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

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).

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* (critical) *temperature*, T_c, a phase transition occurs where the atomic spins are quickly aligned

and the material becomes magnetic. In 1944, Lars Onsager[1] calculated the exact solution for critical temperature 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.

2 Metropolis algorithm

We can numerically simulate Onsager's results using Monte Carlo methods to see the effects his solution predicts via the Metropolis algorithm.

To numerically simulate magnetization in 2D as the temperature increases, we create an $N \times N$ matrix of "atoms" and assign each entry a spin value of +1 or -1. The initial temperature will be $T = 0$, 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_{flip}, is less than zero. If $E_{\text{flip}} > 0$, then the spin direction will change with the probability

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

In other words, the Metropolis algorithm consists of a guided random walk through a stochastic system. This is useful and important because if we wanted to calculate M for each possible state and weight these values by their Boltzmann factor's to find $\langle M \rangle$, we could use a computer to look at a system that is very small. But for a larger system, this is impractical. Even for a 20 $\times$ 20 lattice (much smaller than what I used) of interacting atoms, there are 2^{400} possible states. Rather than looking at all of them, we can choose states based on their Boltzmann factors and then weight them equally. This is the essence of the Metropolis algorithm.

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_{flip} is defined as $E_1 - E_2$. For each incremental increase in temperature, Δt, this algorithm is applied over a certain number of sweeps across the lattice.

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

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 $\Delta t = 0.05$.

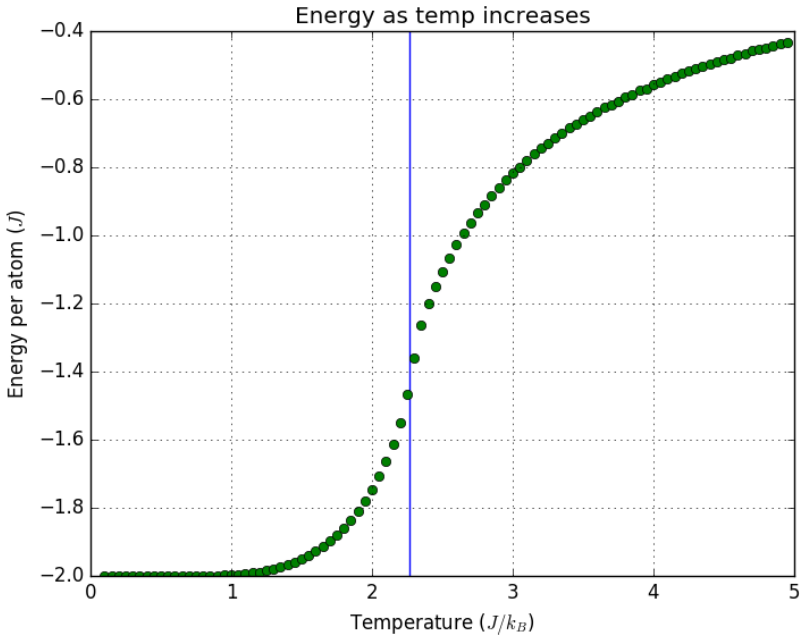

Figure 1: Energy per atom as temperature increases from 0 to 5.

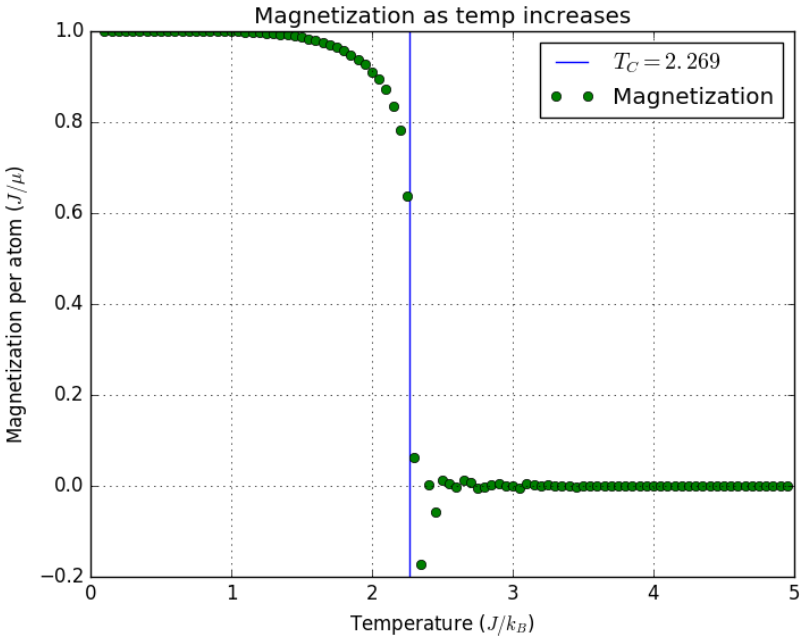

Figure 2: Magnetization per atom as temperature increases from 0 to 5.

The system's energy as T increases is seen in figure (1). There is a clear transition in the system's energy before and after it reaches the critical temperature of $T_C \sim 2.269\, J/k_B$. The energy of the system abruptly increases just before 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 – and increases with T.

