Computer simulation: Computational Methods, assignment 3: Monte Carlo simulations for the 2-D Ising model

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Introduction and Theory:

A material such as a metal or glass has physical properties such as magnetic susceptibility, energy, heat capacity and magnetization. These different properties arise from the composition of the billions of microstates present. These microscopic constituents can couple and interact with each other in many different ways to give rise to different macroscopic properties. The Monte-Carlo method is a famous numerical technique coupled with the established Markov chain processes to analyze these materials. In this report we will specifically be investigating the physics of ferromagnetic materials; examples of these substances are Iron, Cobalt, and Nickel along with metallic alloys and rare earth magnets. The ferromagnetic materials retain magnetization in the absence of an external magnetic field. These materials therefore exhibit a long-range ordering on an atomic level of areas where unpaired electrons have different spins. At a specific temperature (Curie temperature) the system cannot sustain this magnetization and a phase transition occurs.

The Ising model is a simplified model arising from statistical mechanics for the analysis of magnetic structures and interactions of these ferromagnetic substances along with their phase transitions. The Ising model is a square lattice of size N (Nx*Ny) sites with each cell containing a value of +1 or -1, which represents the respective electrons spin in that cell with +1 representing spin up and -1 representing spin down i.e. $\sigma_j \in \{+1, -1\}$. The macroscopic properties of our 2-D Ising system is determined by the nature of the accessible microstates. For simplicity in this report and assignment each spin only interacts with its neighbor's i.e. spins up, down, left and right to itself. We eliminate the effect of the lattice's boundaries by theoretically folding it into a torus. We also assume that there is an absence of an external magnetic field (h=0). The Hamiltonian of the Ising model is given by $H = -\sum_{\langle i,j \rangle} J_{i,j}\sigma_i\sigma_j - B\sum_j \sigma_j$. However there is no external magnetic field which yields the Hamiltonian $H = -\sum_{\langle i,j \rangle} J_{i,j}\sigma_i\sigma_j$. Where $J_{i,j}$ is the exchange energy between the two spins which is also known as the coupling constant. $\langle i, j \rangle$ implies there is 'nearest neighbor interaction only'. If $J_{i,j}$ is positive then the neighboring spins will tend to align giving rise to a ferromagnetic material, we assume that this term is positive and constant for the purpose of this report. Ferromagnetic materials undergo a phase transition at their Curie temperature T_c, which is the temperature above which when the material loses its ferromagnetism and becomes paramagnetic. In this paramagnetic state, the material's magnetic moments are not aligned with each other and the material's magnetization is greatly reduced. The two-dimensional model with no external field was analytically solved by Lars Onsager, showing that the model undergoes a phase transition at the critical temperature given by $(T_{c)} = \frac{2J}{kln(1+\sqrt{2})}$. We allow k the Boltzmann constant to be 1 as well as J =1. The theoretical value calculated is 2.269 for the Curie temperature. At temperatures below the Curie temperature, ferromagnetic materials exhibit long-range magnetic order, meaning that the magnetic moments of the atoms or molecules within the material are aligned with each other over large distances. This alignment of magnetic moments gives rise to the ferromagnetic behavior of the material, such as its ability to be magnetized. At temperatures above the Curie temperature, the thermal motion of the atoms or molecules within the material becomes too great, disrupting the alignment of their magnetic moments. As a result, the material loses its ferromagnetism and becomes paramagnetic, meaning that it is only weakly attracted to a magnetic field, and the

