Computational Physics
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Project 2: Monte Carlo Ising Model

1 Abstract

The ferromagnetism of a material can be defined by the state of discreet spins within the material, known as an Ising Model. While a spin can be randomly changed, there is a dependency on the temperature of the material which affects the ferromagnetism. We create a Metropolis Monte Carlo simulation to replicate this stochastic model and determine the ferromagnetism based on temperature and external magnetic field. Our results demonstrate the predicted phase transition from ferromagnetic to non-ferromagnetic as the temperature increases. The transition is more gradual when an external magnetic field is applied.

2 Introduction

The Ising model is a mathematical model representing the ferromagnetism of a given material. It assigns a discreet spin s, +1 or -1, for the magnetic dipole moments and arranges the spins in a lattice. The energy of the system is given by the Hamiltonian:

$$H = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i \tag{1}$$

Here, $\langle ij \rangle$ is the sum over adjacent neighboring spins, h is an external magnetic field, and J is the degree of ferromagnetism. We interpret the system as ferromagnetic if $J > 0$ and anti-ferromagnetic if $J < 0$; $J = 0$ has non-interacting spins and is non-ferromagnetic. The initial state of the system begins with randomly assigned spins representing a non-ferromagnetic regime. The average magnetization m is

$$\langle m \rangle = \frac{1}{N} \Big\langle \sum_i s_i \Big\rangle \tag{2}$$

for N particles. The ferromagnetism is dependent on temperature with a specific heat c given as

$$c = \frac{k_B \beta^2}{N} (\langle E^2 \rangle - \langle E \rangle^2) \tag{3}$$

for $\beta = \frac{1}{k_B T}$. Combining this dependency on temperature and the magnetization gives the susceptibility χ:

$$\chi = \beta N (\langle m^2 \rangle - \langle m \rangle^2) \tag{4}$$

Our goal for this project is to track the observables in Equations 1 through 4 as well as the lattice of spins for increasing temperatures.

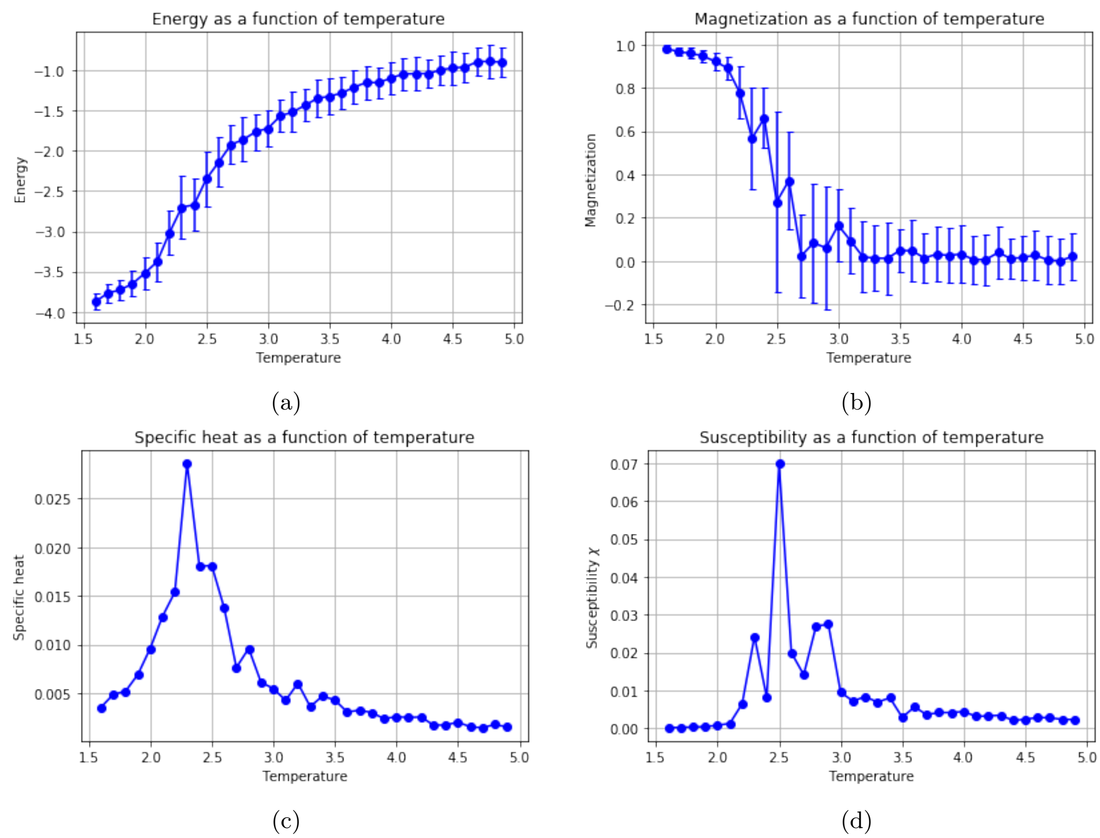
3 Methods

Our simulation establishes a spacial grid of $N = 100$ spins each with an initial random spin value and temperature T (dimensionless) over the entire system. We introduce the Metropolis Monte Carlo algorithm which takes a random particle and flips the spin if the energy E is positive or if a random number is less than $\exp(2E/T)$. Once the system reaches an equilibrium, estimated as time when $t = (n_{time}^2)/3$ for n_{time} time steps, we record the total energy and the magnetization of the system.

