Ising Model

Josh Taylor

January 9th 2017

Abstract

Several variations of the Ising Model were solved using the Metropolis algorithm. After using the algorithm to bring the system to equilibrium, the average magnetization per spin, the average energy per spin, the magnetic suceptbility and the specific heat were calculated and plotted as functions of temperature. The ground state energy of the 2D square lattice was found to be -2.0 J and the critical temperature (T_C) was found to be 2.6 ± 0.1 $\frac{\mathrm{J}}{\mathrm{k_B}}$, which compares well to the expected values 2.269 $\frac{\mathrm{J}}{\mathrm{k_B}}$. For the triangular lattice, the ground state energy was found to be -3.0 J, and T_C was found to be 3.7 ± 0.2 $\frac{\mathrm{J}}{\mathrm{k_B}}$. The simple cubic lattice was found to have a ground state energy of -3.0 J and undergo a phase transition at T = 4.2 ± 0.2 $\frac{\mathrm{J}}{\mathrm{k_B}}$, which is close to the expected value. Finally, the body-centred cubic (BCC) lattice was investigated and found to have a ground state energy of -4.0 J and a critical temperature of T = 5.8 ± 0.3 $\frac{\mathrm{J}}{\mathrm{k_B}}$. The ground state energy was found to increase linearly with the number of nearest neigbours (coordination number) of each point. It was also determined that the critical temperature increased when the coordination number increased.

1 Introduction and Theory

The Ising Model is a model of spin interactions which is used in statistical physics to simulate magnetic systems. It consists of a lattice with a discrete value σ_i assigned to every point. These values can be used to represent whether the site is spin up or spin down, by assigning a value of +1 or -1 respectively. It is commonly used due to its simplicity and its ability to show spontaneous symmetry breaking [1] (a phase transition between order and disorder). The Hamiltonian of this system is given by

$$H = \sum_{ij} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \tag{1}$$

where J_{ij} is the interaction energy between nearest neighbours in the lattice, and h is an external magnetic field. When h = 0 and the interaction energy is positive, the spins in the lattice will tend to align and the system is said to be ferromagnetic. If the interaction energy if negative, the system is said to be antiferromagnetic as the spins will tend to align in opposite directions. In the absence of a magnetic field, h = 0 and so the Hamiltonian is reduced to

$$H = \sum_{ij} J_{ij}\sigma_i\sigma_j \tag{2}$$

Calculating Observables of the System

The Ising Model can be used to investigate physical properties of the system, by calculating several observables & finding when the system undergoes a phase transition.

Energy

The average energy per spin when there is no external field is given by

$$\langle E\rangle = \left\langle \sum_{(i,j)} H_{ij} \right\rangle = \frac{1}{2}\sum_{i\neq j} J_{ij}\sigma_i\sigma_j \tag{3}$$

where the factor of $\frac{1}{2}$ ensures every pair of atoms is only counted once.
In a ferromagnetic system, the expected value of $\langle E\rangle$ is -2J for a square lattice when the spins have all been aligned. It is expected that $\langle E\rangle$ is a continuous function with an inflection point at the value of T_C, which approaches zero for values of temperature higher than this. This would indicate that a phase change has occurred and the system has become paramagnetic.

Magnetization

The net magnetization is the sum of all spins in the lattice. To calculate magnetization per site for an n $\times$ n lattice one can use the formula:

$$\mu = \frac{1}{N^2}\sum_{ij}\sigma_{ij} \tag{4}$$

The magnetization is initially expected to be either 1 or -1 as the system is initially ferromagnetic, however the magnetization is expected to drop to zero when T $> T_C$.

Specific Heat

The specific heat C_V of the system is given by:

$$\begin{aligned} C_V &= \frac{\partial \langle E \rangle}{\partial T} \\ &= -\frac{\beta}{T}\frac{\partial \langle E \rangle}{\partial \beta} = \frac{\beta}{T}\frac{\partial^2 ln(Z)}{\partial \beta^2} \\ &= \frac{\beta}{T}[\langle E^2 \rangle - \langle E \rangle^2] \end{aligned}$$

where Z is the partition function and $\beta = \frac{1}{k_B T}$

Magnetic Susceptibility

The magnetic susceptibility χ can be found with a similar method to the specific heat:

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

The specific heat & magnetic susceptibility are expected to have an infinite discontinuity at T_C, which would show a second order phase transition has occurred.

2 Experimental Method

The Metropolis algorithm was applied to several lattices of different sizes and dimensions to investigate the effect coordination number has on critical temperature. It was expected that T_C would increase with the coordination number.