materials magnetization is therefore greatly reduced. The Ising model is not feasible to evaluate numerically as the number of possible states for an NxN grid is 2^N. We therefore use the metropolis algorithm which is a modified Monte-Carlo method for the system. 4 key steps will provide the framework for the given simulations we will be running. We first prepare an initial configuration of N steps, and then for a particular randomly chosen site we flip the spin and calculate the change in energy dE, where the average energy is given by $(\frac{1}{2}\langle\sum_{i,j} H_{i,j}\rangle)$. If dE is negative, we accept the new configuration and move to the next step. If dE is positive then it is flipped with the probability of $e^{-\frac{dE_j}{kT}}$ where dE_j is the change in energy arising from flipping the spin. This process is repeated as we sweep through the lattice. In this report we will be investigating the magnetization, specific heat, energy and magnetic susceptibility of the system. Partial pseudocode in the form '[ ]' from the full python files submitted will be presented in this report to aid with the explanation of how each task was carried out. The size of the lattice and number of data points were kept relatively small to yield quicker computations which led to some graphs not showing their true theoretical accuracy.

Task 1:

The value for the Curie temperature was calculated to be $(T_c) = \frac{2J}{kln(1+\sqrt{2})} \approx 2.269$ from the analytical derivations calculated by physicist Lars Onsager. We will now try to verify the theory behind this theoretical value temperature T_c of the phase transition between ferromagnetic and paramagnetic phases by plotting the temperature against Energy and Magnetization and analyzing the plots. A lattice of 100 sites (n=100) was initialized by [state = np.random.randint(0, 2, size=(n, n))] and the magnetic field was set to 0 (H=0). The Curie temperature, number of Monte-Carlo steps per temperature, and the temperature increment were all set to the respective values. The initial energy and magnetization was set by [E = -1 * np.sum(state[:-1, :] * state[1:, :])] and [M = np.sum(state)]. The Monte-Carlo simulation we wanted to carry out was defined as well as the change in energy due to flipping the spin at the sight. The spin was flipped with probability $e^{-\frac{dE_j}{kT}}$ and finally the energy and magnetization graphs were recorded and plotted with the arrays the same length as the temperature array.

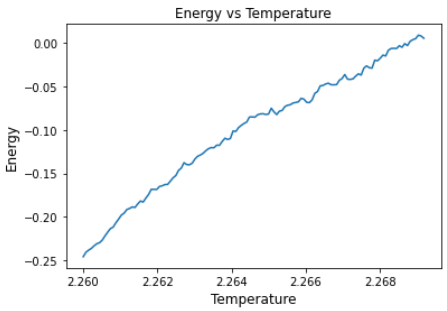

Figure 1 above shows a graph of the energy change during the phase transition for a critical temperature of 2.269.

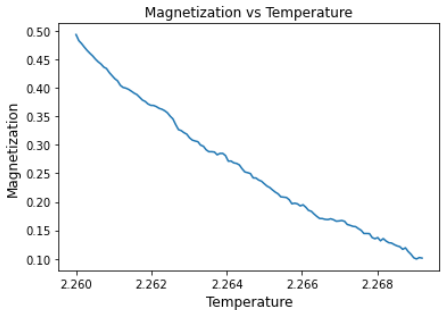

Figure 2 above shows a graph of magnetization change during the phase transition for a critical temperature of 2.269.

As we can see from figure 1 there is a vast change in energy during the phase transition that occurs at a temperature of around 2.269 J/k_B. The energy rapidly increased as there is energy released (typically heat) during this transition. The magnetization against this was also plotted as seen from figure 2 which shows a decrease in magnetization, this is because in a ferromagnetic material, the magnetic moments of the atoms are aligned, which creates a strong overall magnetic field. This alignment requires a certain amount of energy to maintain and when the material transitions to a paramagnetic state, the alignment of the magnetic moments is lost, and then the material's overall

magnetic field is weakened. This task was done to verify the theory discussed in the introduction of this report.

Task 2:

We will now plot the average magnetization per spin over this phase transition given by $\langle M \rangle$ where $\langle M \rangle = \frac{1}{N^2}\sum_{i,j}\sigma_{i,j}$ where N is the lattice size. This will be shown over the range of temperatures (1-4) J/k_B. We once again set the starting size of the lattice to be an 'NxN' lattice. The functions for generating a random spin configurations, Metropolis algorithm, energy configuration and magnetization configuration were all defined. Next the lattice size, computed steps and sweeps were all assigned values. The system was then configured.

