2-D Ising Model in C

Joe Salkeld

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Abstract

The project's aim was to code a two-dimensional Ising model of ferromagnetism using C, and output graphs of the energy, magnetisation, heat capacity and susceptibility of the system as a function of temperature. The code demonstrates the material changing from ferromagnetic to paramagnetic at the Curie temperature. The critical exponent values for heat capacity, magnetisation and susceptibility (α, β and γ respectively), were found to be $\alpha = 0.02 \pm 0.01$, $\beta = 0.11 \pm 0.03$ and $\gamma = -1.6 \pm 0.3$, which are within the error of accepted values. The behaviour of the material changed from ferromagnetic to paramagnetic around the Curie temperature as expected, with the paramagnetic magnetisation as a function of applied field approximating a Brillouin function. The code could execute lattice sizes of 50x50 to calculate critical exponents with a runtime of 175 seconds, and when plotting the spatial magnetisation of the lattice, could output a 300x300 system in 26 seconds.

1 Introduction

A code was written to solve the two-dimensional Ising model for ferromagnetism, and check the relations between temperature and the magnetic properties of the material: magnetisation, heat capacity and susceptibility. The code uses the Metropolis algorithm for random sampling to evolve the system into a relaxed magnetic state. Graphs of the magnetic quantities as a function of temperature were plotted to determine their relationship, which were then compared to the scaling laws found by Lars Onsager [1]. The code was also used to predict the behaviour of the magnetisation both below, at and above the Curie temperature.

2 Method

2.1 Magnetic Quantities

The two-dimensional Ising model is based around the calculation of the total energy of the magnetic system. This is given by an equation of N spins $\boldsymbol{s}_i$

$$E = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(n(i,j)\boldsymbol{s}_i \cdot \boldsymbol{s}_j) - \mu_B \sum_{i=1}^{N} \boldsymbol{B} \cdot \boldsymbol{s}_i, \qquad (1)$$

which is comprised of two terms. The first is the exchange energy of the atoms, which only interacts with the nearest neighbours. J is the strength of this interaction and the factor of a half avoids double counting. The value of J is something which is found experimentally, and can vary based on the bulk properties of the material, but is on the order of ≈ 10 meV. The values of J from [2] are used, for Iron, Cobalt and Nickel. μ_B is the Bohr magneton, and

$$n(i,j) = \begin{cases} 1, & \text{if } \boldsymbol{s}_i \text{ and } \boldsymbol{s}_j \text{ are nearest neighbours,} \\ 0, & \text{otherwise .} \end{cases}$$

The second term in the equation is the Zeeman energy which adds the effect of an applied magnetic field $\boldsymbol{B}$.

The system itself is a two dimensional square matrix with randomly assigned values of +1 and -1 representing spin orientation. The orientation is randomly generated using a Mersenne Twister RNG [3], and implemented using the GSL RNG Library [4]. As the code is attempting to model an infinite lattice, periodic boundary conditions are imposed on the system to eliminate edge effects. This is done by allowing the matrix to 'wrap around' when calculating $n(i,j)$, so the edges of the matrix affect each other. In this way all atoms in the lattice have four nearest neighbours, and the two dimensional system acts like it was on the surface of a torus.

The system is evolved by selecting a spin at random and then calculating the change in energy ΔE that would be required to flip it. The Metropolis algorithm is then used to decide whether the spin is flipped or not.

Algorithm 1 Metropolis Algorithm on Spin Flip

```
if ΔE <= 0 then
    Flip the Spin
else
    generate a random number between 0-1
    if random number < exp^(-ΔE/(k_B T)) then
        Flip the Spin
    end if
end if
```

This extra chance for the spin to flip employs a Boltzmann factor allowing the temperature T to affect the evolution. This evolution is iterated N times, and then the energy is calculated. This is repeated 5000 times to allow the energy to average out.

The three quantities of interest are the Magnetisation $\boldsymbol{M}$, the Heat Capacity C and the Susceptibility χ. These are cal-

culated as follows:

$$\boldsymbol{M} = \frac{1}{N}\sum_{i=0}^{N} \boldsymbol{s}_i, \tag{2}$$

$$C = \frac{\partial}{\partial T}\langle E\rangle = \frac{\sigma_E^2}{k_B T^2}, \tag{3}$$

$$\chi = \lim_{H\to 0}\frac{\partial}{\partial H}\langle M\rangle = \frac{\sigma_M^2}{k_B T}, \tag{4}$$

where σ_E and σ_M are the standard deviation of the fluctuations in energy and magnetisation respectively.

The Curie temperature T_c of the system (where the material transitions from ferromagnet to paramagnetic) can also be found by examining the graphs these three quantities produce when plotted against temperature.

According to theory, the magnetic quantities are linked to the Curie temperature by the following relations

$$\begin{aligned} C &\propto |T - T_c|^{\alpha}, \\ M &\propto |T - T_c|^{\beta}, \\ \chi &\propto |T - T_c|^{\gamma}, \end{aligned} \tag{5}$$

with the critical exponents having values of

$$\alpha = 0, \beta = \frac{1}{8}, \gamma = -\frac{7}{4}, \tag{6}$$

For a finite system however, the heat capacity C is not a constant value and actually varies with the dimensions of the system D with a linear relationship

$$C_{\max} \propto \ln(D), \tag{7}$$

and this code will calculate and verify this behaviour.