With the total energy and magnetization for a given temperature, we calculate the spatial average and variance over time. We use the bootstrapping method to also calculate the specific heat and susceptibility. Bootstrapping is the method of re-sampling a set of results multiple times and calculating an observable each time. In the end, this method allows us to calculate the errors of the specific heat and the susceptibility for each temperature. However, the errorbars we calculated were very small and are not visible in the figures (Section 4), contradicting the noisy results. Finally, we continue this process for different temperatures and different external magnetic field strengths. Our final results reflect the temperature dependency of these variables.

4 Results

We track the change of energy, magnetization, specific heat, and susceptibility as the temperature increases. In Fig. 1a we see a negative energy, or potential energy, decrease in magnitude. Similarly, the magnetization in Fig. 1b decreases from 1.0 (very magnetic) to 0.0 (not magnetic). Both of these point towards the system losing magnetization and the potential energy that is associated with it. We see a peak in specific heat (Fig. 1c) and susceptibility (Fig. 1d) around a temperature of 2.3 or 2.5. While the energy and magnetization do not show a similar spike in activity, this is the turning point for the system and is an indication of the phase change.



(a) (b) (c) (d)

Figure 1: Observables as a function of temperature for no external magnetic field.

Fig. 2 shows a map of spins at the end of a simulation (having reached equilibrium time) with $T = 1.5$, which is on the low end of the temperatures tested. We see a high correlation of negative and positive spins grouped together, indicating a high degree of magnetization. Testing higher temperatures shows less structure and more randomized spin values throughout the spacial grid even after equilibrium time.

Finally we manipulate the external magnetic field to monitor the change in ferromagnetism. The magnetic field stays constant as we run the simulation and increase the temperature as usual. The observables are shown in Fig. 3, 4, and 5 as the strength of the external magnetic field is increased. Immediately we see the specific heat and susceptibility varying more, no longer as a single peak but instead changing almost constantly. The magnitudes of the specific heat and susceptibility, however, are relatively low compared

