Simulating Ising Model

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Abstract

Ising model is a mathematical tool for approximating ferromagnetism behaviors. This paper will examine the theory behind this model, how it works, and how to compute macroscopic observable quantities from the model. Monte Carlo and Markov Chain algorithms are used to simulate the models. The models were simulated with different parameters and we will observe the different characteristic that each parameter in the model possess. In addition, hexagonal antiferromagnet Ising model will be simulated. Plotting the hexagonal antiferromagnet model as a function of external magnetic field results in a magnetization plateaus.

Contents

1 Introduction

In this paper, I will discuss about Ising model, how I simulate the model, and applying it with different constraints. We will first develop a basic understanding of Ising model and how it relates to the physical world. We then will implement an algorithm that simulates the Ising model. Next, hopefully with a working algorithm, we can start applying different constraints (temperature, interaction coupling constant, lattice shape) to see the affects of each constraints. A video of the simulation is also represented in this project. It shows what the algorithm is doing at each iteration for better understanding and also an incentive to learn how to properly visualize and present data. (Beneficial as a Data Science student)

2 Background Information

In this section, we will go over the definition of Ising model, Onsager's exact solution for observable quantities for a 2D lattice, and a quick overview of Monte Carlo and Markov Chain. With Onsager's exact solution, after we simulate our model, we can use it to check if our simulation is working as expected. Monte Carlo and Markov Chain are the main algorithm scheme that is used to implement this algorithm, thus it is crucial to review them.

2.1 Ising Model

The Ising Model is developed by a a German physicist, Ernst Ising. It is a simplified mathematical model to represent properties of ferromagnetism. A ferromagnetic material is where the material has magnetic properties. Iron, nickel, cobalt are some examples of ferromagnets. To understand their magnetic properties, we need to examine their microscopic atomic spins. The Ising model is essentially a representation of the atomic spins of a material.

A simple case of Ising model is represented by a lattice $N \times N$ square grid. In the lattice square, single atomic spins occupy the lattice sites. The atomic spins can be in two states: spin up and spin down, which we will denote by $+1$ and -1 respectively.

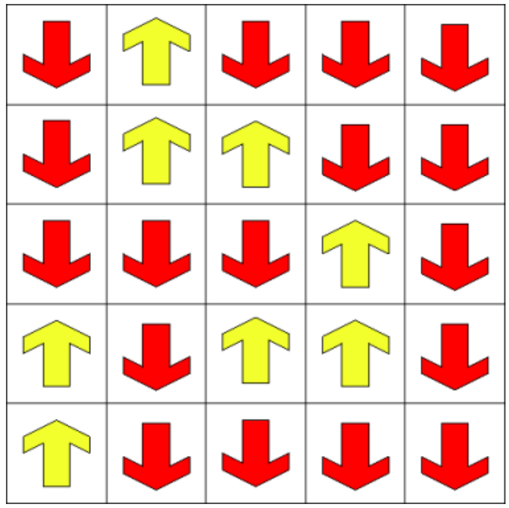


Figure 1: Sample of 5×5 square lattice

Each spin in the lattice sites represents the microscopic state. To make observations in the macroscopic world, we need to consider all the microscopic states. For instance, to calculate the overall magnetization of this model, we can sum up all the spins in each lattice sites.

This brings up another question, given a simulated Ising Model, what quantities can we calculate in the macroscopic world?

2.1.1 Observable Quantities

Let's first start with aforementioned quantity of *magnetization*. We can calculate the total magnetization or average magnetization per spin as

$$M = \frac{1}{N} \sum_{i=1}^{N} S_i \tag{1}$$

where S_i is the spin at site i.

Another quantity we can calculate is the *total energy*. The Hamiltonian at site j is given as

$$H_j = -J \sum_{<ij>} S_i S_j - k \sum_{j} S_j \tag{2}$$

where J is the coupling interactions between the neighbor sites, the notation $\sum_{<ij>}$ means the sum of the four neighbor around our site (top bottom, left right), k represents the external magnetic field applied on lattice site j.