2.2 Magnetisation at Constant Temperature

For a ferromagnet, the spins align due to the exchange interaction. However, above the Curie temperature, the material becomes paramagnetic, and the magnetisation becomes a function of the applied field at a constant temperature. This function is known as a Brillouin function [5]; it only depends on the ratio of B to T and describes the magnetisation of an ideal paramagnet as a function of applied field.

More detail on Brillouin functions is not necessary as in the Ising model the function simplifies to

$$M = \tanh(x) \tag{8}$$

where x is proportional to $\frac{B}{T}$. This function is a useful way to show that the behaviour of the material for temperatures above T_c is paramagnetic and not ferromagnetic. Graphs of varying temperatures above T_c will be plotted and shown to reflect hyperbolic tangent functions.

2.3 Domain Imaging

Another way to view the magnetic behaviour of the material is by plotting the magnetisation spatially, with +1 and -1 being represented by different colours. This goes some way to displaying the domain behaviour of the material. It is energetically favourable for a material to have regions of magnetisation oriented in the same direction, which reduces the stray field. For the 2-D Ising model the magnetisation is only in one of two states, so cannot rotate from one to the other over any spacial distance. By visualising the spins at different temperatures, the breakdown of magnetic order can be seen around the Curie temperature. Below T_c the magnetisation will tend to be uniform (ferromagnetic). As T_c is neared, domains will begin to form and eventually, once T_c is surpassed, the domain structure of the system will break down and the magnetisation will be proportional to the applied field (paramagnetic).

3 Results

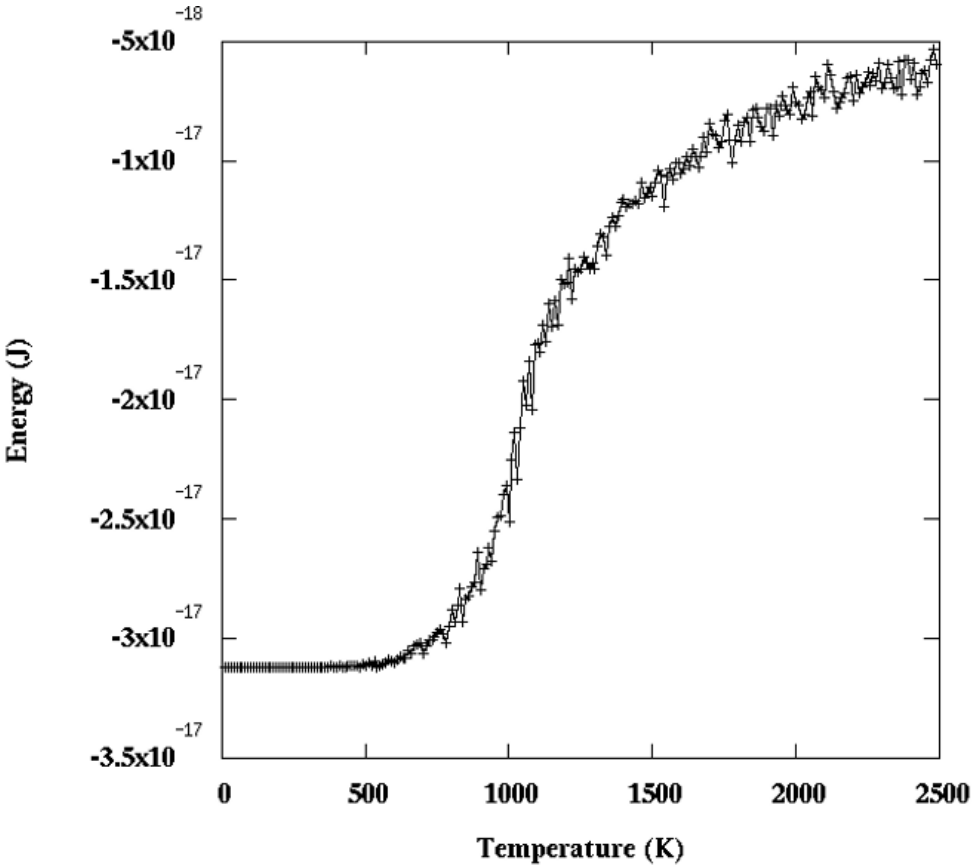

Figure 1: The energy dependence on temperature in zero applied field, for a lattice of 50x50.

The total energy of the system increases as the temperature increases due to the breakdown of ferromagnetic behaviour, resulting in a larger exchange energy term. The system wants to minimise its energy, and spins which are aligned parallel to each other have a smaller exchange energy than those which are anti-aligned [6]. Therefore at low temperatures when the system is a ferromagnet, the spins are all aligned and the energy is at a minimum. As the temperature increases, the spins begin to flip due to the Boltzmann factor, which leads to neighbouring spins being oriented in opposite directions, increasing the energy.