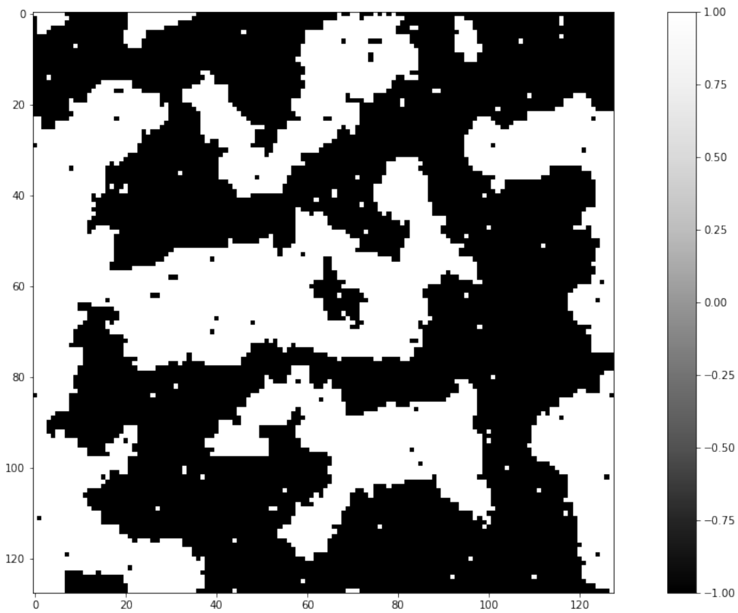


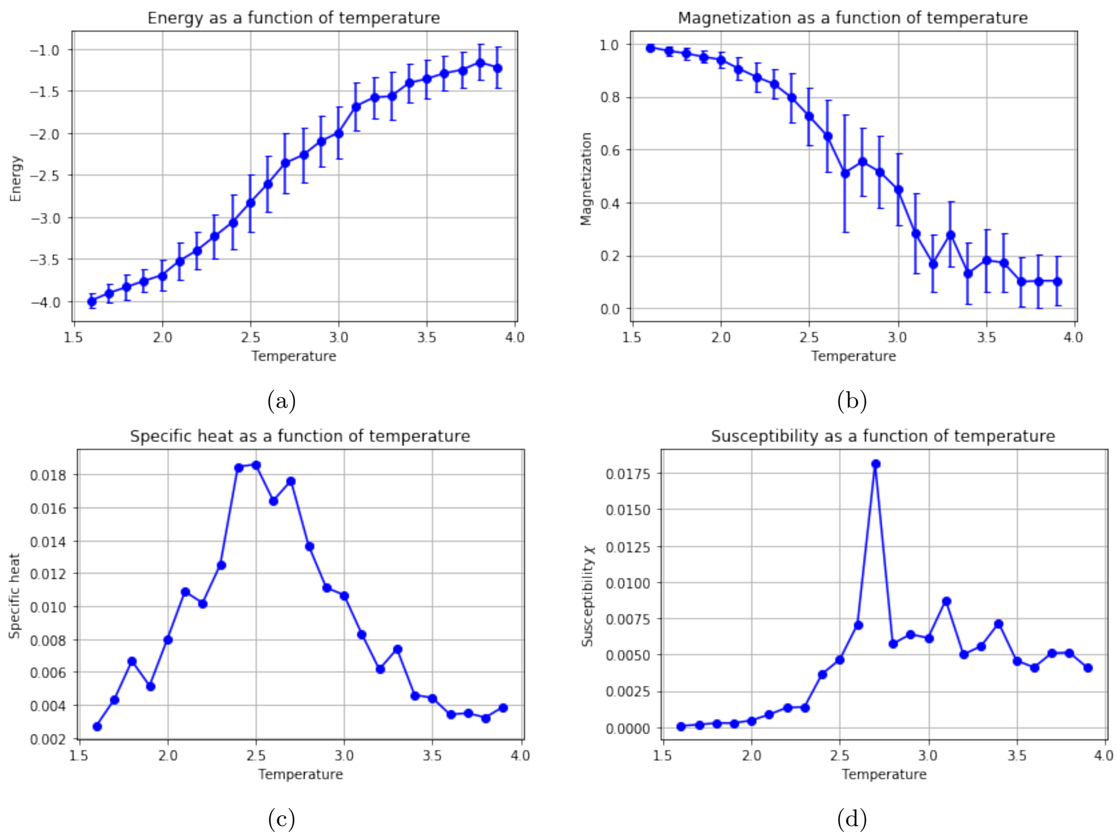
Figure 2: An example of a map of the spins after a Monte Carlo simulation.

to no external field: specific heat in Fig. 1c has a maximum of 0.025 and susceptibility in Fig. 1d has a maximum of 0.07, while their respective counterparts in Fig. 5c and Fig. 5d have maxima at 0.012 and 0.003 when $\mu = 0.5$.

This is also reflected in the energy and magnetization plots as the slopes are straighter and more gradual. Overall this shows a smoother phase transition from ferromagnetic to non-ferromagnetic as the temperature increases.

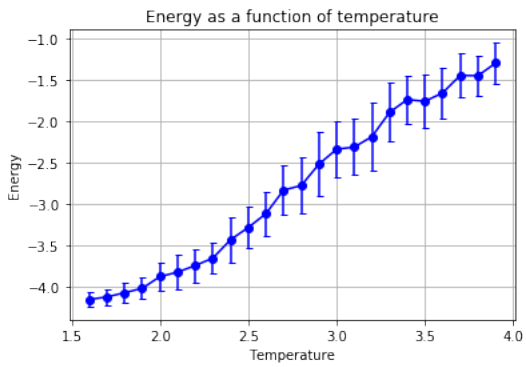
5 Conclusion

We successfully created a simulation of the Ising model by using the Metropolis Monte Carlo algorithm. Using this simulation, we were able to calculate the magnetization, energy, specific heat, and susceptibility as a function of temperature. The results clearly outline a phase transition from ferromagnetic to non-ferromagnetic as the temperature increases, which is consistent with theoretical models. Applying and increasing the strength of an external magnetic field generally decreases the specific heat and susceptibility, and demonstrates a more gradual phase transition. Further work can include other observables to monitor and incorporating a more advanced algorithm, such as the Swendsen-Wang or Wolff algorithm.



(a) (b) (c) (d)

Figure 3: Observables as a function of temperature for an external field of $\mu = 0.1$.



