**Computational Physics - Final Project Report - 2D Ising Model**

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# 1 Introduction

Ferromagnetic materials are commonly modeled using the Ising model. These materials are made up of atoms arranged in a lattice. Each atom in this lattice has a spin state, either up or down, which interacts with the spins of its immediate neighbors. At high temperature, these spins are all in random directions but as the temperature decreases, the magnetic interactions align the spins. The magnetization of the material is determined by the number of atoms with spins that are parallel to their neighbors.

Ernst Ising solved this model in his 1924 thesis for 1D, which was found to have no phase transition. In his thesis he wrote that this model doesn't have a phase transition in any dimension. We're going to demonstrate that he was wrong! A phase transition means a sudden change in the properties of the system as when there is a small change in a certain parameter, in this case, temperature. One example is water transitioning from liquid to solid when it's temperature drops below 0°C.

In the Ising model, the spins can have a value of either +1 (up) or -1 (down). For $N$ atoms in the ferromagnetic material we're modeling, the spin values are $\{s_i\}$ for $i = 0, 1, 2, \ldots,$ N-1. Because we're looking at interactions of an atom's nearest neighbors in the $x$ and $y$ directions, the total energy of the material can be computed as

$$E = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_{i=0}^{N-1} s_i \tag{1}$$

where $J$ is the *exchange energy* (strength of the interaction, set to $J = 1$) and $H$ is an externally applied magnetic field (set to 0 initially). For our experiment, we will look at the case where there is no external magnetic field ($H = 0$), so the last term of (1) can be disregarded.

Note that there's a minus sign before the $J$. The lowest energy state of the system occurs when all the spins are parallel, when there product is +1. By using $-J$, we will have the lowest energy. For this reason, the Ising model is initialized at $T = 0$ which all the spins aligned at +1.

If we define the overall magnetization as

$$M = \sum_{i=0}^{N-1} s_i$$

then at high temperatures, the spins will vary randomly and we'll have $\langle M \rangle = 0$ (the *paramagnetic* phase). Once the temperature drops below a critical point called the *Curie temperature*, $T_c$, a phase transition occurs where the atomic spins are quickly aligned and

the material becomes magnetic. In 1944, the exact solution for critical temperature was calculated as

$$T_c = \frac{2}{\log(1+\sqrt{2})} = 2.2691853142118531421\frac{J}{k_B},$$

where $k_B$ is Boltzmann's constant, $k_B = 1.3806503 \times 10^{-23}$ J/K. This was calculated in 1944 by Lars Onsager[1].

# 2 Metropolis algorithm

The work behind Onsager's analytical solution is immensely complicated, but we can use Monte Carlo methods to see the effects his solution predicts numerically via the Metropolis algorithm.

The general algorithm consists of a random walk through the system. In the Ising model, the direction of spin can be switched with a probability that's a function of the spins of it's neighbors.

To numerically simulate magnetization as the temperature increases in 2D, we create an $N \times N$ matrix of "atoms" and assign each entry a spin value of +1 or -1. Initially, we will start at $T = 0$, so all spins will be aligned with $s_i = +1$ and the material will be magnetized. As the temperature increases, the changes in spin are simulated using the Metropolis algorithm. A number of "sweeps" will occur and the spin in each atom will "flip" if the energy required, $E_{\text{flip}}$, is less than zero. If $E_{\text{flip}} \neq 0$, then the spin direction will change with the probability

$$P_{\text{flip}} = e^{-E_{\text{flip}}/k_B T}. \tag{2}$$

Remember that if the algorithm is evaluating whether to transition from state 1 to state 2 when $E_1 > E_2$, then $P_{\text{flip}} = 1$. In the case where $E_2 > E_1$, then $P_{\text{flip}} = e^{-E_{\text{flip}}/k_B T}$. $E_{\text{flip}}$ is defined as $E_1 - E_2$.