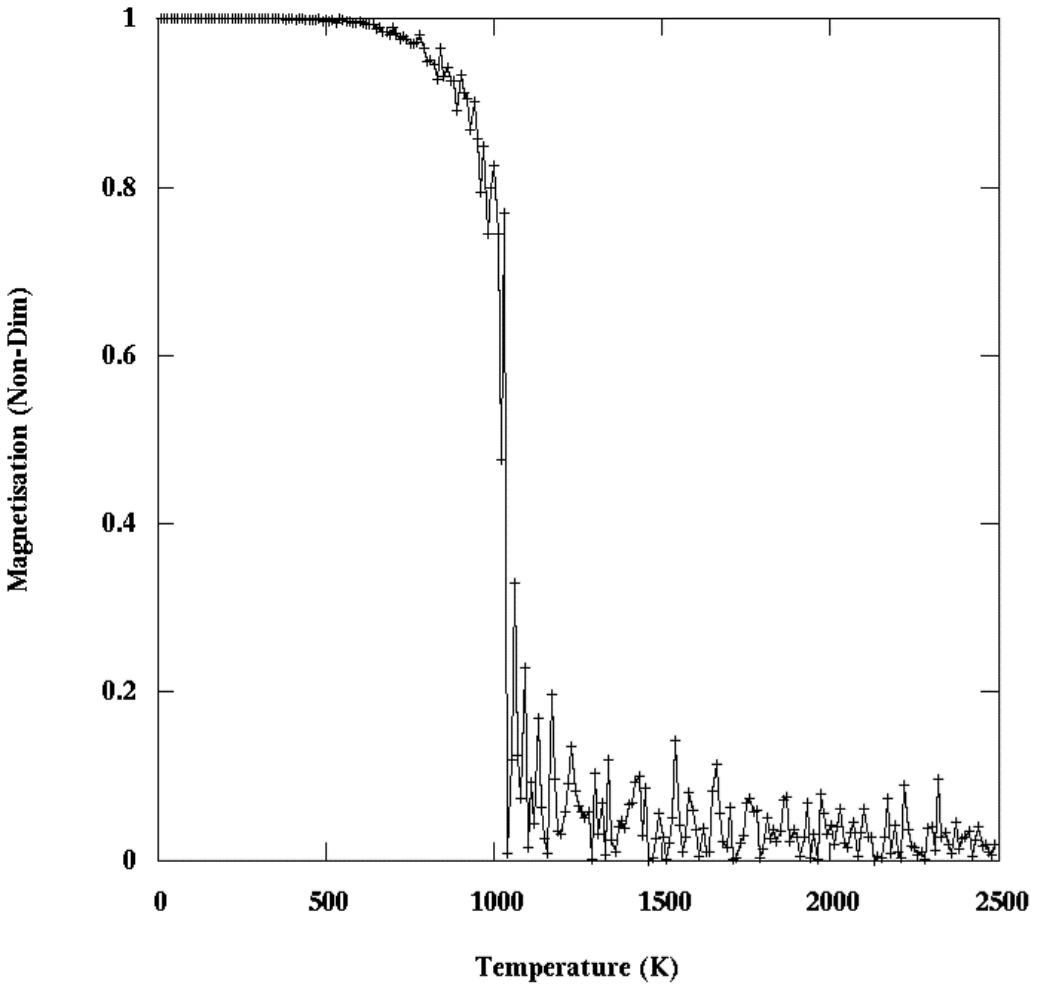

Figure 2: The absolute value of the magnetisation at zero applied field, with varying temperature for a lattice of 50x50.

The sample is uniformly magnetised at temperatures below T_c, but as it approaches the Curie temperature the magnetisation becomes less uniform. Above the Curie temperature of around 1000 K, the material behaves paramagnetically, with magnetisation only arising with an applied field, hence the drop to zero. The theoretical critical exponent is $\beta = 0.125$, with the code producing $\beta = 0.11 \pm 0.03$.