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 fully magnetic, yet slowly decreases as T increases. The phase transition, again, occurs abruptly around $T \sim 2.269$. The transition is so steep that the system briefly becomes anti-magnetic, meaning there are a higher number of -1 spins than +1 spins. The system then stabilizes with $\langle M \rangle = 0$. Again, this matches the theoretical prediction that magnetization is highest at low temperatures and decreases as T increases.

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

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

ΔT	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	2.26918531421185314215	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:

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

This measures the fluctuation of energy at each step. We see in figure (3) that there is also a very sharp transition as the temperature approaches T_C. This tells us that the largest shifts in system energy are occurring close to T_C. As with the other plots, I used a Δt 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. Figure (4) shows 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

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

[2]I would have liked to create a convergence plot but these calculations in Python took very, very long to complete. Lowering ΔT 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.

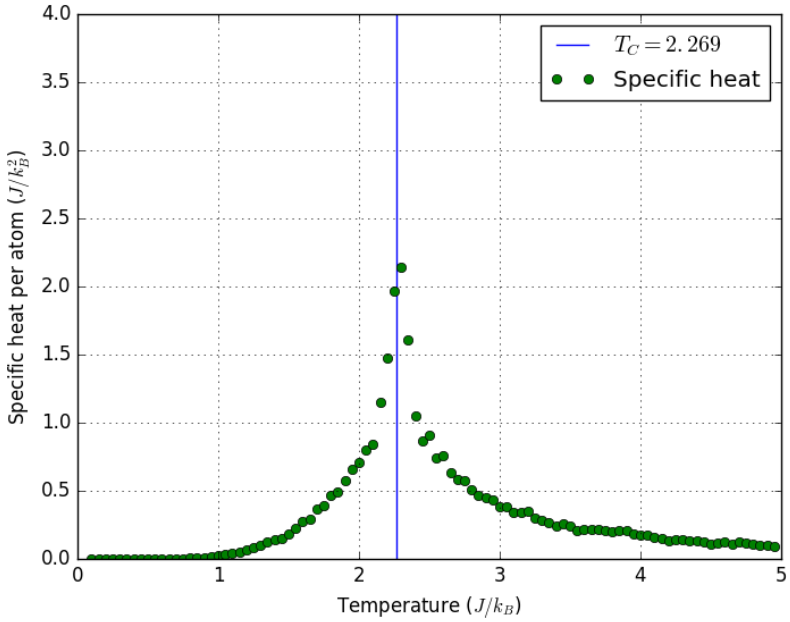

Figure 3: Specific heat per atom as temperature increases from 0 to 5.

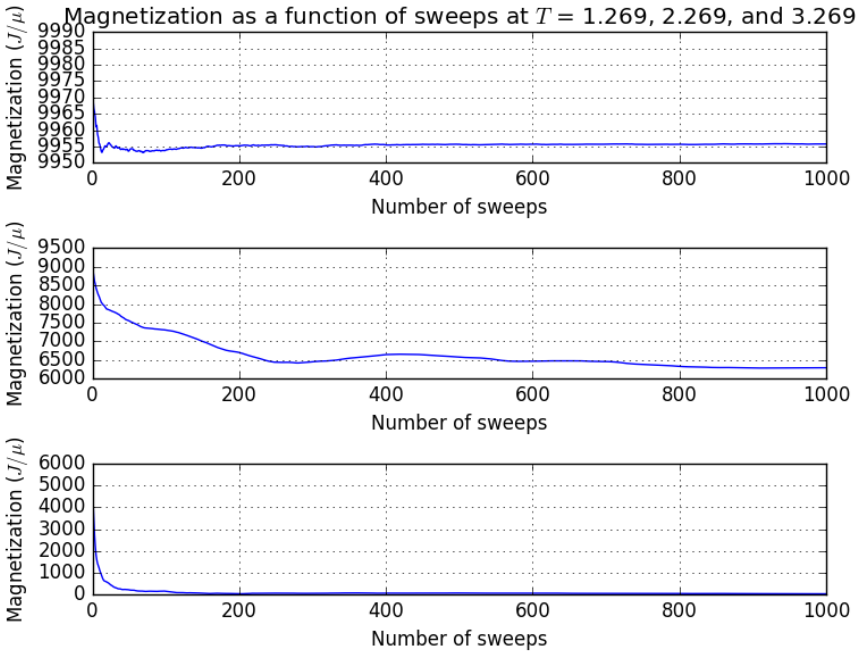

Figure 4: Change in net magnetization over 1000 sweeps at $T = 1.269, 2.269,$ and 3.269.

temperature is still well below the critical temperature, and predictably, the magnetization is still very high. Recall that my experiment used an array of 100×100 atoms, giving us a total of 10,000 spins. Even after 1000 sweeps, 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. In the next plot, 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 ~ 0 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.