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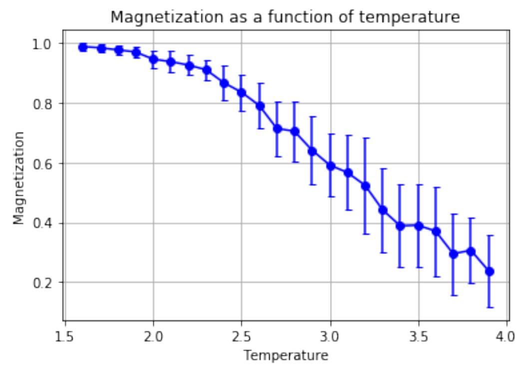
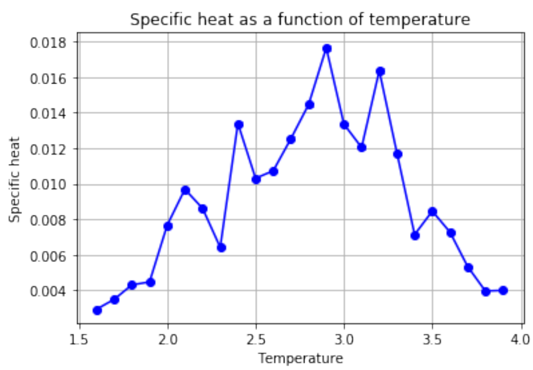


(b)



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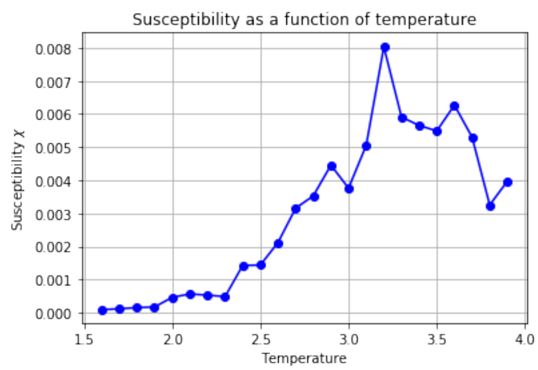
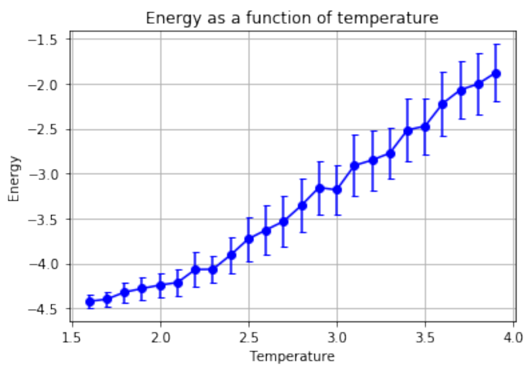
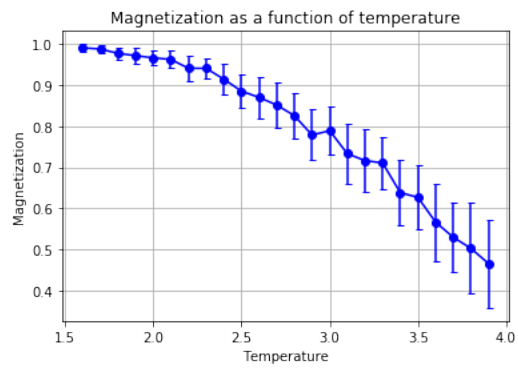


(d)

Figure 4: Observables as a function of temperature for an external field of $\mu = 0.25$.



(a)



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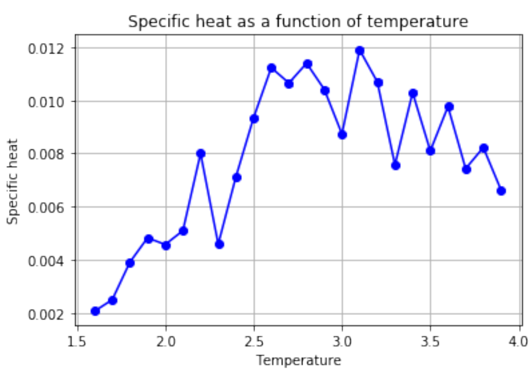

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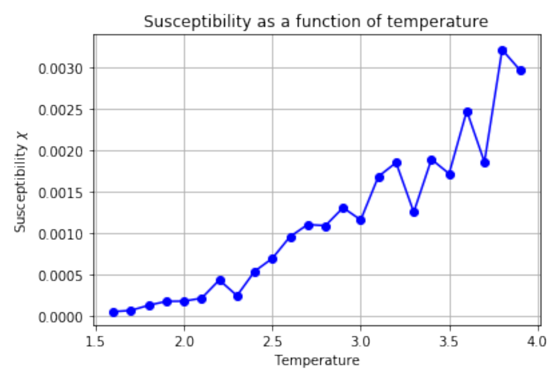

(d)

Figure 5: Observables as a function of temperature for an external field of $\mu = 0.5$.