If H_j represents the energy at each sites, then the total energy of the model is

$$E = \frac{1}{N} \sum_{i=1}^{N} H_j \tag{3}$$

$$E = \frac{1}{N}\sum_{i=1}^{N}(-J\sum_{<ij>} S_i S_j - k\sum_{j=1}^{N} S_j)$$

Other observable quantities we can derive given *magnetization* and *energy* is *magnetic suspectibility* and *specific heat*.
Mangetic suspectibility measures the tendency of a material to become magnetized when applying a magnetic field. *Magnetic suspectibility* of a given Ising Model can be found as

$$X = \left(\frac{1}{N}\sum_{i=1}^{N} S_i^2\right) - M^2 \tag{4}$$

Specific heat, a quantity that determines the amount of heat needed to raise the material by a degree, can be calculated as

$$C = \left(\sum_{i=1}^{N} H_j^2\right) - E^2 \tag{5}$$

We will simulate our Ising model and calculate the observable quantities (M, E, X, C) to compare it to Onsager's exact solutions. If the results agree, we can start applying different alterations to the model.

2.2 Onsager's Exaction Solutions

In 1944, Lars Onsager obtained the analytical expression for the Ising Model constrained with a square lattice with magnetic field $k = 0$, and assuming the horizontal and vertical coupling interaction energy between neighbors are J_1 and J_2 respectively.

The exact solution for critical temperature T_c or the temperature where we see a phase transition is given as

$$\sinh\left(\frac{2J_1}{k_B T_c}\right)\sinh\left(\frac{2J_2}{k_B T_c}\right) = 1 \tag{6}$$

where k_B is Boltzmann's constant.
For simplicity, we set $J_1 = J_2 = J$ and with a little bit of algebra we come to the solution,

$$T_c = \frac{2J}{k_B \ln(1+\sqrt{2})} \tag{7}$$

The equation above means that the critical temperature is only dependent on coupling interaction J, which means different material will have different critical temperatures.

In addition, Onsager also solved the analytical expression of magnetization, and it is given as

$$M = \left(1 - \left[\sinh(2\beta J_1)\sinh(2\beta J_2)\right]^{-2}\right)^{\frac{1}{8}} \tag{8}$$

where $\beta = \frac{1}{T}$ which T is temperature measured in Kelvin.

Again, for simplicity, we set $J_1 = J_2 = J$ and the analytical expression for magnetization becomes

$$M = \left(1 - \left[\sinh(2\beta J\right]^{-4}\right)^{\frac{1}{8}} \tag{9}$$

for $T < T_c$ and 0 for $T > T_c$.

The quantity magnetization is a function of T (embedded in β), thus, we should hypothesize that at certain temperature, we see a change in the magnetic property.

2.3 Monte Carlo & Markov Chain

The algorithm to simulate an Ising model requires the use of Monte Carlo and Markov Chain. This section will briefly explain the two algorithm schemes.

2.3.1 Monte Carlo

Monte Carlo is an algorithm and utilizes a series randomization to approximate certain behaviors. In each iteration, the process is independent of each other. Monte Carlo is applicable in many fields such as statistical mechanics, climate change and computational biology.

2.3.2 Markov Chain

Similarly to Monte Carlo, Markov Chain is also an randomize algorithm, but the main difference is that in Markov Chain, the the $(i+1)^{th}$ iteration is dependent on the i^{th} iteration. Thus Markov Chain is a stochastic model with predefined probabilities for each state. In short, simulating with Markov Chain algorithm will force the model to regions with higher probability.

3 Algorithm

In this section, we will go over the main algorithms for simulating a Ising Model.
The pseudo-code for the main simulating function is given below.

