PYU33C01 Computational Methods Assignment 3

Completed by Seán Alexander 21364546

Simulating the Ising Model Using Object Orientated Programming

The ising model is a model in statistical physics which described the magnetic spin micro-states of a system. In order to determine how a two dimensional lattice submerged in a heat bath behaves, it is modelled as a lattice of classical spins $\pm S_j$ with nearest-neighbor interaction with periodic boundary conditions. Each lattice site has a finite probability of changing spin which is affected by the spin states of its nearest neighbours and therefore any given unlikely micro-state will likely dynamically adjust to more likely permutations given the temperature and value of any present applied magnetic field. To determine quantities such as the average energy, average magnetisation, magnetic susceptibility and heat capacity of a physically relevant micro-state of such a system, one must apply Markov-chain Monte Carlo methodology to a provided micro-state. This is also known as the metropolis algorithm. The methodology involves iteratively applying spin changes to each site of a micro-states in line with the probabilities that they should change.

This is computationally complex and requires the information of each iteration be the input for each subsequent operation. When one is intending to apply this methodology to different instances of a lattice in order to quantify its properties, it is appropriate to use object orientated programming. One may define a class of objects which give the properties of a particular randomly generated lattice and methods which apply the metropolis algorithm to it and determine its physically relevant properties. This is what was achieved to allow the explorations of the ising model which are detailed below. A method which plots a given lattice object was also programmed.

Computing Observable Quantities

The average magnetisation ($\langle M \rangle$) of the system was determined by summing the normalised magnetizations of each of the lattice sites and averaging the value of each of these summations for each micro-state for each metropolis sweep beyond the initial sweeps which bring the initial state closer to more likely permutations. The associated formula is provided below:

$$\langle M \rangle = \frac{\sum_S M(S) e^{-E(S)/(k_B T)}}{Z} \tag{0.1}$$

The average energy ($\langle E \rangle$) was calculated similarly except the normalised coupling energy was what was summed across for each site of the lattice. The energy is for each spin site S formula is included below:

$$E(S) = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \tag{0.2}$$

Where J is the coupling constant and h is the applied magnetic field.

The magnetic susceptibility (χ) was then determined using the following formula:

$$\chi = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{0.3}$$

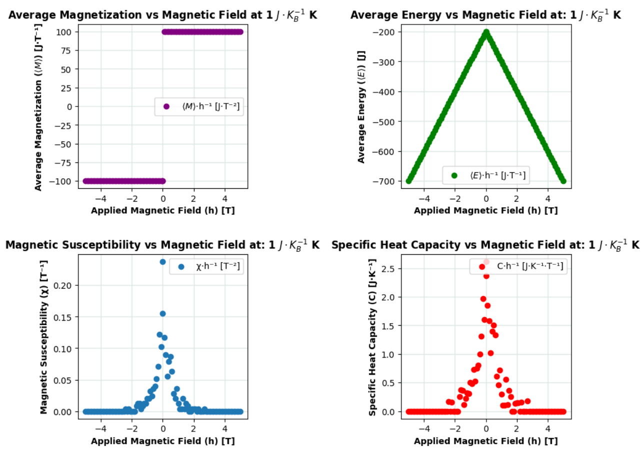
The formula being the variance of the magnetization divided by the temperature and Boltzmann's constant.

Similarly the specific heat capacity (C) of the system was determined using the formula below:

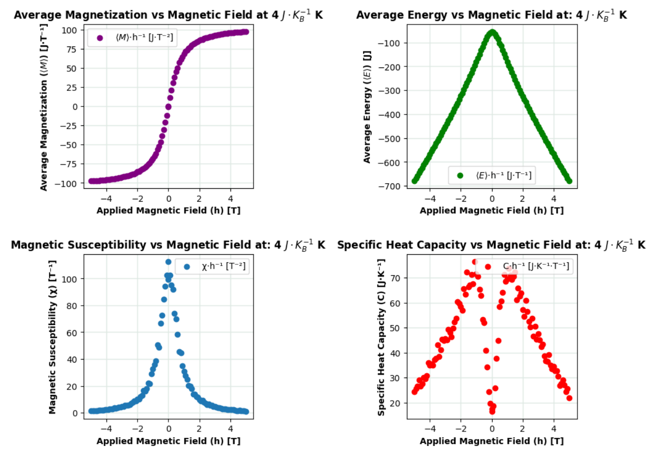
$$C = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{0.4}$$