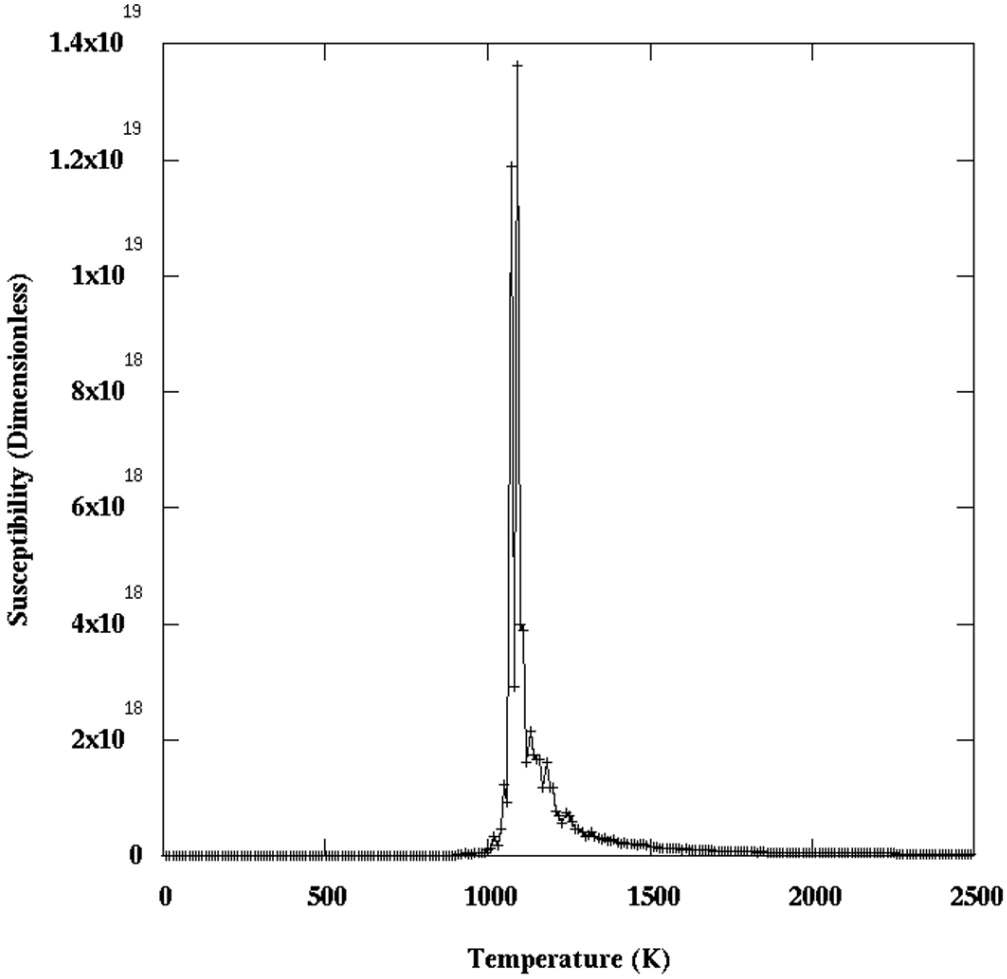

Figure 3: The susceptibility of a sample with no applied field, for a lattice of 50x50.

The susceptibility of the material is directly linked to the standard deviation of the magnetisation, as can be seen in equation 4. When the magnetisation is uniform at temperatures much below T_c, this standard deviation is zero, and the same applies when the material is behaving paramagnetically, for temperatures much larger than T_c. The region around the Curie temperature is important, as this is where the magnetic behaviour transitions from ferromagnet to paramagnet, and so the magnetisation changes. This gives rise to a steep peak at T_c, followed by a quick decrease, with a theoretical critical exponent of $\gamma = -1.75$. This model gave a critical exponent of $\gamma = -1.6 \pm 0.3$.

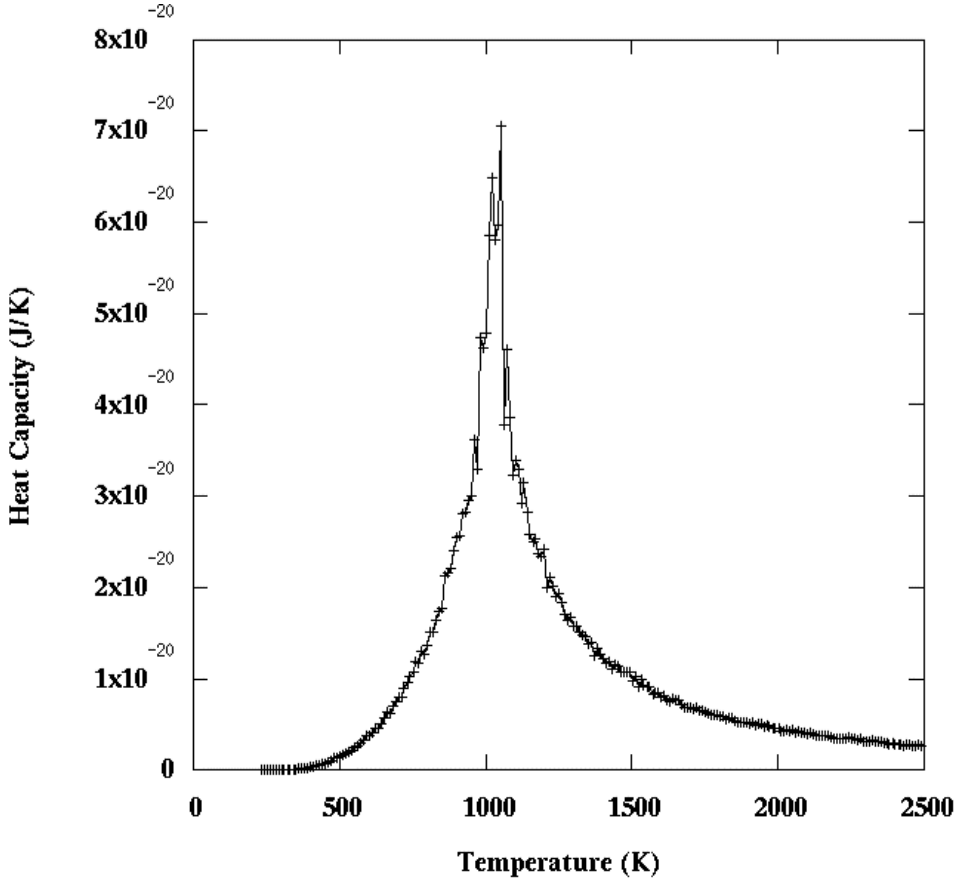

Figure 4: The heat capacity as a function of temperature in zero applied field for a lattice of 50x50. The peak in the heat capacity occurs at the Curie temperature.