Another important point is that this model uses periodic boundary conditions, meaning $s_{N+1} = s_1$.

At a non-zero temperature, there is a chance that an atom will transition to a higher energy state. For each incremental increase in temperature, $\Delta t$, this algorithm is applied over a certain number of sweeps across the lattice.

# 3 Results

I ran the Metropolis algorithm on an $N \times N$ array with $N = 100$ for 1000 sweeps for each increase in temperature starting at $T = 0 \ldots 5$ where $\Delta t = 0.05$. The results for energy per atom and magnetization per atom were plotted as the temperature increases. As we see

[1] Onsager won the 1968 Nobel Prize in chemistry for his work.

in figure (1), there is a clear transition in the system's energy before and after it reaches the critical temperature of $T_C = 2.2691853142118531421\, J/k_B$. The energy of the system abruptly increases around this point. This is consistent with the theoretical prediction that the system's energy state is lowest at $T = 0$, when 100% of the spins are aligned in the $+1$ direction.

The phase transition is even sharper when looking at the magnetization per atom in figure (2). Starting at $T = 0$, we see that the system is strongly magnetic, yet slowly decreases as $T$ increases. The phase transition occurs abruptly around $T = 2.2691853142118531421$. The transition is so abrupt that the system briefly becomes anti-magnetic, then stabilizes with $\langle M \rangle = 0$. Again, this matches the theoretical prediction that magnetization is highest at low temperatures and decreases at $T$ increases.

We can also compare the numerical critical temperature with the analytic solution by looking at the difference between the two magnetization values with the largest derivatives of

$$\frac{\partial M}{\partial T} = \frac{M_i - M_{i-1}}{\Delta T}.$$

| $\Delta T$ | Numerical $T_C$ | Error ($\lvert$Analytic $T_C -$ Numerical $T_C\rvert$) |
|---|---|---|
| 0.5 | 2.200 | 0.06918531421 |
| 0.1 | 2.224999999999999645 | 0.04418531421 |
| 0.05 | 2.269185314211853142149999999992523 | 0.00031468578 |

From the above table[2], we see that the numerical $T_C$ quickly converges to Onsager's analytic $T_C$ as $\Delta T \to 0$. This is the result we were hoping for and demonstrates that the Metropolis algorithm works as expected.

Another useful quantity which illustrates the phase transition is the system's specific heat, which tells us how much the energy changes as the temperature increases:

$$C = \frac{1}{T^2}[\langle E^2 \rangle - \langle E \rangle^2].$$

We see in figure (3) that there is also a very sharp transition as the temperature approaches $T_C$. As with the other plots, I used a $\Delta T$ of 0.5.

We can see another very illustrative example of how the Metropolis algorithm works if we look at how the net magnetization of the system, $\langle M \rangle$, changes with the sweeps that occur at each time step. Remember that a sweep is when the algorithm evaluates the energy required to flip an atom's spin. My code applies 1000 sweeps per time step. Figures (4-6) show how $\langle M \rangle$ changes as these sweeps occur at $T = 1.269, 2.269$, and $3.269$. At $T = 1.269$, the system's temperature is still well below the critical temperature, and predictably, the magnetization is still very high. Recall that my experiment used an array of $100 \times 100$ atoms, giving us a total of 10,000 spins. Figure (4) shows us that even after 1000 sweeps,

[2]I would have liked to create a convergence plot but these calculations in Python took very long to complete. Lowering $\Delta T$ even further would have taken several hours and a table seemed like a cleaner way of presenting the data rather than making a plot of only three points.

the magnetization fluctuates slightly but remains very high, converging to around 9,955. This means that 9,955 of 10,000 atoms had spins in the +1 direction at this temperature. If we look at figure (5), we see the change in $\langle M \rangle$ at the critical temperature, $T = 2.269$. As expected, we see a sharp decrease in magnetization as the sweeps occur, dropping from nearly 9000 to approximately 5600. At this point, the net magnetization is still positive but quickly decreasing. If we increase to $T = 3.269$, we see another sharp decline in magnetization, dropping to `1.7e-13` after 1000 sweeps. Since the temperature is now well past $T_C$, the system is fully demagnetized.