Plotting Observable Quantities Against the Applied Magnetic Field

The observable quantities outlined above were plotted against the applied magnetic field (h) for a system size of 100 at temperatures $1\,J \cdot K_B^{-1}$ K and $4\,J \cdot K_B^{-1}$ K. These plots are included below:



(a) Temperature: $1\,J \cdot K_B^{-1}$



(b) Temperature: $4\,J \cdot K_B^{-1}$

Figure 1: Observable Quantities vs Applied Magnetic Field (h)

The difference between the observable quantities at these two quantities can be explained by the fact that the lattice which is at $1\,J \cdot K_B^{-1}$ K behaves in its ferromagnetic phase and the lattice which is at $4\,J \cdot K_B^{-1}$ K behaves in its paramagnetic phase. The lattice was plotted in its initial random state (sweep 0), and a micro-state post metropolis (sweep 1000) for different applied magnetic fields. The transition between directions of the magnetic field (h) can describe the difference between the two phases.

In the Ferromagnetic case the spins (s_j) of the lattice sites align with the magnetic fields close to $h = 0$ while they fail to do this completely in the paramagnetic case.

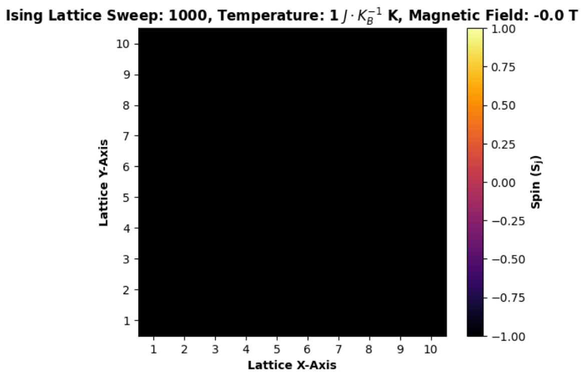
The average magnetisation ($\langle M \rangle$) appears to behave like a a step function in the ferromagnetic phase but like a sigmoid function in the paramagnetic phase.

The average energy ($\langle E \rangle$) appears to behave similarly with different bounds and sharpness due to the temperature difference in each phase.

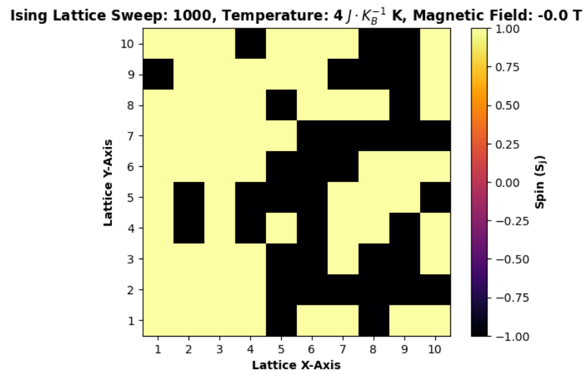
The magnetic susceptibility appears to behave similarly which much larger magnitude in the paramagnetic phase.

The specific heat capacity has a much larger magnitude a the paramagnetic phase with it troughing instead of peaking as it approached a magnetic field (h) of 0.

