Ising Model

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1 Introduction

The Ising Model is a model of ferromagnetism in statistical physics. The model, in 2D, describes a square lattice in the $x - y$ plane with one spin per lattice point, where only nearest neighbour spins interact, and spins can only point 'up' or 'down' along the z-axis. This report investigates the use of Monte Carlo simulations as a way of evaluating the observables of a ferromagnetic material, and the use of the Metropolis algorithm for evolving the system over a range of temperatures, during which we expect a phase transition to occur. We can then use finite size scaling analysis to evaluate the critical exponents of the system, and can compare our results to Onsager's exact solution [1]. All simulations are run with zero external magnetic field.

2 Theory

There are various quantities that can be extracted from the system. We can calculate the energy of the system by summing the spin exchanges between lattice points.

$$E = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(nn(i,j)\mathbf{s_i}\cdot\mathbf{s_j}) - \mu_0\sum_{i=1}^{N}(\mathbf{B}\cdot\mathbf{s_i}) \tag{1}$$

where $nn(i,j) = 1$ when $\mathbf{s_i}$ and $\mathbf{s_j}$ are nearest neighbours, and 0 otherwise. Furthermore, the magnetisation of the system can be calculated by summing the values of spin, and dividing by the number of lattice points,

$$\mathbf{M} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{s_i}. \tag{2}$$

From these two quantities the susceptibility and heat capacity can be calculated,

$$\chi = \frac{1}{k_B T}(\langle M^2\rangle - \langle M\rangle^2) \tag{3}$$

$$C = \frac{1}{k_B T^2}(\langle E^2\rangle - \langle E\rangle^2) \tag{4}$$

The system is expected to undergo an abrupt transition between magnetised and un-magnetised states at a critical temperature T_C. Onsager's exact solution [1] finds the relationship between critical temperature T_C and spin-spin exchange energy J to be

$$T_C = \frac{2J}{k\ln(1+\sqrt{2})}, \tag{5}$$

which is used by the program to define J corresponding to a user defined critical temperature T_C. The program also compares its results to Onsager's exact relationship between M and T,

$$M_0 = (1-k^2)^{1/8} \tag{6}$$

where

$$k = [\sinh(2J/k_BT)\sinh(2J'/k_BT)]^{-1} \tag{7}$$

and $J = J'$, given that the interaction energies of our model are equal in the x and y directions. This exact solution can be simplified through a Taylor expansion into the relationship eq. (9) for temperatures close to T_C, but was used in its original form. The value 1/8 in eq. (6) corresponds to the critical exponent α in eq. (8).
The relationship between T, T_C, and the quantities listed in eqs. (2) to (4) are

$$C \propto (T-T_C)^{-\alpha} \qquad (8) \qquad\qquad M \propto (T-T_C)^{\beta} \qquad (9) \qquad\qquad \chi \propto (T-T_C)^{-\gamma} \qquad (10)$$

Given the difficulty in calculating the exponents of eqs. (8) to (10), due to conditions of approaching from below and above T_C [2], we can instead employ a finite size scaling method [3, 4] to evaluate them.
It has been shown [3, 4] that the side length L of the lattice, in 2D, is inversely proportional to the difference in the exact critical temperature, and the one at which critical behaviour is observed. Thus it is possible to substitute the quantity

$$L \propto |T_C(L=\infty) - T_C(L)|^{-\nu} \tag{11}$$

into eqs. (8) to (10) to get a relationship between L and C, M, χ.

$$C(T_C) \propto L^{-\alpha} \qquad (12) \qquad\qquad M(T_C) \propto L^{\beta} \qquad (13) \qquad\qquad \chi(T_C) \propto L^{-\gamma} \qquad (14)$$

The exponents are now much more easily extracted by plotting logarithmic plots of the respective values at T_C against lattice length.