The heat capacity of the material is related to the standard deviation in the energy of the material, from equation 3. The energy increases as the Curie temperature is approached, before stabilising out at temperatures much greater than T_c. This graph has a theoretical critical exponent of $\alpha = 0$, as there should be a single peak at the Curie temperature, and this model gives an $\alpha = 0.018 \pm 0.009$.

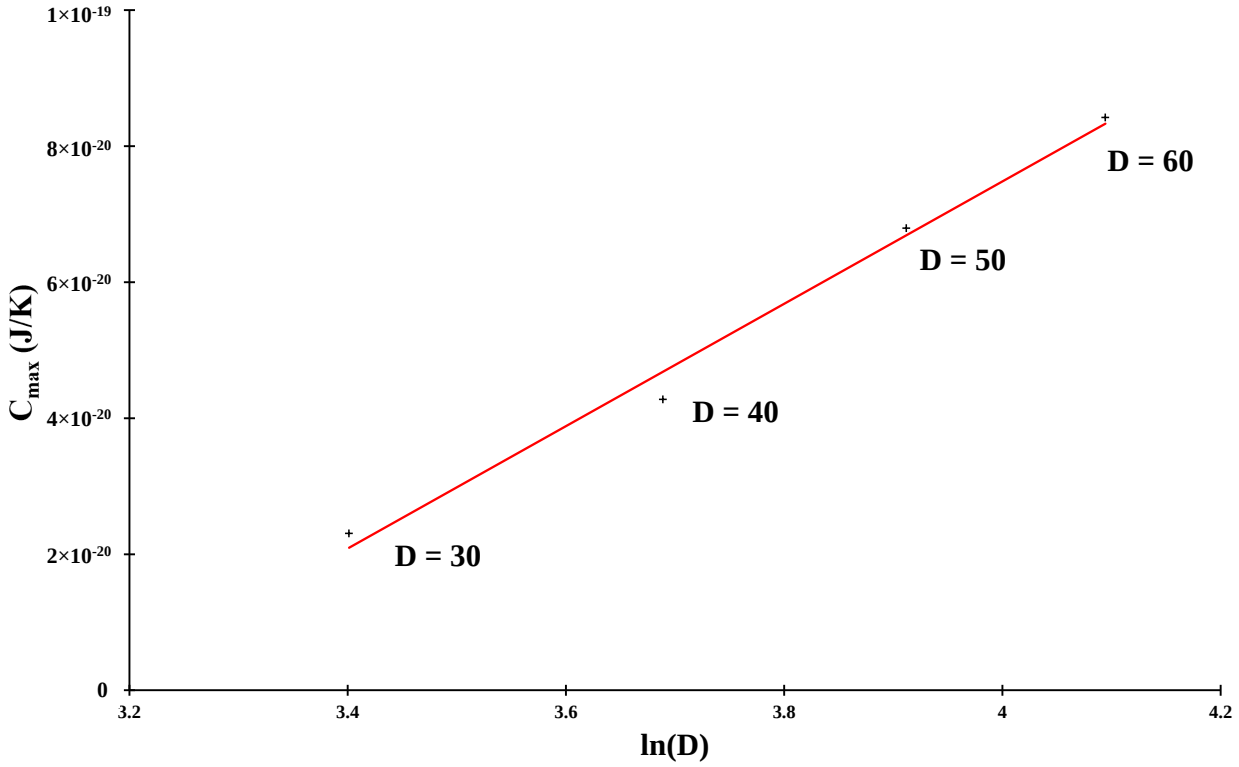

Figure 5: The linear relationship between the maximum value of the heat capacity and the natural logarithm of the system dimensions DxD.

From equation 7 it is expected that the maximum heat capacity of a sample will vary linearly with the natural logarithm of the system dimensions. Figure 5 demonstrates this with values in the lattice size from 30x30 to 60x60. The largest lattice sizes were chosen because the error in the maximum value of the heat capacity is smaller for larger values of D.

