Implementation of the Metropolis Algorithm for investigation of the two dimensional Ising Model.

Jeffrey Lyons 13325575 lyosnj4@tcd.ie

January 18, 2017

Abstract

The following investigation made use of the Metropolis Algorithm to numerically solve the 2D Ising model for an arbitrary number of lattice sites. The Metropolis Algorithm was utilized succesfully and allowed for the observation of phase changes around the critical temperature of 2.269 J/k_b. In particular, the observables, energy per site, mean magnetization per site, and specific heat capacity were investigated for their dependence on temperature. All showed clear phase change behaviour at the critical temperature. As expected the lattice magnetized quickly at temperatures much lower than T_c, while negligable net magnetic moment was observed for temperatures at and above T_c. Results are depicted graphically so that the reader may easily visualize the behaviour of a ferrous system.

1 Introduction

First formulated by Ernest Ising and Willhelm Lenz in 1920, the Ising model attempts to rigourously describe the macroscopic behaviour of ferrous materials. The ferrous material is modelled as a lattice, arbitrarily large, whose sites are populated by discrete variables which can take one of two values. The value of these variables corresponds to the orientation of electron magnetic momenta in a magnetic material, aligned parallel or anti-parallel to an external magnetic field. The spin excess of the system determines its macroscopic properties.

As T $\rightarrow$ 0K macroscopic alignment is observed as it is energetically favourable for an individual spin to align parallel to its nearest rectilinear neighbours. This is due to the form of the spin Hamiltonian which may be expressed as,

$$H = -J \sum_{\langle i,j \rangle} S_i \cdot S_j$$

in the absence of an external magnetic field, where J is the coupling parameter between neighbouring spins. Taking the inner product of the choosen spin with the spin orientation of its nearest neighbours and multiplying by the coupling parameter produces the energy of the spin. This may be expressed as,

$$E = \sum_{\langle i,j \rangle} H_{i,j}$$

At higher temperatures spins may spontaniously align antiparallel to their neighbours as a result of their increased thermal energies. The probability of a spin flip spontaneously occuring is given by the Boltzmann factor and may be written as,

$$P_{flip} = e^{(\beta \Delta E)}$$

where $\beta = 1/k_bT$ and ΔE is the change in energy of the spin neighbour system as a result of the flip. Above T_c, the critical temperature of the system, magnetization will not occurr in the absence of a driving field as the thermal energy of the spins overcomes any tendency to mutually align. The critical temperature of the Ising model for a square lattice has been derived analytically to be,

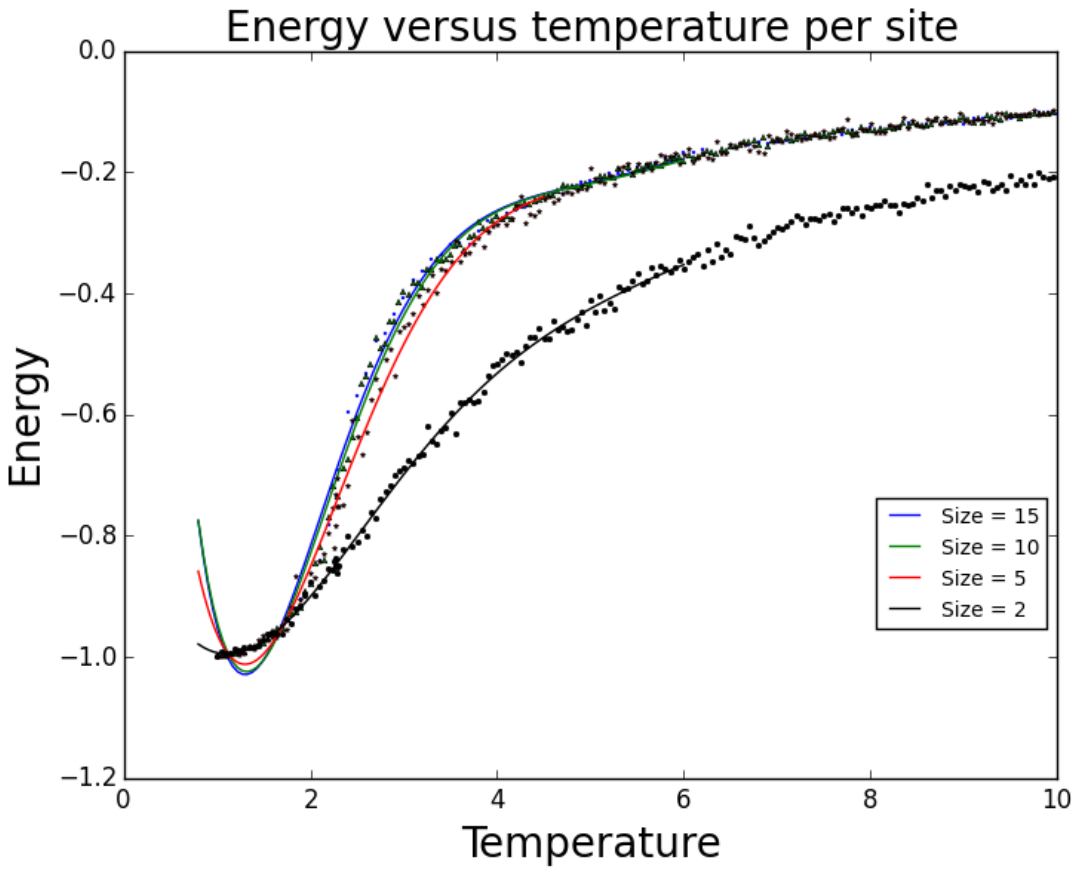
$$T_c = \frac{2}{\ln(1+\sqrt{2})} k_b/J$$

