomaly can be explained by looking again at Figure 9.
In this graph, there is a small peak at around 0.5, thought to be due to the formation of small areas of alignment or 'domains'. Figure 6 shows that T_c increases with lattice size for 2D lattices. If 1D lattices were to follow the same trend, for small 1D lattices this

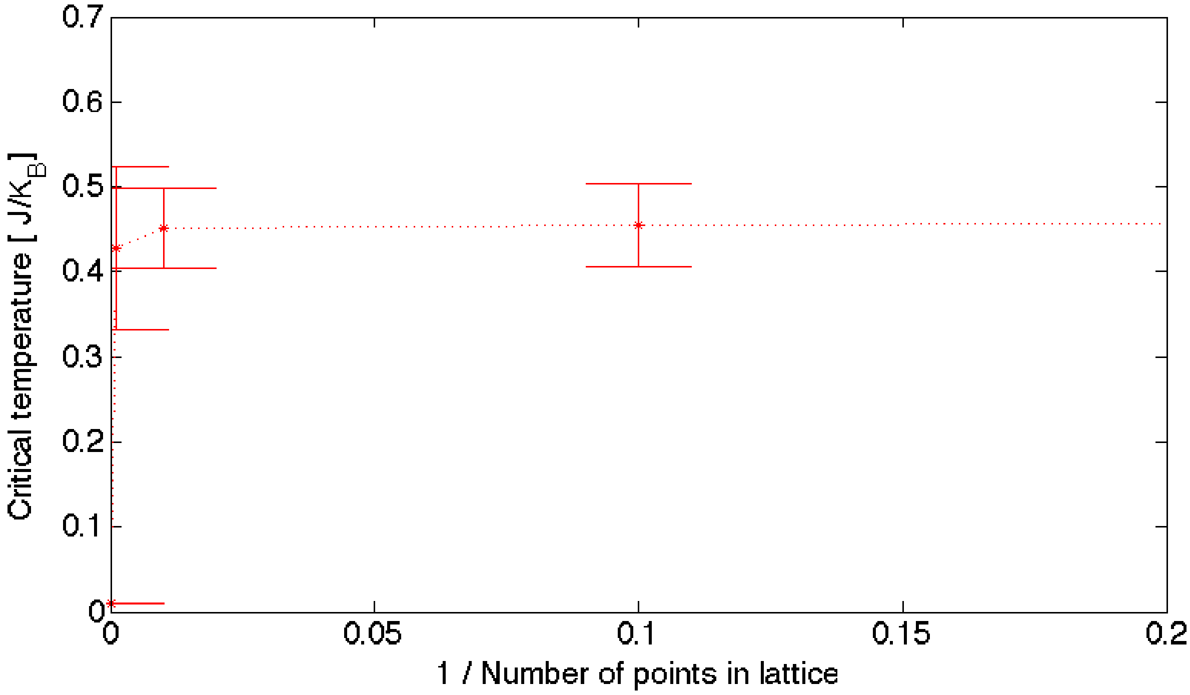


Figure 10: Graph of 1D lattice size against critical temperature as determined by highest value of magnetic susceptibility in a 1D lattice.

would mean that T_c is negative. The calculations did not cover temperature less than 0 and so the main peak was missed. Instead a minor secondary peak was reported, resulting in the plateau seen in Figure 10.

3.3 The 3D Lattice

Following the consideration of the effect of interactions on T_c in 1D; it can be predicted that the critical temperature of a 3D lattice is higher than that of a 2D lattice. The number of nearest neighbours is 6 rather compared to 2D's 4, and so the ordering effect should be stronger. This means that it will take a higher thermal energy to promote disorder in the lattice.

Figure 11 confirms this prediction, demonstrating a convergence with increasing lattice size to $T_c = 4.543 \pm 0.035$ J/K$_B$.