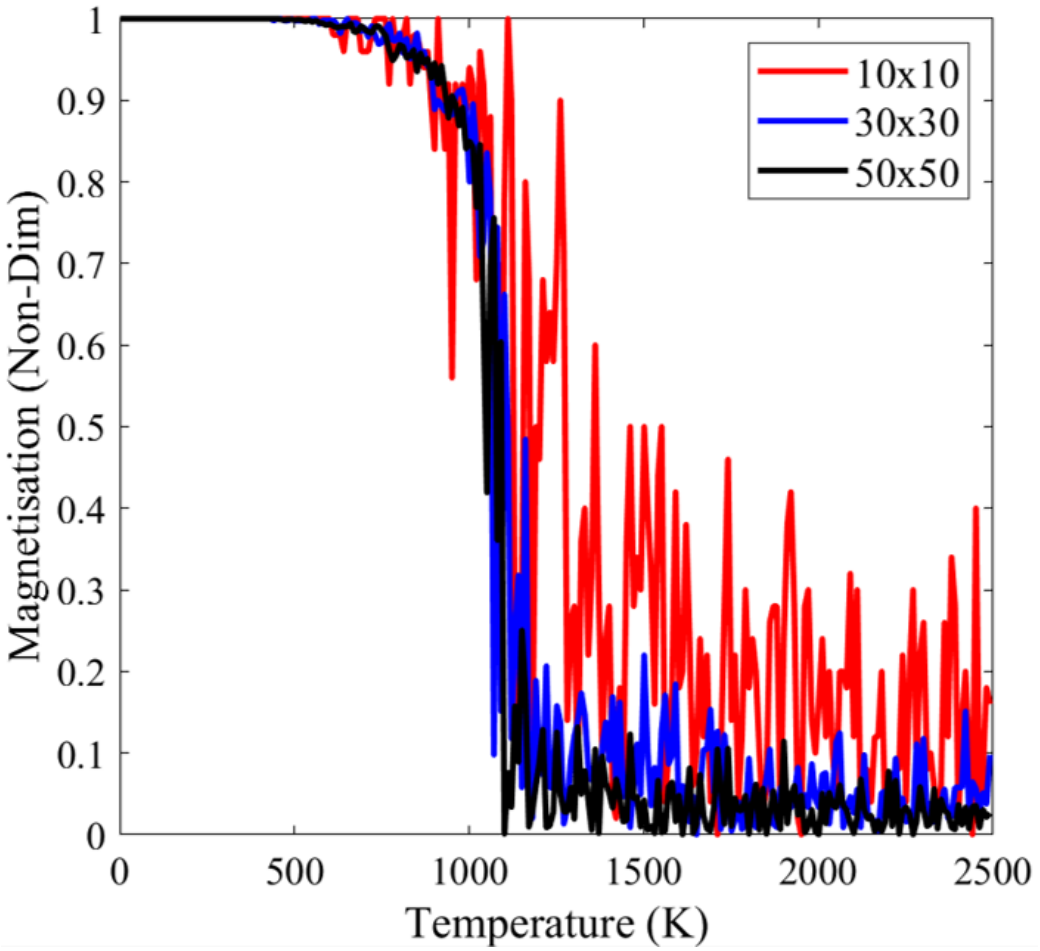

Figure 6: The effect of an increased lattice size on the smoothness of the graphs produced, with the magnetisation graph from Figure 2 used.

Figure 6 demonstrates the effect of increasing the lattice size in the Ising model code. Increasing the number of lattice points in a system decreases the chance that a single lattice point will be selected multiple times, which results in the system having a more well defined average value for each specific parameter set. Here, the magnetisation has a much more defined curve for the larger lattice size, most notably when the material is paramagnetic, above $\approx$ 1000 K. The fluctuations in the 10x10 lattice are on the order of 0.4 compared to the 50x50 lattice which only fluctuates around 0.1.