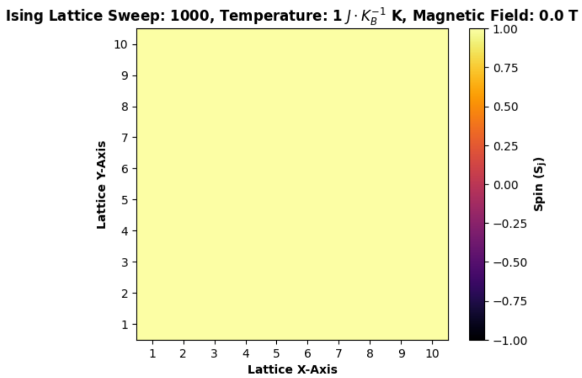
Plots of the lattices at the applied magnetic field $h = 0$ transition plotted using a method "plot_lattice(self,label):" are included below:



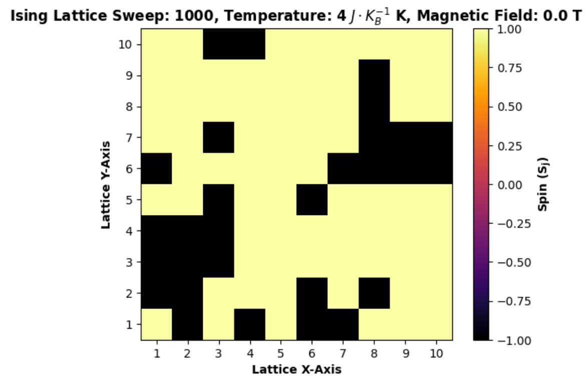
(a) Metropolis State Below 0 T at 1 $J \cdot K_B^{-1}$ K



(c) Metropolis State Below 0 T at 4 $J \cdot K_B^{-1}$ K



(b) Metropolis State Above 0 T at 1 $J \cdot K_B^{-1}$ K



(d) Metropolis State Above 0 T at 4 $J \cdot K_B^{-1}$ K

Figure 2: The Metropolis States of the Ising Lattices in the Ferromagnetic and Paramagnetic Phases

Once it was understood that the difference in physical properties of the lattice between the two phases was dictated by the temperature of the bath, the critical temperature (T_c) between the transition was then determined. The physical properties of the lattice were then plotted for different temperatures to find this critical temperature (T_c) as shown below:

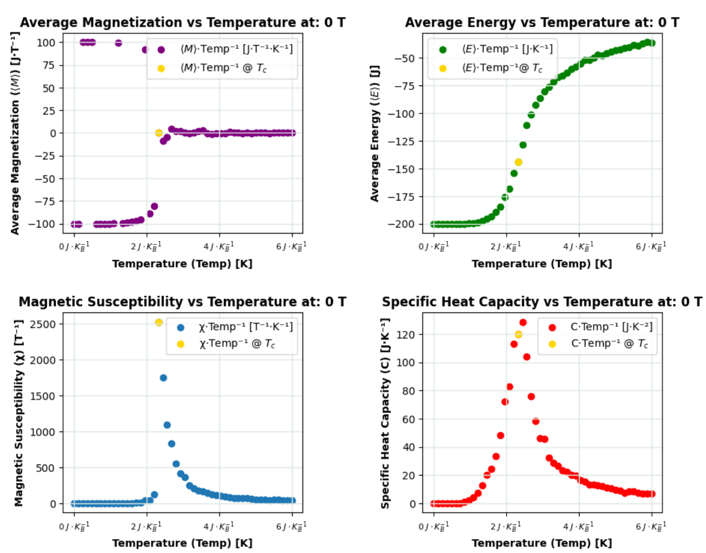


Figure 3: *Observable Quantities vs Temperature (T)*

The critical temperature (T_c) was determined to be roughly 2.3 $J \cdot K_B^{-1}$. This was determinable because the physical properties: χ and C peak at this temperature, $\langle M \rangle$ approaches 0, and $\langle E \rangle$ has an inflection point at this temperature. In order to determine the affect the critical temperature (T_c) and the system size (L^2) have on the observable quantities, The properties were plotted against the system size at the critical temperature (T_c). This is shown below:

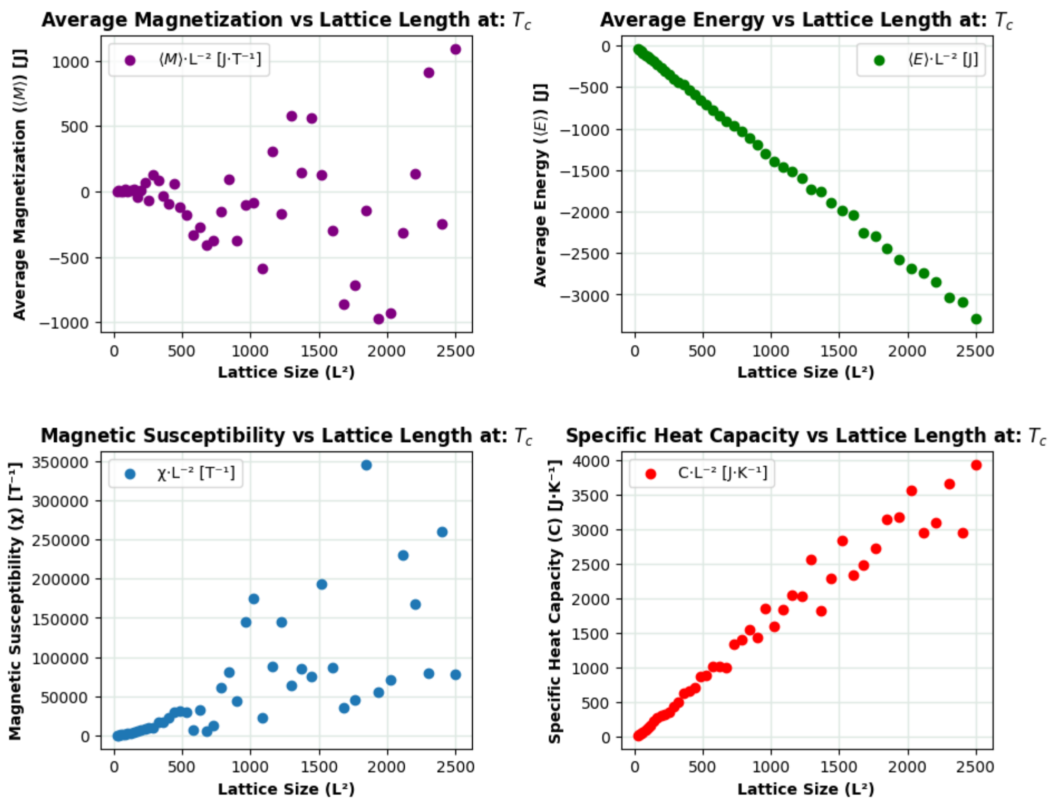


Figure 4: *Observable Quantities vs System Size at* T_c

The average magnetisation ($\langle M \rangle$) appears to roughly increase in magnitude as the system size increases as there are more sites to contribute to this value. As it is at the critical temperature (T_c) the lattice behaves both like it is in a ferromagnetic and paramagnetic phase interchangeably.

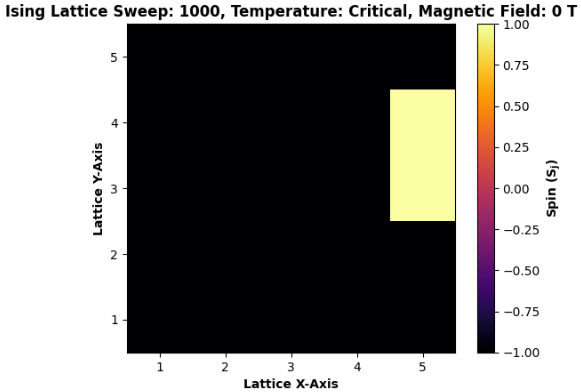
The average energy ($\langle E \rangle$) appears to decrease linearly as the system size increases as there are more sites to contribute to the energy. As the lattice size increases the ($\langle M \rangle$) and ($\langle E \rangle$) are affected more by the initial state and the number of samples required to get an accurate average is larger and therefore increasing that number would smoothen the curve.

The magnetic susceptibility (χ) appears to increase linearly up until the lattice reaches roughly 500. As the lattice size increases the number of sweeping states required to reach physically relevant micro-states is increased and therefore more sweeping states are required to get accurate results.