The Metropolis Algorithm

The Metropolis Algorithm was applied to the system as follows:

- The n $\times$ n matrix was initialised to a random configuration of up & down spins
- The algorithm is more accurate at large n, however in order to reduce computation time, periodic boundary conditions were introduced by using the modulo operator for neighbouring sites.
- A lattice site is randomly selected and the energy change Δ E if the spin flips is calculated. If $\Delta E < 0$, the spin is flipped. Otherwise, it is flipped by comparing the probability $e^{-\Delta E/k_B T}$ to a random number on the interval [0,1].

- This process is randomly repeated for the desired number of times and a new matrix is returned

A flow chart for the Metropolis algorithm is provided in the Appendix (Fig 1).

Calculating Observables

Several functions were designed to calculate the average magnetization per spin, average energy per spin, the magnetic susceptibility and the specific heat of the system. When the system reached equilibrium, the Metropolis algorithm was used to calculate these observables over a certain number of steps.

3 Results & Analysis

3.1 Simulating Ising Model

The program was initially run for a 2 dimensional system at a temperature of $1\,\frac{\mathrm{J}}{\mathrm{k_B}}$. Since the value of temperature was less than T_C, the system was expected to be ferromagnetic for J > 0. From the updated configuration of the matrix (see Fig 2), it is obvious that this is the case, as domains are beginning to form between neighbouring spins. For values of J < 0, the system was found to be anti-ferromagnetic, due to the alternating pattern of spins (see Fig 3). A 100×100 matrix was used to minimize computing times. Using a larger matrix would have improved the accuracy of the results, however the computational time would have been significantly increased. A 100×100 matrix was used to reduced computing time while still yielding accurate results.

3.2 Calculating observables for different lattice types

The program was run to calculate the observables after equilibrium was reached. The magnetic field was left at 0 & J was set equal to 1 throughout the computation. Phase transitions can be identified by inflection points of energy & magnetization, and discontinuities in their derivatives; heat capacity & magnetic susceptibility. The plots of the various observables for the different lattice types are in the appendix below (Fig 4-7)

3.2.1 Square Lattice - 4 nearest neighbours

The transition occurs at around T = $2.2 \pm 0.1\ \frac{\mathrm{J}}{\mathrm{k_B}}$, which agrees with the exact value of 2.269185 calculated by Onsager (1944).[2] As the temperature approaches zero, the energy approaches a ground state energy of -2J as predicted by the theory. The magnetization per spin was seen to be 1 until the critical temperature, when it suddenly dropped to zero. This shows the system becomes highly disordered at temperatures higher than T_C.

3.2.2 Triangular Lattice - 6 nearest neighbours

Figure 5 shows the plots of the observables for the triangular lattice. A phase transition can be seen at T = 3.7 $\pm$ 0.2 $\frac{\mathrm{J}}{\mathrm{k_B}}$, which compares well with the value of 3.6410 given by Fisher (1967)[3]. It is higher than the critical temperature for the square lattice because it has more nearest neighbours. The ground state energy was -3.0J as expected.

3.2.3 Cubic Lattice - 6 nearest neighbours

For a simple cubic lattice, there is a phase transition at T = 4.2 $\pm$ 0.2 $\frac{\mathrm{J}}{\mathrm{k_B}}$, which is close to the values of 4.5103 given by Fisher (1967)[3] and 4.5115 obtained by Heuer (1993)[4]. This is larger than the value of T_C for the square lattice, which is expected as it has more nearest neighbours. The ground state energy was found to be -3.0 J as expected.

3.2.4 Body-Centred Cubic Lattice - 8 nearest neighbours

At T = 5.8 $\pm$ 0.3 $\frac{\mathrm{J}}{\mathrm{k_B}}$, a phase transition in the BCC lattice can be seen. This value of T_C is higher than that of the simple cubic lattice, which again suggests that the higher the coordination number of the lattice, the higher its critical temperature will be. The energy of the system was found to approach -4.0 J when temperature approached zero, which agrees with the theory.

4 Discussion and Conclusions

The Metropolis algorithm was successfully implemented to update the spin configuration of a system. It was discovered that, although they would be more accurate, larger systems would be impractical to use as they require a significant number of iterations to reach equilibrium. Smaller systems result in much quicker computation times at the cost of accuracy, but are far more practical to use. One disadvantage of this is that the plots of magnetization & susceptibility do not yield very accurate results for some of the lattices with a larger coordination number which may indicate the algorithm needed to be run for a higher number of iterations. A potential solution for this is to run the program for longer or use ssh to run it on multiple computers simultaneously.