3 Method

Since the program simulates an infinite lattice, periodic boundary conditions are used for a finite lattice as an approximation, which can be visualised as a 3D torus with the spins on the surface of the structure.
Each point on the lattice is then randomly assigned a spin of 'up' (+1) or 'down' (−1), and then the system is evolved using the Metropolis algorithm [5].
The algorithm functions as follows:

1. Make a trial change in the system by selecting a random spin and flipping it.

2. Compute the change in energy ΔE of the site using (1).

3. If the state is energetically favourable, i.e. $\Delta E \leq 0$, accept change.

4. If $\Delta E > 0$, generate a uniform random number U.

5. If $U < \exp(-\Delta E/k_B T)$, accept change.

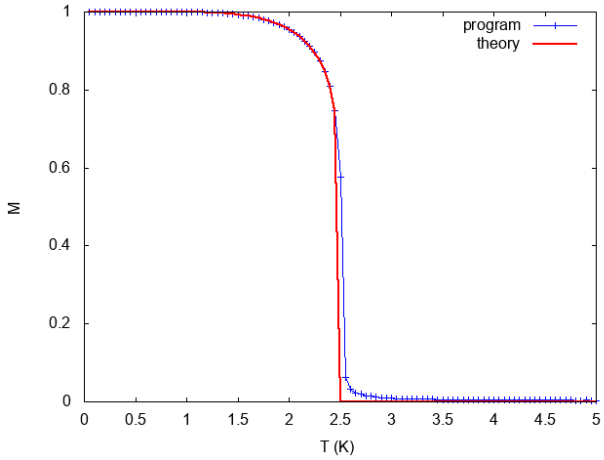
The equation in step 5. in the algorithm represents the system changing due to thermal noise. Significantly below the critical temperature, this effect is negligible, however above T_C it becomes much more pronounced. After evaluating N sites on the lattice, we evaluate the quantities (1) and (2), and periodically compute averages over lattices until the system appears to be fluctuating randomly about an average. This program calculates this by calculating the gradient of each value of M and E over several lattices, and when the gradient is sufficiently close to zero, the set of values is accepted, from which χ and C can be calculated from eqs. (3) and (4) respectively. The sites for the algorithm can either be selected randomly, which represents a more physical system, or in order, to reduce running time. All values calculated were done so using an ordered selection of sites for this reason. Given that energy and magnetisation are calculated as 'per site', care must be taken in calculating χ and C with eqs. (3) and (4), and should me multiplied by number of sites to preserve the 'per site' dimensionality.

4 Results and Discussion

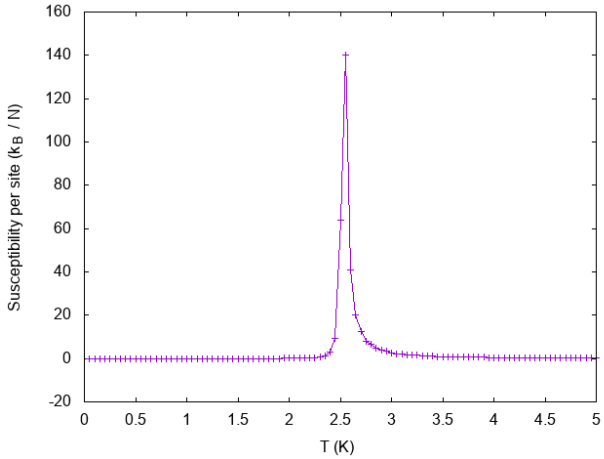
Table 1: Table displaying the critical exponents derived from the graphs in Figure 2 for eqs. (8) to (10).

Quantity	Exponent	Finite Size Scaling	Theoretical
Grid Length	ν	1.06 ± 0.06	1
Heat Capacity	α	$\alpha \to 0$	0
Magnetisation	β	0.122 ± 0.003	0.125
Susceptibility	γ	1.80 ± 0.01	1.75