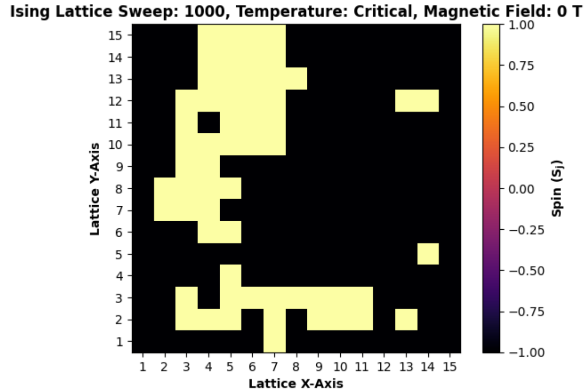
However the specific heat capacity (C) of the lattice does not appear to lose its linear relationship as quickly as the magnetic susceptibility (χ) does.

Sweeping randomly rather than sequentially would defeat the purpose of the metropolis algorithm and would just produce observable quantities which are not physically relevant.

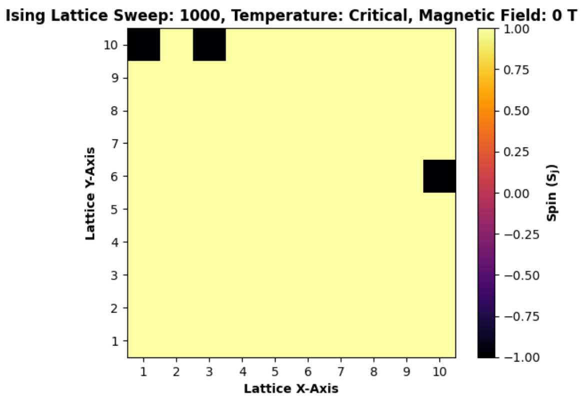
Some metropolis states of these lattices at different sizes are also included below:



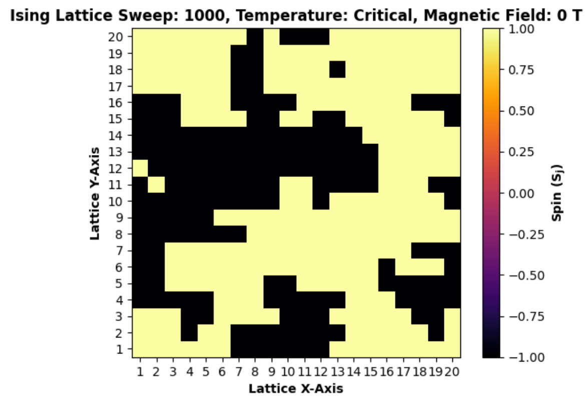
(a) Metropolis State at Lattice Size 25 at (T_c)



(c) Metropolis State at Lattice Size 225 at (T_c)



(b) Metropolis State at Lattice Size 100 at (T_c)



(d) Metropolis State at Lattice Size 400 at (T_c)

Figure 5: The Metropolis States of the Ising Lattices at different Lattice Sizes (L^2) at Critical Temperature (T_c)

Conclusion

In summary, the application of object-oriented programming and the Metropolis algorithm to simulate the 2D Ising model yielded valuable insights into its behavior. By exploring observable quantities such as average magnetization, energy, magnetic susceptibility, and specific heat capacity, distinct patterns emerged, revealing phase transitions at critical temperatures. The critical temperature ($T_c \approx 2.3\, J \cdot K_B^{-1}$) played a crucial role, influencing the system's response to applied magnetic fields. The study also investigated the impact of varying system sizes (L^2) on observable quantities, indicating the importance of system size in obtaining accurate results. Metropolis states at different lattice sizes provided visual representations of microstates, illustrating the evolving configurations at the critical temperature. Overall, the computational methods employed provided a comprehensive understanding of the Ising model's macroscopic behavior, contributing to the broader field of statistical physics and computational simulations of complex systems.