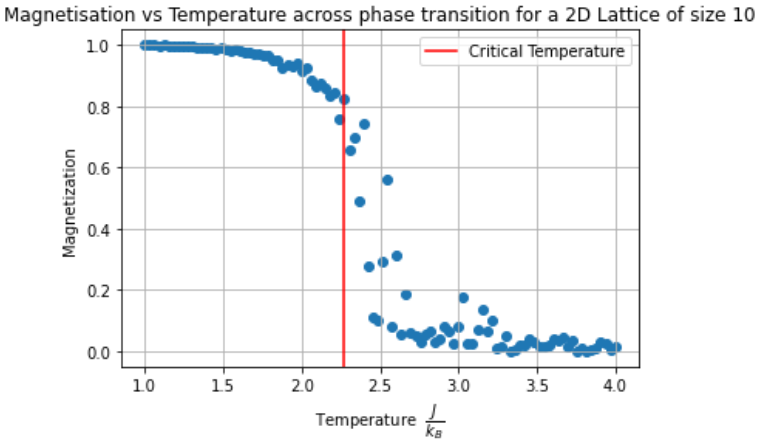

Figure 3 above shows the average magnetization per spin across the phase transition for a 2D lattice of size 20

From figure 3 we can clearly see how the average magnetization spin is an average of 1 until the phase transition temperature where afterwards it rapidly decreases. This agrees with our theory already described, where the critical temperature line will include the point of inflection of the graph. The system is randomized hence why some points may not agree completely with what a theoretical graph should look like.

Task 3:

Next we will plot the specific heat capacity as a function of system size for a temperature of T = T_c. The specific heat capacity of the system is given by $c_v = \frac{1}{T^2}[\langle E^2 \rangle - \langle E \rangle^2]$. The same Metropolis algorithm was set up, the values updated and specific heat capacity defined.

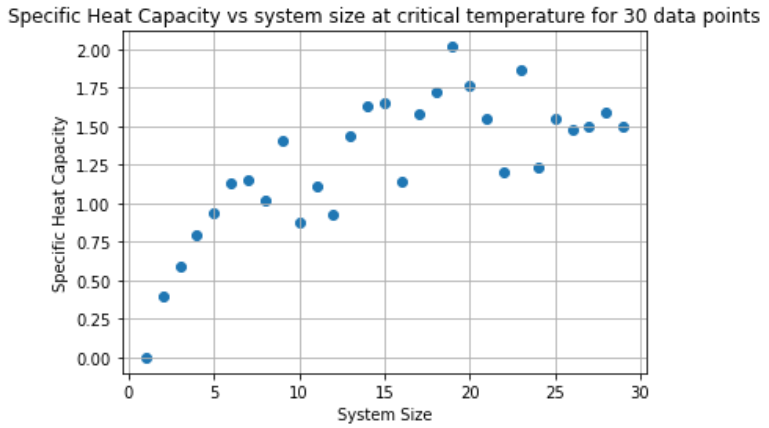

Figure 4 above shows the specific heat capacity of the system at the critical temperature plotted for 30 data points.

From figure 4 we can see a rough relationship between the specific heat capacity of the system at the critical temperature. At the critical temperature where a phase transition occurs, the relationship between the system size and the specific heat capacity can vary depending on the details of the system and the phase transition. In general, the specific heat capacity of a substance is a fundamental property that is independent of the size of the sample, so the two variables would not be directly related at the critical temperature. However, for systems that exhibit phase transitions, the specific heat capacity will show a sharp peak at the temperature where the phase transition occurs, and the size of the system could affect the magnitude of this peak or jump. Larger systems may show a more pronounced effect, with the peak or jump in the specific heat capacity becoming more pronounced as the system size increases. However our graph does not show the most profound peak where the system size it largest, it does show a general trend of how the specific heat capacity increases as the system size increases. This relationship may vary depending on the materials involved and their individual properties such as the rate at which the temperature of the system is changed, as well as other factors such as the presence of external fields (in our system there is none) or the type of boundary conditions.