If we consider the magnetization as a function of temperature, T, we have the relationship

$$M \propto |T - T_C|^{\beta} \tag{3}$$

Another of Onsager's findings is that the critical exponent for the magnetization has the analytic solution, $\beta = 1/8$. His original derivation came from

$$M = [1 - \sinh^{-4}(2J/k_B T)]^{1/8}.$$

I was able to numerical solve for the critical exponent β using finite size scaling[3] and placed a nonlinear fit for the data. Since the relationship in (3) only holds when $T \lesssim T_C$, I used 40 data points just to the left of T_C for the fit. I ran this for lattice of size $N = 20, 50$ and 100.

N	Numerical β	Error ($\lvert\beta_{\text{Numerical}} - \beta\rvert$)
20	0.100	0.025
50	0.111	0.014
100	0.129	0.004

The above results were computed with a 95% confidence interval. We see a plot of the fit for $N = 100$ in figure (5).

I also tried to solve for β numerically using a least squares fit of a `loglog` plot of the magnetization vs. $|T - T_C|$. For these trials, I used $\Delta t = 0.00625$ for the 40 points in the range $T = 2.0, \ldots, 2.265$. The results are below:

N	Numerical β	Error ($\lvert\beta_{\text{Numerical}} - \beta\rvert$)
20	0.100	0.025
50	0.085	0.040
100	0.100	0.025
200	0.111	0.014

As we can see, this method converge much slower. A plot for the results for $N = 200$ is seen in figure (6).

[3] `http://www.helsinki.fi/~rummukai/simu/fss.pdf`

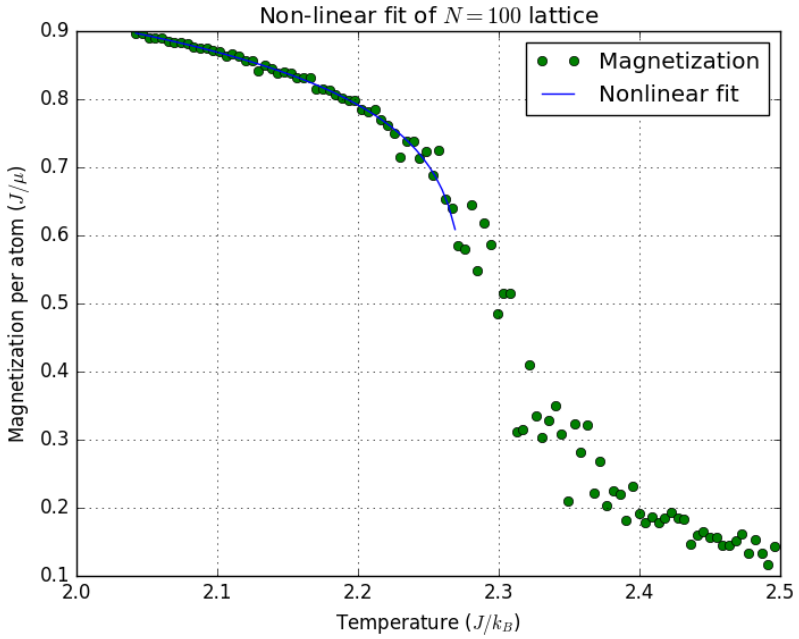

Figure 5: Plot of magnetization vs. temperature with a nonlinear fit.

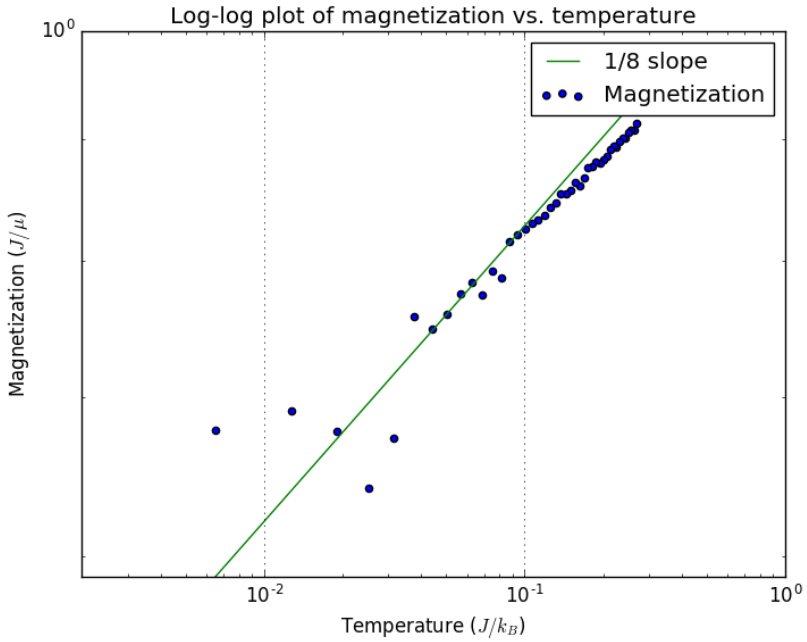

Figure 6: Loglog plot of magnetization vs. temperature using a least squares fit.

3.1 Animation

I've included an animation (*parghi-film.mp4*) which shows the phase transition in action. It shows how the spin directions change in a 100×100 lattice as the temperature increases. Initially, we see solid red at $T = 0$. 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. The film visually demonstrates that there is an abrupt change after the critical temperature, going 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 $\langle M \rangle \sim 0$.