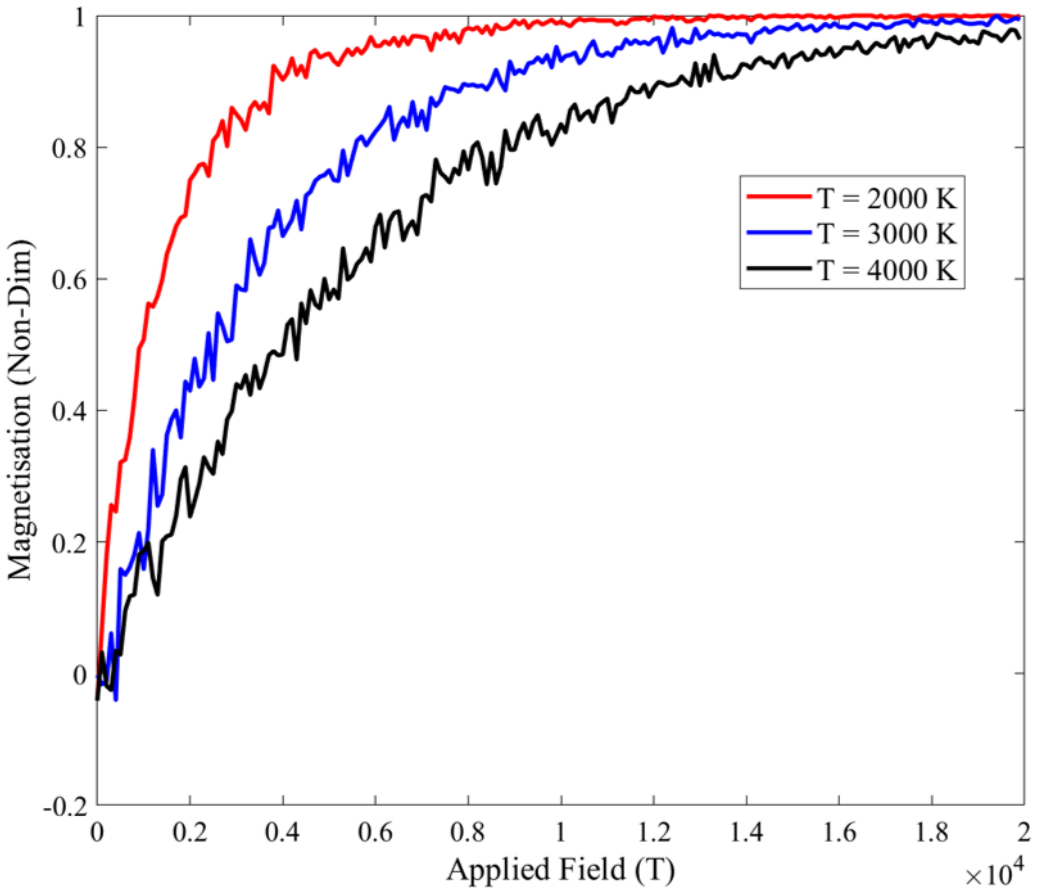

Figure 7: The magnetisation as a function of applied field for different temperatures above T_c and a lattice size of 40x40. These functions follow the predicted theory from equation 8, displaying hyperbolic tangent curves.

In equation 1, the exchange term has the order of ≈ 10 meV due to the exchange constant, whereas the Zeeman term for 1 T is on the order of a Bohr magneton, or ≈ 0.006 meV. This leads to an applied field needing to be on the order of 10^4 T, as is seen in Figure 7, to dominate the energy equation. As the temperature increases, the coefficient x from equation 8 which is proportional to $\frac{B}{T}$ decreases, so for larger temperatures the curve should tend to a straight line, as can be seen.

Table 1: Table showing values calculated for the critical exponents from equation 6 compared to their predicted values, calculated for a lattice size of 50x50.

Critical Exponent	Predicted Value	Simulated Value
Heat Capacity, α	0	0.018 $\pm$0.009
Magnetisation, β	0.125	0.11 $\pm$0.03
Susceptibility, γ	-1.75	-1.6 $\pm$0.3

Table 2: Table showing values calculated for the Curie temperature of the three ferromagnetic elements, calculated from the peaks of the Heat Capacity graph, with lattice size of 50x50.

Material	Accepted Value (K)	Simulated Value (K)
Iron	1044	1050 $\pm$ 90
Cobalt	1388	1420 $\pm$ 120
Nickel	631	470 $\pm$ 70

Errors for the Curie Temperature were calculated by running the simulation 50 times and calculating the standard deviation in the temperature at which the peak heat capacity occurred.

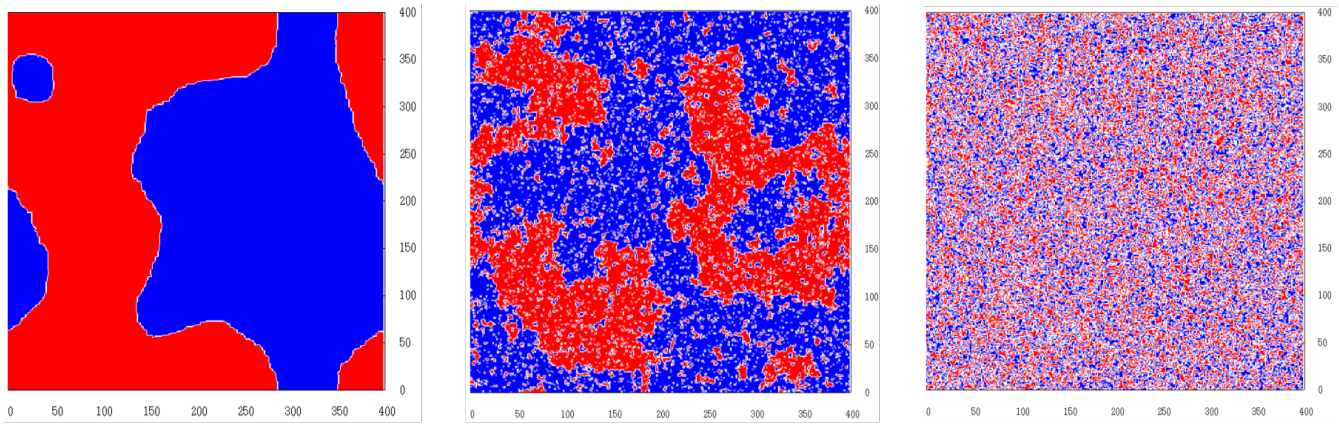

Figure 8: Images of the magnetisation after 5000 iterations for a lattice size of 400x400 with zero applied field. Regions with opposite magnetisation are represented in blue and red, with the region between neighbouring opposing spins in white. The three regions shown represent ferromagnetic ($T < T_c$), Curie temperature ($T = T_c$) and paramagnetic ($T > T_c$) regimes.