Thus we see how 1,000 applications of (2) impact $\langle M \rangle$ at different temperatures.

## 3.1 Animation

I've included an animation (*parghi-film.mp4*) which shows the phase transition in action. It shows the spin directions changing in a 100 × 100 array as the temperature increases. Initially, we see solid red. This means that every atom is spinning in the +1 direction. Slowly, spots of blue appear which means that those atoms have flipped their spin direction to -1. Without any calculations, the film visually demonstrates that there is an abrupt change after the critical temperature. The array quickly goes from mostly red to a nearly even mix of red and blue. This tells us that there is a mix of -1 and +1 spins, resulting in a net magnetization $\langle M \rangle \sim 0$.

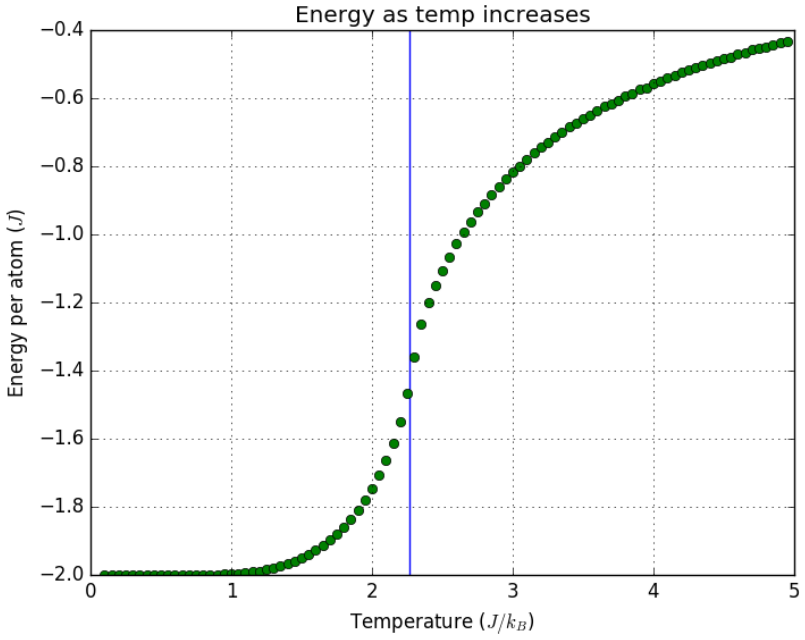


Figure 1: Energy per atom as temperature increases from 0 to 5.

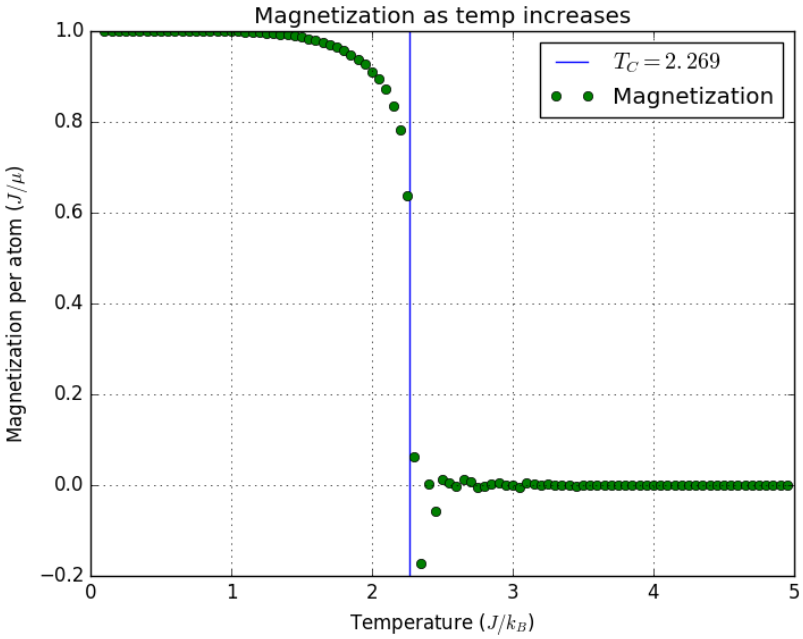


Figure 2: Magnetization per atom as temperature increases from 0 to 5.