3.4 The Shape of lattices

As a further investigation, the effect of 2D lattice shape on T_c was observed. Figure 12 shows the results of this investigation. Side lengths are on the x and y axes, and colour gives an indication of relative T_c. Darker squares indicate a lower T_c. This graph supports the hypothesis laid out at the end of section 3.1, linking T_c to correlation. It can be seen that although there is some small rise in T_c produced by increasing just x or y, the greatest changes occur when both are increased. This implies that the main factor that governs the

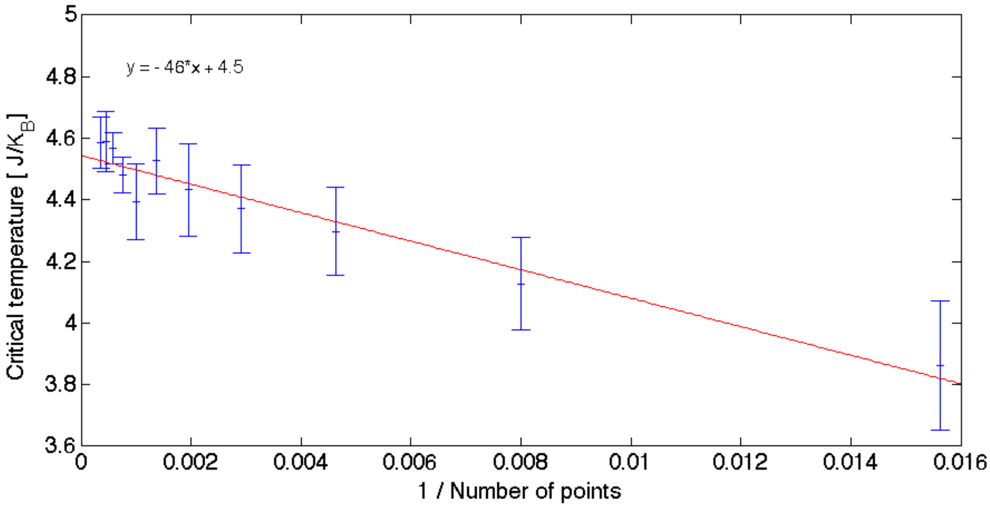


Figure 11: Graph showing convergence of T_c of cubic lattices with increasing lattice size. y intercept gives an estimate of $T_c = 4.543 \pm 0.035$ J/K$_B$ with $\chi^2 = 3.034$

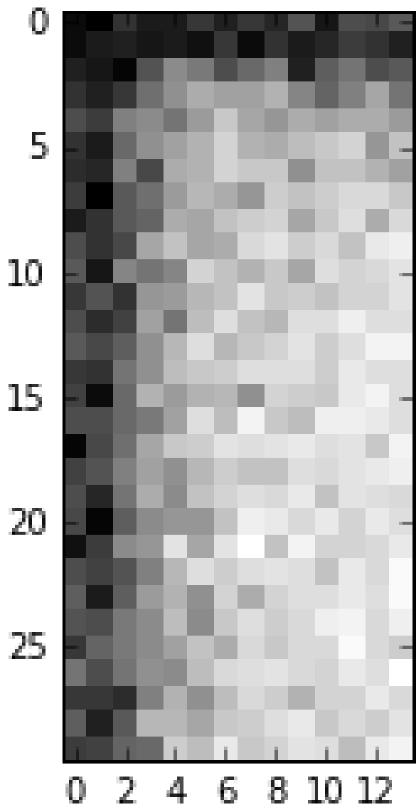


Figure 12: Graph displaying how relative critical temperature changes for different widths and lengths of a lattice. For example the bottom right square represents a 14x30 lattice. Darker squares indicate a lower T_c.

T_c of a lattice is minimum side length, not number of sites as might be surmised if one were to just observe square lattices.

Similarly to Figure 7, the colour gradient is clearly seen to level out when both x and y are more than 3; i.e. the effects of correlation are minimal in the lattice. This implies that the smallest 2D lattice that will still accurately simulate an infinite lattice is 4x4.