Figure 8 shows the change in the magnetic ordering of the material below and above the Curie temperature. Below the Curie temperature the magnetisation of the material is very uniform, with formations of a few stable domain regions of uniform magnetisation. As the temperature is only below T_c and not close to zero, the Boltzmann factor is still creating some fluctuations which is why the magnetisation is not uniform. At the Curie temperature the material has regions of uniform magnetisation which are constantly fluctuating, and above T_c, the material is in the paramagnetic regime. As the field is zero here, the magnetisation is randomly oriented.

4 Discussion

The two-dimensional Ising model reproduces graphs for the energy, magnetisation, heat capacity and susceptibility of magnetic materials. Although the values which the graphs give are largely arbitrary, due to a lack of physical constants involved in the model, the shape of them allow for analysis into the behaviour of the magnetic ordering at the Curie temperature. Figure 1 shows how the total energy of a system increases when the temperature is increased above the Curie temperature, demonstrating the importance of the exchange energy when looking at ferromagnets. With a temperature above the Curie temperature, the energy dependence on temperature, which in this model is a Boltzmann factor, begins to dominate over the ferromagnetic exchange energy wanting spins in the same orientation, leading to the observed shift in minimum energy and paramagnetic behaviour. This transition is clear in Figure 2 as well, with the inflexion point of the curve showing the change from ferromagnetic ordering to paramagnetic disorder. This inflexion point is what leads to the peak in the heat capacity and susceptibility at the Curie temperature, as they are defined as the differentials of the energy and magnetisation respectively, seen in equations 3,4.

Figure 6 shows the effect of an increased lattice size, and how for larger lattice sizes the noise on the graphs is reduced, as the curves become smoother. As a Metropolis algorithm is used to select lattice points to examine and potentially flip, a larger lattice size decreases the chance that the same point is selected multiple times, which would lead to larger fluctuations in the value. In reality, a system of 30x30 is large enough that these fluctuations do not obscure the importance in the shape and behaviour of the graph. Practically, these fluctuations can be ignored, as when measuring actual materials, the lattice size is on the order of N_AxN_A, Avogadro's number, or 10^{23}, so the behaviour will produce a smooth curve.

The Metropolis algorithm selecting the spins at random does occasionally lead to a state at low temperatures where the system is not uniformly magnetised. This can happen because the spins split into two or more regions of opposite orientation, but the system stabilises because all the spins on the boundary have three of their four nearest neighbours oriented in the same direction. This results in a non uniform magnetisation until the temperature is high enough that the Boltzmann probability flips these spins and the ferromagnetic uniform order is restored. This could potentially be eliminated by initially running through the matrix in order rather than randomly, before evolving it randomly for the calculations. It appears as though this occurs more often at larger lattice sizes, although further investigation is needed to quantify this.

The values of the critical exponents were all found to be in agreement with previously established values, as can be seen in table 1. A large lattice size was used to make the curve as smooth as possible. The values were found by using Gnuplot's fit function, which employs a nonlinear least-squares Marquardt-Levenberg algorithm [7]. This was given the form of the data with fitting parameters matching the critical exponents, and then run to find the parameter values. The error in the data is a result of running the same program for all three ferromagnetic materials and then calculating the deviation in exponents.

The runtime of the code varies greatly depending on the parameters for which it is required to run. All the graphs and output produced in this report were calculated and printed in less than a five minute runtime. A short list of suggested parameters and runtimes are included in the header of the code, to allow for a user to check the code works before changing the variables to suit their needs. For the graphs with constant applied fields and varying temperature, a maximum temperature of 2500 K with steps of 10 K was used, and for a lattice size of 50x50 the runtime was on average 175 seconds. These parameters were found to produce an acceptable quality of graph whilst still having a reasonable runtime. For a constant temperature and varying applied field, the code runs at around the same speed, provided the number of points measured is roughly the same. When producing the domain images, the calculations go much faster, as the code does not calculate any values of the system, but simply evolves it, outputting as many images as the user requires. Due to this, a lattice size of 300x300 can be run in 26 seconds to output 5 images. The number of iterations of the evolution is set at 5000. The first 1000 evolutions are run without any further calculations being done to allow for the system to reach equilibrium, and then the subsequent 4000 are run with all properties calculated to keep track of the average and standard deviation of the magnetisation and energy. The number of iterations per evolution can be changed, but 5000 was used for this code because it allowed enough time for the magnetic properties of the system to fluctuate around an average, whilst being small enough that the code could run in an acceptable time.

5 Conclusion

The code written simulates a two-dimensional Ising model for lattice sizes of at least 50x50 in acceptable runtimes, giving values for the critical exponents of the magnetisation, heat capacity and susceptibility of the material which were within the error of expected values. The Curie temperatures of the three ferromagnetic elements Iron, Cobalt and Nickel were calculated from the point at which the Ising model transitions from ferromagnetic to paramagnetic behaviour, and were found to be within the expected errors of the accepted values. The system also accurately predicts paramagnetic behaviour above the Curie temperature, with the relationship between the applied field and the magnetisation following a Brillouin function. The transition from ferromagnetic order to paramagnetic disorder in zero field was observed for lattice sizes up to 400x400. The code and model are a good approximation for the basic behaviour of a uniaxial magnetic material following classical mechanics, giving accurate predictions of the material's critical exponents and Curie temperature.

References

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