Task 4:

Now we will further investigate how this system behaves with regards to magnetic susceptibility, specific heat capacity and energy over the phase transition. To show these on various plots the same code was used as in task 2 and 3 however we needed to define magnetic susceptibility and energy which was done through python. Magnetic susceptibility X was given by $X = \frac{\langle M^2 \rangle - \langle M \rangle^2}{N^2 T}$, where $\langle M \rangle$ is the average magnetization per unit spin, T the temperature and N the lattice size.

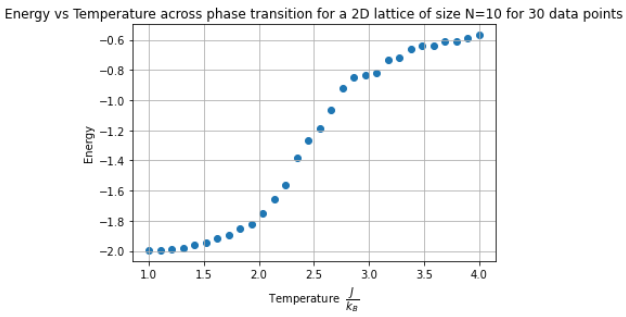

Figure 5 above shows a graph of the energy plotted across the phase transition.

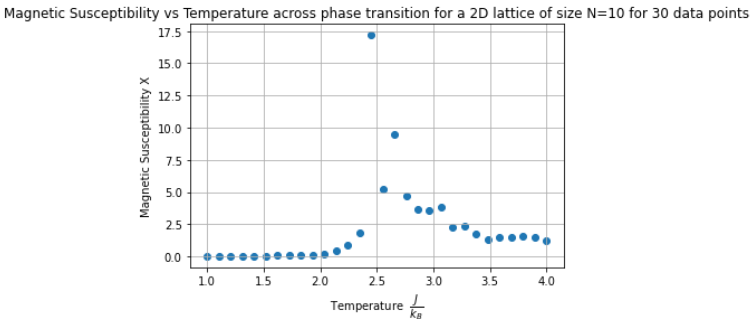

Figure 6 above shows a graph of the magnetic susceptibility plotted across the phase transition.

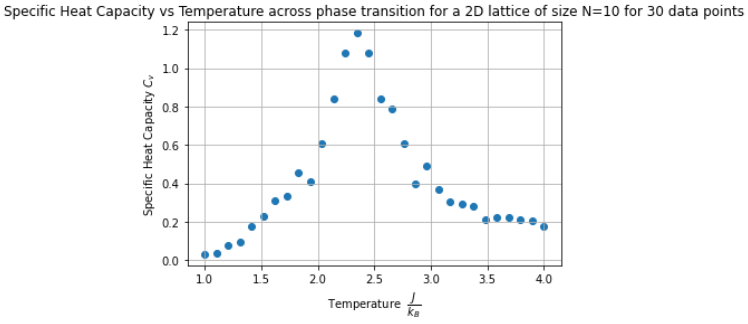

Figure 7 above on the previous page shows a graph of the specific heat capacity plotted across the phase transition.