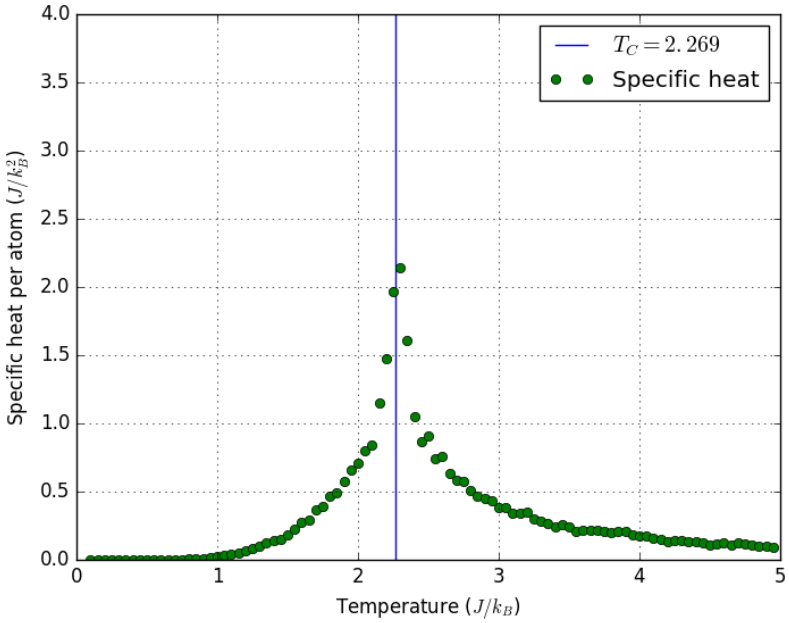


Figure 3: Specific heat per atom as temperature increases from 0 to 5.

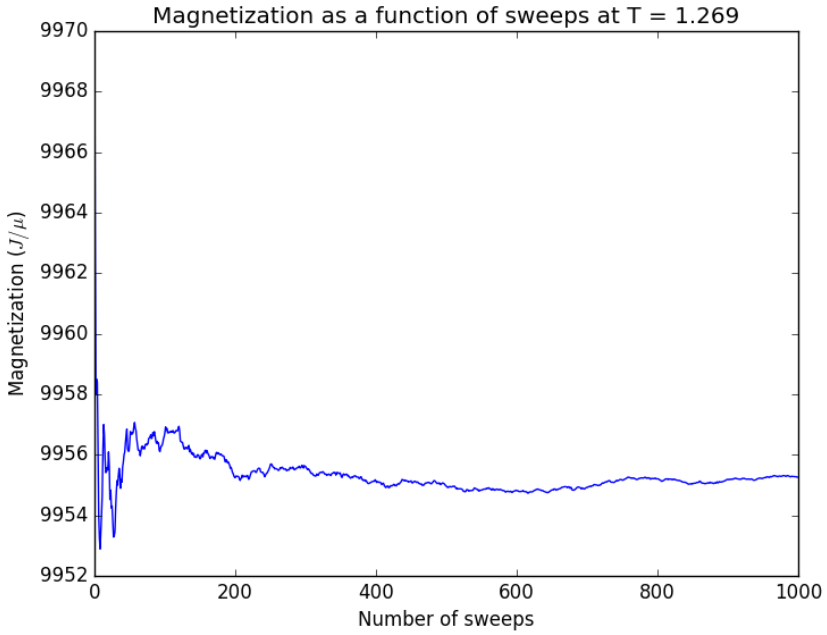


Figure 4: Change in net magnetization over 1000 sweeps at $T = 1.269$.