The values of the observables for each lattice type are shown in the table below:

Lattice	T_C (J/k$_B$)	Ground State Energy (J)
Square	2.2 $\pm$ 0.1	-2.0
Triangular	3.7 $\pm$ 0.2	-3.0
Simple Cubic	4.2 $\pm$ 0.2	-3.0
BCC	5.8 $\pm$ 0.3	-4.0

The values of critical temperature T_C were found to agree well with the theory. They could have been made more accurate by increasing the size of the lattice or by averaging over several simulations, however this would come at the cost of significantly increased computation times. The discontinuities of magnetic susceptibility & specific heat at T_C for the four lattices indicated that the phase transitions were of second order. The lattices were determined to represent ferromagnetic systems, as the plots of magnetization against temperature showed second order phase transitions at the critical temperature. It appears as though the increase of T_C for more complex lattices & lattice in higher dimensions is related to the increase in coordination number of each point.

References

1. Strocchi F. (2008), Symmetry Breaking in the Ising Model. In: Symmetry Breaking. Lecture Notes in Physics, vol 732. Springer, Berlin, Heidelberg

2. Onsager L. (1944), ”Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition”, Phys. Rev., Series II, 65: 117149

3. Fisher, M.E., 1967, ”The theory of equilibrium critical phenomena”, Rep. Prog. Phys., 30, 615-730

4. Heuer, H.O., 1993, ”Critical crossover phenomena in disordered Ising systems”, J. Phys. A, 26, L333-L339

Appendices

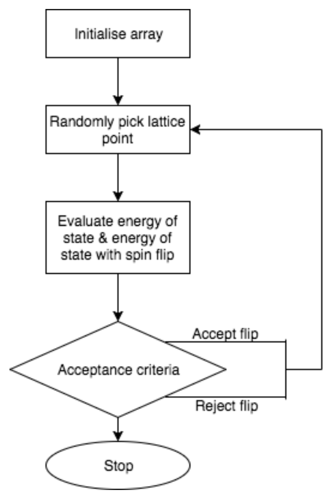

Figure 1: Flow Chart showing evolution of Metropolis Algorithm as it iterates over the lattice

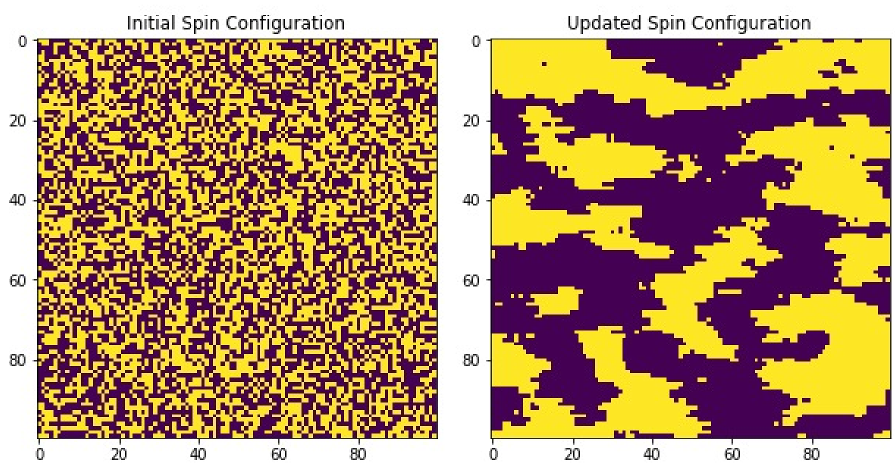

Figure 2: Comparison of the random initial configuration (left) & the updated system (right) for a 100 $\times$ 100 matrix with T = 1 $\frac{\mathrm{J}}{\mathrm{k_B}}$

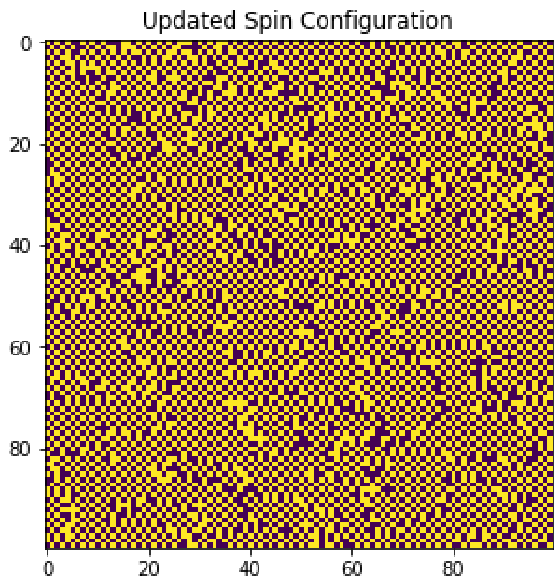

Figure 3: Graph showing the updated lattice for a paramagnetic system, ie: J $<$ 0