Figure 5 in general shows us that the energy of a system is related to the temperature through the laws of thermodynamics. As the temperature of a system increases, the energy of the system also increases, and vice versa. However the effects of temperature on the energy of a system are not always straightforward, and can be influenced by a number of factors such as the size and composition of the system. From figure 6 we can see the relationship between magnetic susceptibility and temperature across the phase transition. Magnetic susceptibility is a measure of how easily a material can be magnetized, and it is related to the temperature of the material through the laws of thermodynamics. As the temperature of a material increases, its magnetic susceptibility typically decreases, meaning that it becomes less easily magnetized. At the critical temperature, the behavior of the material is changes dramatically, and it becomes more susceptible to being magnetized as the material goes from being ferromagnetic to becoming paramagnetic. We can clearly see this spike on the graph at the critical temperature point of $T \approx 2.269$. From figure 7 we can clearly see how the specific heat capacity is increasing until the temperature of the system reaches the critical value. Specific heat capacity is a measure of the amount of heat energy required to raise the temperature of a substance by a given amount and this shows how more energy is required to raise the temperature of a ferromagnetic material compared to a paramagnetic material. Ferromagnetic materials are typically composed of atoms with unpaired electrons, which gives rise to their magnetic properties. The unpaired electrons can align with each other to create a strong magnetic field, however they also require a significant amount of energy to rearrange and as a result, it generally requires more energy to raise the temperature of a ferromagnetic material compared to other materials, such as paramagnetic ones where this is not the case.

Discussion and Conclusion:

One may wonder what effect does changing the initial state have on the system. The initial state of a 2-D Ising model with no external magnetic field can have a significant effect on its behavior. We know that the initial state of a system refers to the arrangement of its components at the start of a given process or simulation and in the case of a 2-D Ising model, the initial state refers to the initial alignment of the atoms within the model. If we varying the initial state of the model we can affect its behavior in a number of ways, one such example is the temperature at which it undergoes a phase transition and the overall behavior of the system. For example if we start the model with all of the atoms aligned in the same direction we may get a different result in the phase transition temperature compared to starting the model with the atoms randomly aligned. Following from this the rate at which temperature the system undergoes phase transition, magnetic susceptibility and specific heat capacity will also have changed. In this system we have assumed there is no external field but from our knowledge we can intuitively think what may happen if this was not the case. For example if an external magnetic field is applied to a 2-D Ising model, it can have a significant effect on the behavior of the system. The external field can influence the alignment of the atoms/electrons within the model, which will affect the critical temperature at which the system undergoes a phase transition. For example, if the external field is strong enough, it may be able to induce a phase transition at a lower temperature than would be possible without the field. We have already discussed in task 3 how varying the system size might affect the temperature at which the system undergoes a phase transition with regards to the specific heat capacity, however a larger system size may also make it more susceptible to the influence of an external magnetic field.

Varying the sample size and update method used in the Metropolis algorithm can affect the behavior of the 2-D Ising model. We can intuitively think how using a larger sample size can increase the accuracy of the simulation, but that then this can also make the simulation more 'computationally expensive'. Using too small of a size for the system may also lead to the system not showing a phase transition. Varying the random update method for the Metropolis algorithm can affect the speed at which the algorithm converges to the equilibrium state of the Ising model and using different update methods will use different strategies for selecting which spins to flip, which can affect the overall behavior of the system like its magnetization. If we use a sequential update method, which means that the atoms are updated in a fixed order, we will improve the efficiency of the simulation, but this may also affect the accuracy of the results. In general, the accuracy of a simulation is determined by how closely the results of the simulation match the behavior of the system being modeled. The sequential update method updates the atoms in a fixed order, rather than randomly selecting them as in the standard Metropolis algorithm which can affect the way the atoms interact with each other yielding a different overall behavior of the system. Additionally, the sequential update method may also affect the convergence of the simulation, which is the point at which the system reaches equilibrium and the simulation results become accurate.

In conclusion the physics of a 2-D Ising model on a square lattice in the absence of a magnetic field h=0 was studied with particular attention given to the phase transition that occurs between the ferromagnetic and paramagnetic states for a particular temperature. The magnetic susceptibility, specific heat capacity, and energy of the system was further studied and analyzed using various plots, while more information was grasped about the effects of varying different conditional aspects to the metropolis algorithm used.