2 Monte Carlo simulation

The 2D square lattice Ising model may be solved numerically through the implementation of Monte Carlo methods. The metropolis algorithm used to simulate the random fluctuations of spin orientations in a lattice is an iterative method which relies on the production of pseudo-random numbers. A site is first choosen at random. If the energy cost of flipping the choosen spin is negative the spin is flipped. If it is non-negative, ie not energetically favourable, the spin is flipped with P_{flip} as outlined above.

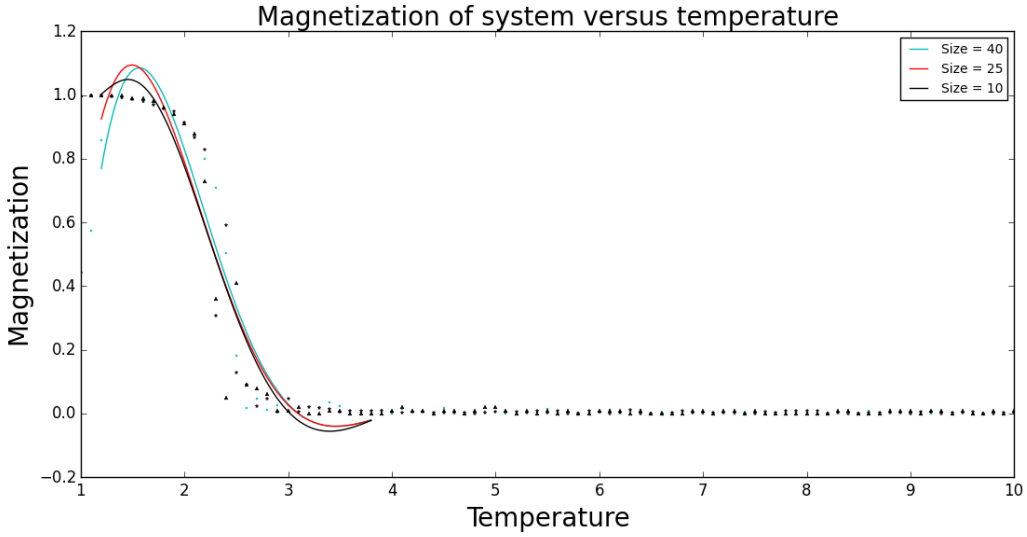
3 Results

3.1 Energy.

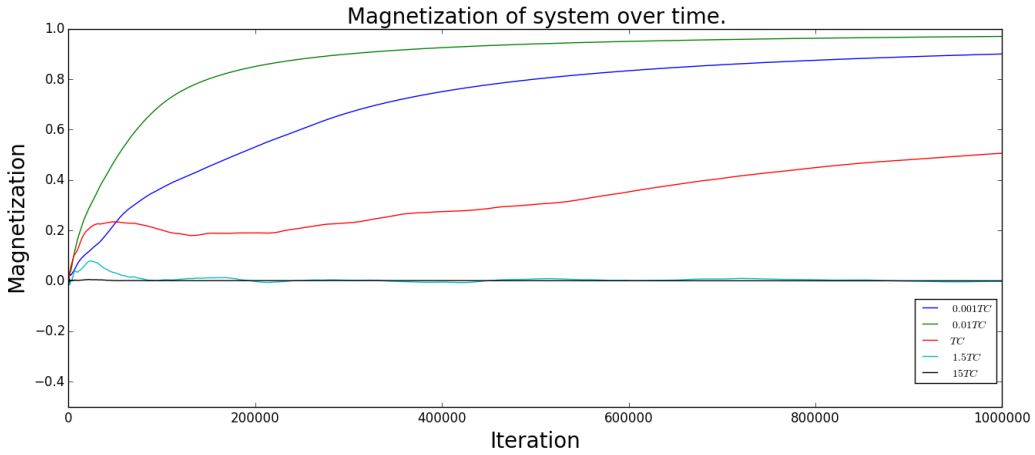


The above graph demonstrates the dependence of lattice energy per site on the ambient temperature. A phase change is observed for $T = T_c$ where rapid demagnetization of the lattice occurs. Initially the lattice is fully magnetized with all spins mutually aligned producing an energy per site equal to unity. As $T \to T_c$, the effects of thermal fluctuations become more apparent and the lattice begins to demagnetize. For temperatures in the upper limit the energy per site tends toward zero as each spin will have, on average, two parallel neighbours and two antiparallel neighbours.