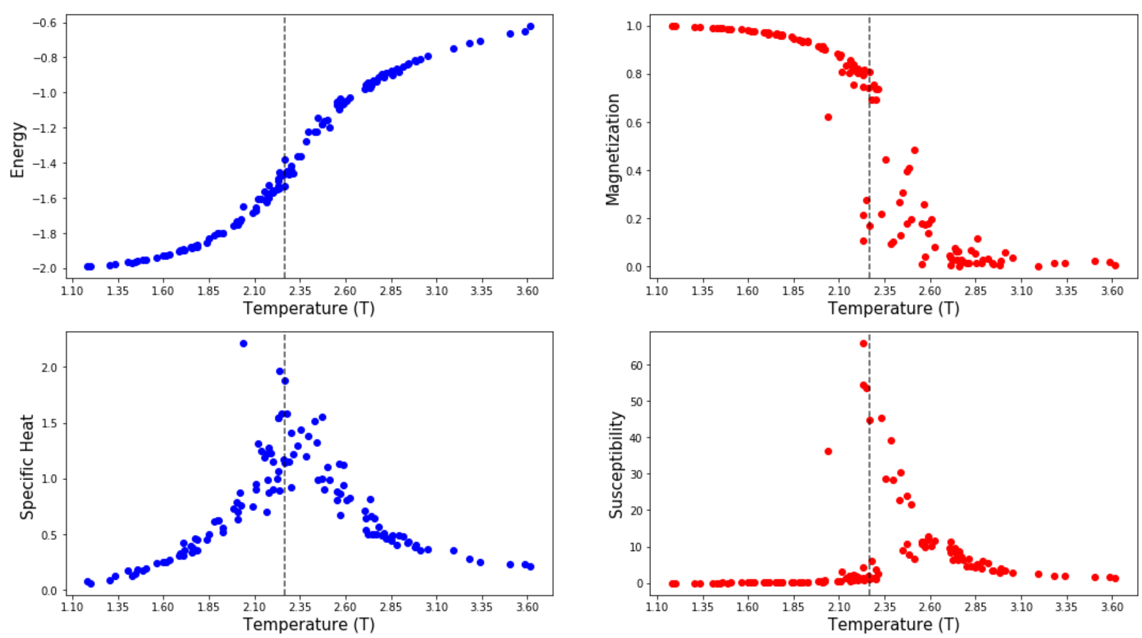

Figure 4: Graphs showing how the energy, magnetization, heat capacity & magnetic susceptibility of a 16×16 square lattice change with temperature

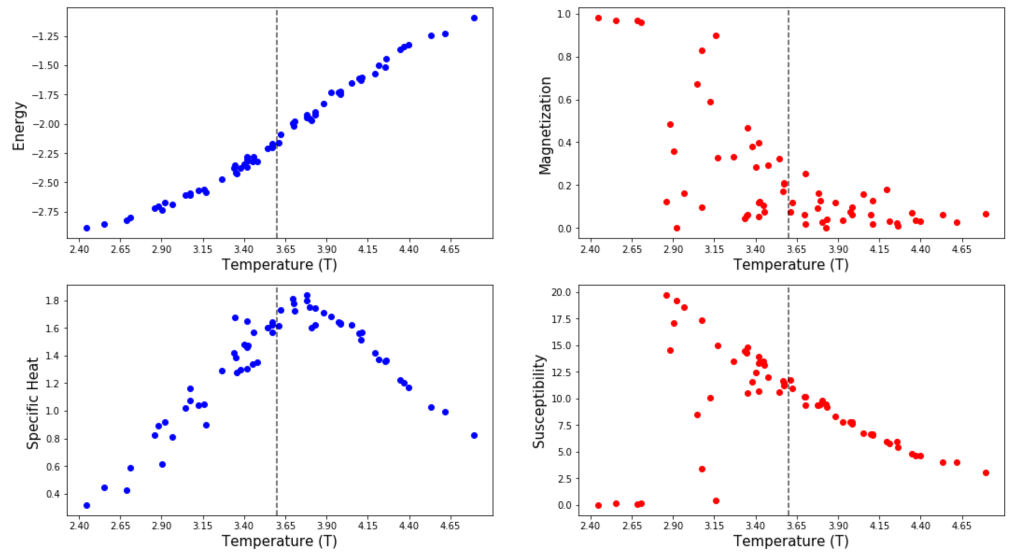

Figure 5: Graphs showing how the energy, magnetization, heat capacity & magnetic susceptibility of a 8 × 8 triangular lattice change with temperature