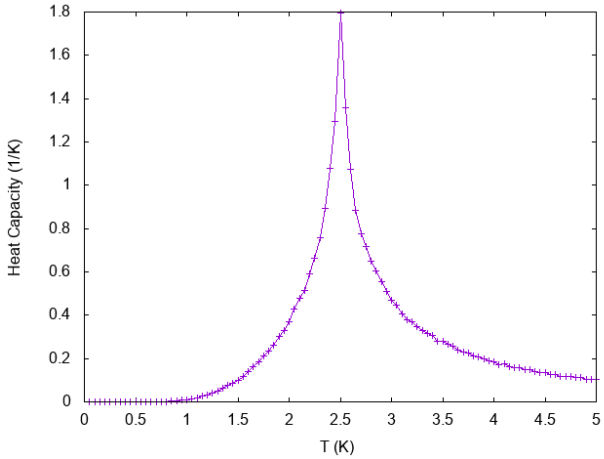
Figure 1a shows the magnetisation of the system at temperatures above and below the critical temperature, in this case $T_C = 2.5K$. The plot shows a clear change from magnetised state $\langle M \rangle = 1$ below T_C to an un-magnetised state $\langle M \rangle = 0$ above T_C. This graph plots the magnitudes of M, since for small, non-infinite lattices, there is a finite chance that the magnetisation of the system can flip spontaneously [3, 4], which is uncharacteristic of a real system. This however results in weaker statistics at higher temperatures, which is why our system takes longer to decay to $\langle M \rangle = 0$ than otherwise. This will also have an affect on our variances for χ, given that it is calculated using M.
Figure 1b shows the susceptibility of the system above and below the critical temperature. The plot shows a clear jump at T_C, after which it returns back to zero. This is as we would expect, given that the system is only changing at this exact temperature. Ideally, for an infinite lattice, we would expect this graph to be a Dirac delta function $\delta(T - T_C)$.
Figure 1c shows the specific heat capacity of the system around the critical temperature. For figs. 1b and 1c the peak value scales with grid size, with larger lattice lengths corresponding to larger peaks. For an infinite lattice, there is a discontinuity at these points, and the function is undefined/infinite at the critical temperature given that in theory the transition occurs instantaneously.



(a) Magnetisation M over T.



(b) Susceptibility χ over T.



(c) Heat Capacity C over T.

Figure 1: The plots above were produced with 1000 saved values over 100 iterations between $0 < T < 5$K at a grid size of $L = 400$. The critical temperature is set to 2.5K using eq. (5).