Performing the same investigation with 3D lattices, Figure 13 shows a similar trend as for 2D lattices in which the largest changes in T_c occur when x, y and z are all increased. The gradient is visibly very similar to Figure 12.

One key difference is that the gradient is much more regular for increasing individual side lengths. However this could be attributed to a smaller range in axes lengths investigated.

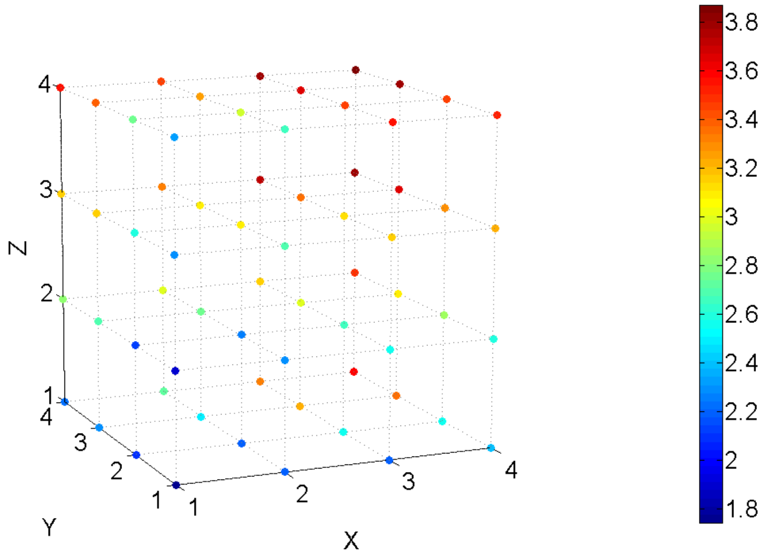


Figure 13: Graph displaying how relative critical temperature changes for different maximum x, y and z values of a lattice. The scale goes from cooler blue points around $(1,1,1)$ to warmer red points around $(4,4,4)$. The warmer a T_c is on this graph, the closer it is to the true value of T_c for 3D lattices.

4 Conclusion

In this report, important insights were made into the effect of shape, size and dimensionality on the properties of the ISM.

It was found that the T_c of 2D lattices converges to a temperature of $T_c = 2.301 \pm 0.038$. A hypothesis was made that this convergence could be related to long distance interaction between points on the lattice, as displayed by the correlation function.

The 1D lattice was briefly covered, with a plot showing phase transition at 0. An interesting anomaly was highlighted where the critical temperature graph didn't show convergence of T_c with increasing lattice size. It was thought that this may be due to the critical temperature increasing to 0 with increasing lattice size, as this was the trend shown for 2D and 3D T_c plots. If this was the case, the actual T_c values were outside of the range of temperatures investigated.

The 3D lattice was found to have $T_c = 4.543 \pm 0.035$ by the same method of convergence as for 2D. It was decided that the increase of T_c with growing dimensionality was likely to do with the increasing number of nearest neighbours for each point.

An investigation into the effect of shape and size on the T_c of lattices made clear the importance of minimum side length in the accuracy of T_c estimates. The minimum side length in order to accurately simulate an infinite lattice was found to be 4. This also served to further strengthen the link between the correlation and lattice size.

References

[1] Niss, M. Archive for History of Exact Sciences. *History of The Lenz - Ising Model 1920–1950: From Ferromagnetic to Cooperative Phenomena*. Springer. 2005; volume 59, No. 3

[2] Brush, S. Reviews of Modern Physics. *History of the Lenz–Ising Model*. American Physical Society. 1967; volume 39, No. 4

[3] Huang, K. *Statistical Mechanics*. John Wiley and Sons, Inc. 1987

[4] Reichl, L. *A Modern Course in Statistical Physics*. Wiley-VCH. 2009

[5] Huang, K. *Introduction to Statistical Physics*. Taylor and Francis. 2001