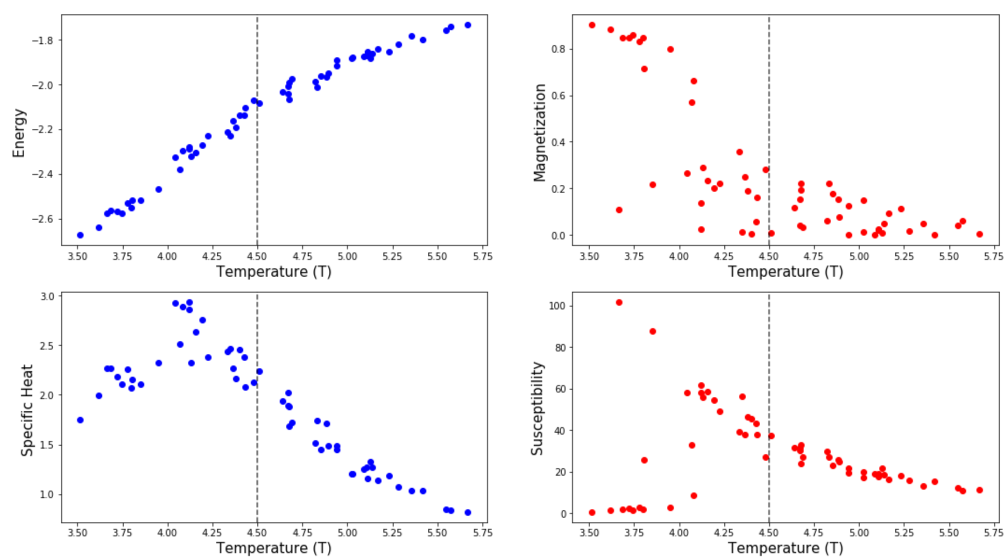

Figure 6: Graphs showing how the energy, magnetization, heat capacity & magnetic susceptibility of a simple cubic lattice of length 8 change with temperature

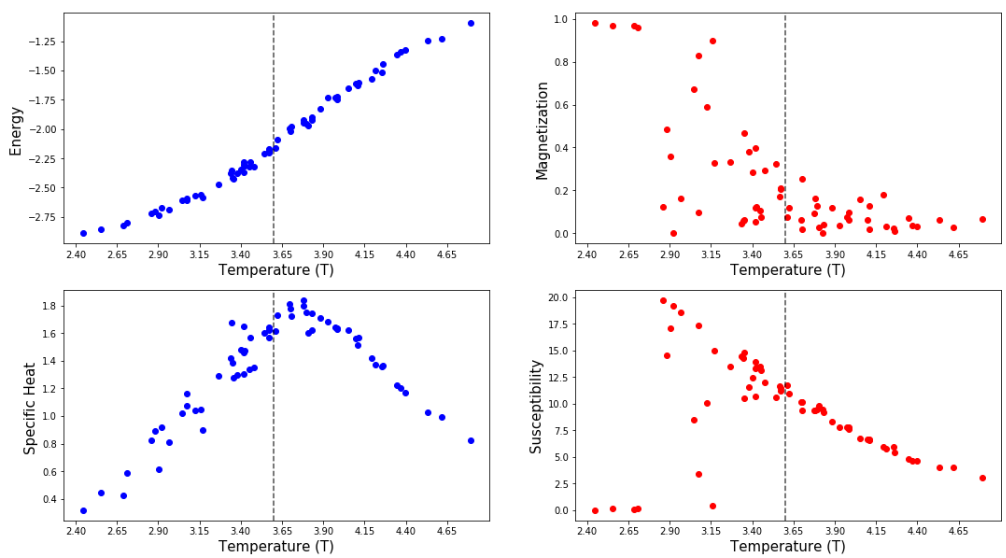

Figure 7: Graphs showing how the energy, magnetization, heat capacity & magnetic susceptibility of a BCC lattice of length 8 change with temperature