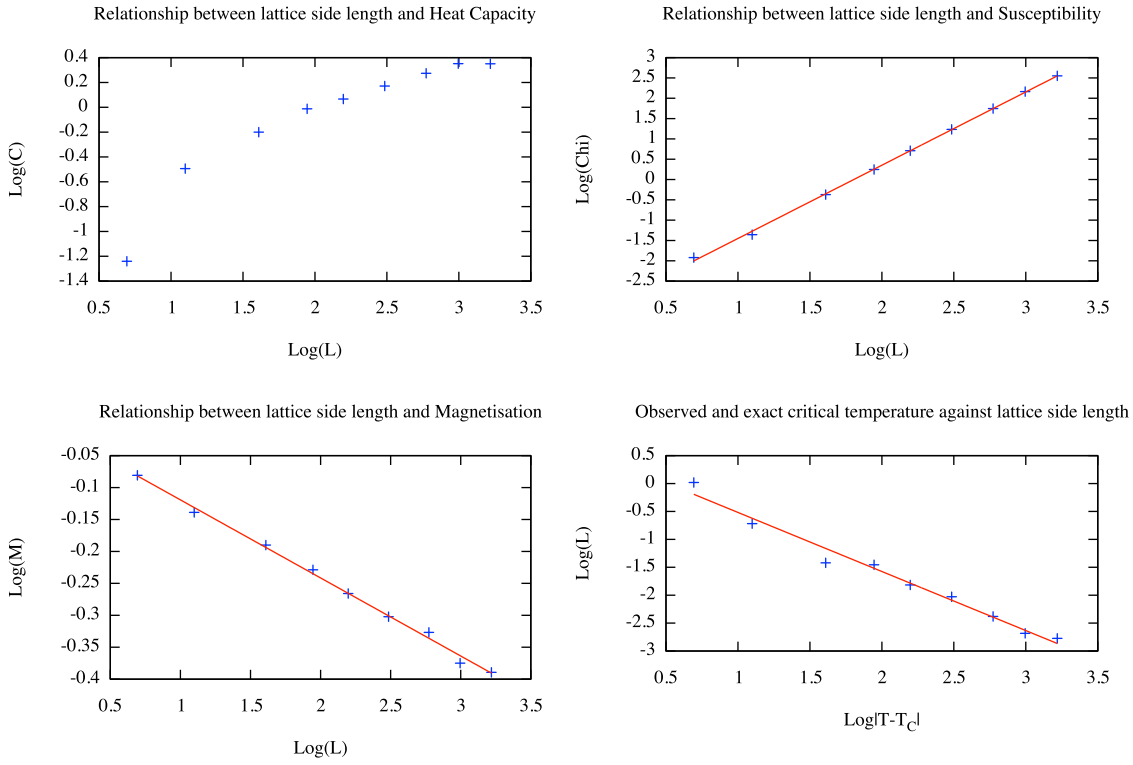


Figure 2: From these four graphs we can extract the gradients and this evaluate the critical exponents given in eqs. (11) to (14). The gradients are shown in Table 1. The lattice length varied between $2 < L < 35$, and the values were obtained from 10000 saved values over 1000 temperature iterations.

From figs. 1a to 1c we can calculate the value of each variable at the critical temperature, and then, using eqs. (12) to (14), we can plot the logarithm of each and extract the exponent from the gradient. This has been done in the graphs in Figure 2. The data was collected using small lattices with $2 < L < 35$, but with a high number of quantities saved, and thus a larger number of values of M and E to calculate χ and C from, improving accuracy. The first graph shows a gradient that tends towards zero as the lattice length increases. Thus we can assume that for infinitely large lattices, this coefficient is zero. The final graph in Figure 1a is used to prove the relationship that $\nu = 1$ for a 2D lattice, and thus justify the use of eqs. (12) to (14).

Table 1 contains the observed values for the critical exponents. The theoretical values for ν and β lie just within our error bounds, however χ lies outside by $-0.04 k_B/N$. Given the shift of observed critical temperature as seen in eq. (11), this means that our desired quantities for analysis will not lie exactly at the $T_C = 2.5K$ temperature, and thus a very small temperature step is required in order to observe the maximum quantities at these shifted temperatures. The graphs in Figure 1b were plotted with a temperature step of $0.005K$, which is why lattice sizes were limited to below $L = 35$, which would correspond to a shift by $0.03K$. However, much higher resolution is likely required to observe the exact point of phase change,

and thus much more time to run the program.

5 Conclusion

Given the large approximations that the model takes, including limiting spin to 'up' or 'down', only allowing nearest neighbour interactions, and using a finite lattice, the Ising model has been able to calculate a critical exponent β for M containing the true value within its error boundaries, and has shown that the heat capacity exponent α tend to to zero for infinitely large lattices. The largest limit in calculation of these exponents is the temperature step used. A smaller step would have yielded much more accurate results, at the significant cost of program running time. On a 3rd generation intel i7, for $L = 400$, $T_{STEP} = 0.005$ for $0 < T < 5K$, and 10000 values saved at a time, the process took at least 6 hours to run. Efficiency improvements in the program could be implemented with a dynamically sized number of values stored, to minimise attention on $T << T_C$ and $T >> T_C$.

References

[1] L. Onsager, *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*, Phys. Rev. 65 117 (1944)

[2] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press (1982).

[3] J. Kotze, *Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet* (2008) `https://arxiv.org/pdf/0803.0217.pdf` (accesed 27 Feb 2017).

[4] `http://fraden.brandeis.edu/courses/phys39/simulations/advancedlab1_Part1.pdf` (accesed 27 Feb 2017).

[5] H. Gould, J. Tobochnik, and W. Christian, *An Introduction to Computer Simulation Methods: Applications to Physical Systems Chapter 17 Monte Carlo Simulation of the Canonical Ensemble*, Addison-Wesley (2006).