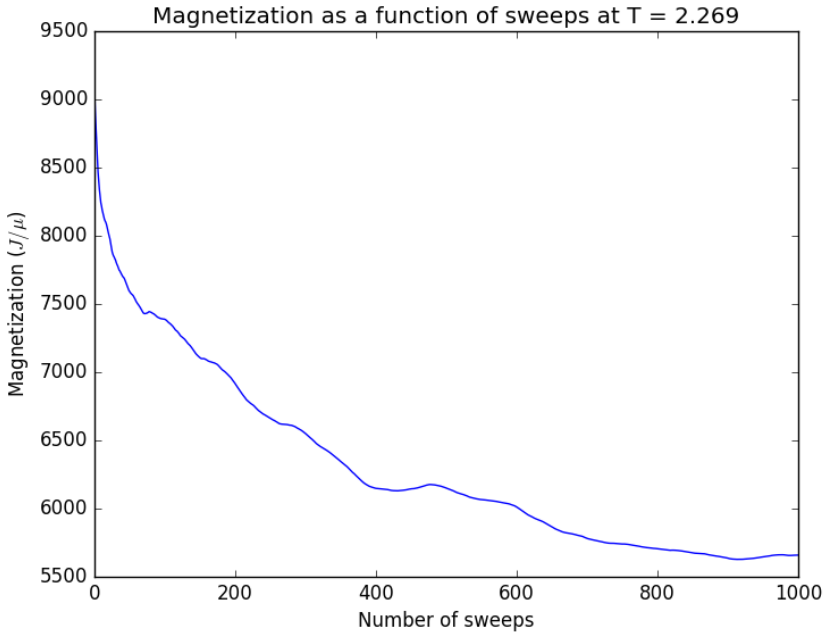


Figure 5: Change in net magnetization over 1000 sweeps at $T = 2.269$.

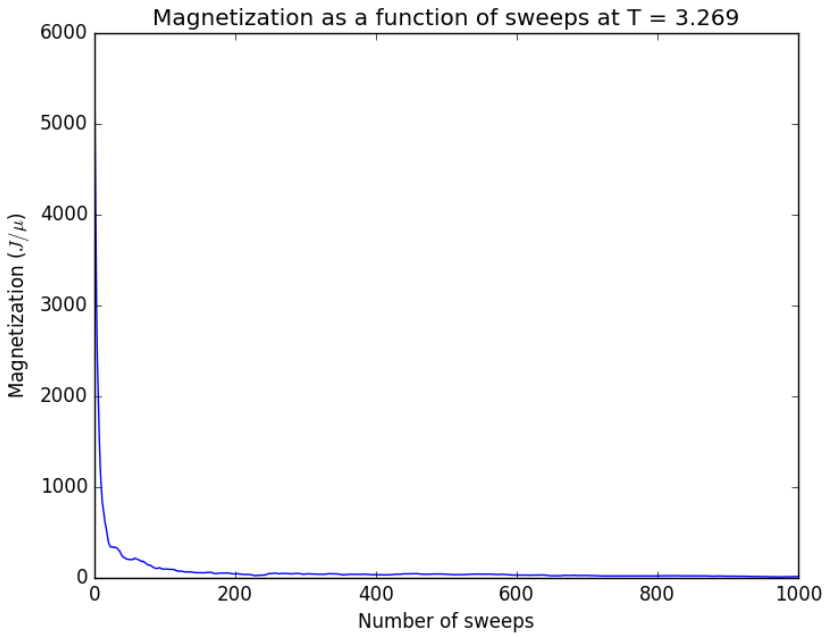


Figure 6: Change in net magnetization over 1000 sweeps at $T = 3.269$.