3.2 Magnetization.



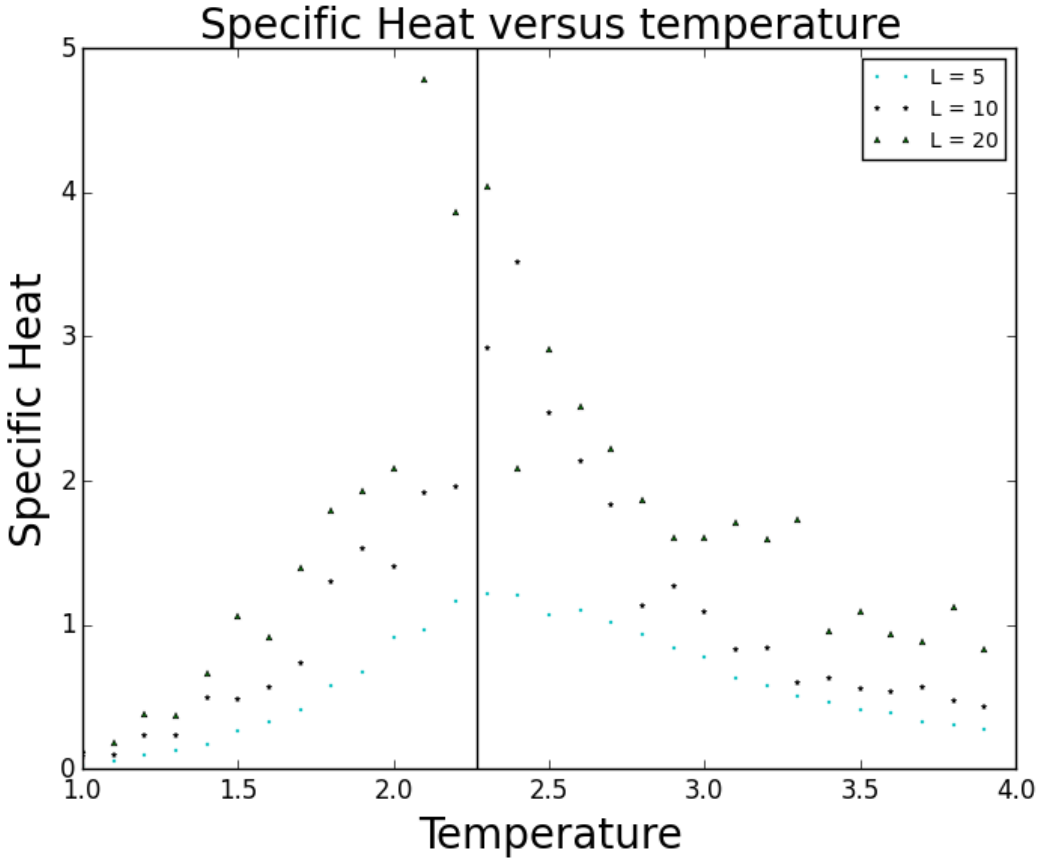
The above graph demonstrates the relationship between magnetization per site and temperature for three distinct lattice types. There is a clear inverse correlation between the above graph and that was discussed in the previous section. Again, we witness a substantial phase change as the ambient temperature approaches T_c and the lattice begins to fully demagnetize as the magnitude of the Boltzmann factor increases.



We now plot the magnetization per spin for four different lattice sizes as a function of the

iteration count. The iteration count in this case is a good proxy for time. For temperatures well below T_c we observe magnetization tending toward unity very quickly. Again, this is due to the absence of thermal energy. Each succesive increase in the ambient temperature results in a simulation which approaches magnetization faster. For $T = T_c$ we observe very slow magnetization with saturation at 0.5. For temperatures in excess of T_c magnetization does not occur and the value of the observable proceeds to randomly walk around net zero magnetization.

3.3 Heat Capacity.



As expected, a significant change in the heat capacity of the system is observed as $T \to T_c$. Here the critical temperature is plotted as a vertical line to illustrate the sharpness of the peak at $T = T_c$.

4 Conclusion

The Ising model was numerically solved and significant phase changes were observed in three major thermodynamic observables for $T = T_c$. The preparatory work undertaken helped foster a better understanding of both Monte Carlo methods and the statistical thermodynamics that was the backbone of our algorithm.

My initial decision to take this course was based on the understanding that a concerted effort had to be made to learn a programming language and that a module long course such as this

would be the perfect opportunity. My scientific programming skills are now greatly improved and I retain an active interest in mathematical programming, having not long ago registered for Project Euler.

5 Bibliography.

- Dr Thomas Archer, PY3C01, Computational methods.
- Dr Stefan Hutzler, PY3C01 Computer Simulations I, Numerical and Statistical Methods.
- //docs.scipy.org/doc/numpy/reference/
- Kittel, C., Hill, R. W. (1970). Thermal Physics. Physics Today, 23(8), 6163