Algorithm 1 Ising Model Simulation

Create a 2D lattice of size $N \times N$
Fill the lattice with $+1$ and -1 randomly
Randomly select a site on the lattice
Flip the spin of the selected site and calculate the change in energy ΔE using eqn (2).
if $\Delta E \leq 0$ **then**
  return we want to permanently flip the spin
else
  Calculate the Boltzmann Probability p

$$p = e^{-\beta \Delta E}$$

  Generate the random number u between 0 and 1
  if $u \leq p$ **then**
    return we want to permanently flip the spin
  else
    return Revert back to the original spin
  end if
end if
Repeat steps $3 - 6$ (randomly selecting a site) until convergence.

Examining the algorithm, we can identify the implementations of Monte Carlo and Markov Chain. The steps where we randomly choose a site in the lattice is a Monte Carlo, where each iteration does not affect each other. Whereas in the second *if* condition, we calculated the Boltzmann probability p to determine whether to flip or not to flip the spin. The Boltzmann probability serves as a predefined probability that tries adjust to our state to regions dictated by the Boltzmann probability.

3.1 Boundary Conditions

When I first implemented this algorithm, I defined my boundaries as having a finite space. Which means, if the algorithm selects a site on the boundaries, only 3 (or 2) neighbors where taken into account when calculating the Hamiltonian. The imposed boundary condition does not make the model converge into an expect state.

I tried the algorithm again, but now assuming the material as having infinite space. Thus I imposed the boundary conditions using *periodic boundary conditions*. The *periodic boundary condition* sets the ghost cells using the values from the opposite cells. For instance if a site is selected at the left boundary, then this site does not have a left neighbor. To overcome is, we use the value on the right boundary for the left neighbor. Thus using this boundary conditions give me a better solution which will be discussed in the following sections.

4 Simple Ising Model (No external magnetic field)

In this section, we will use the the algorithm above to simulate the Ising Model. With the simulated system, we can calculate its observable quantities and compare it to the exact solutions.

4.1 Simulation

The following figures are simulating the Ising model with different values for J and T. Let's first setup the initial spins for a lattice grid.

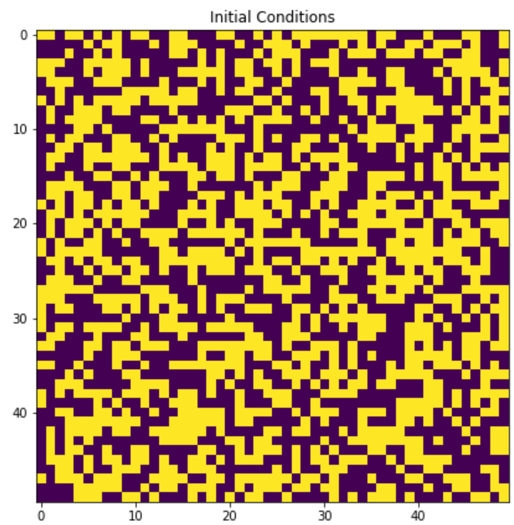
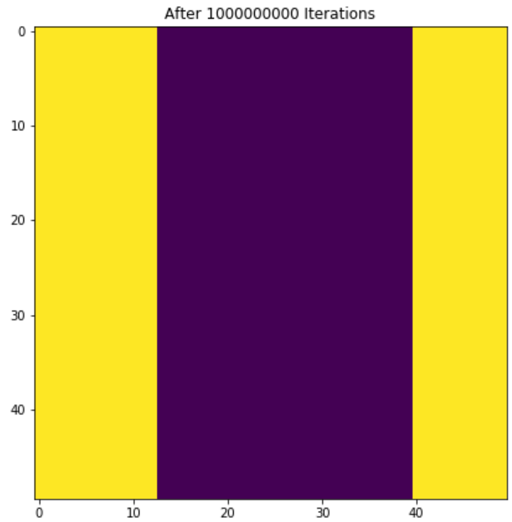


Figure 2: Initial spins in each lattice sites

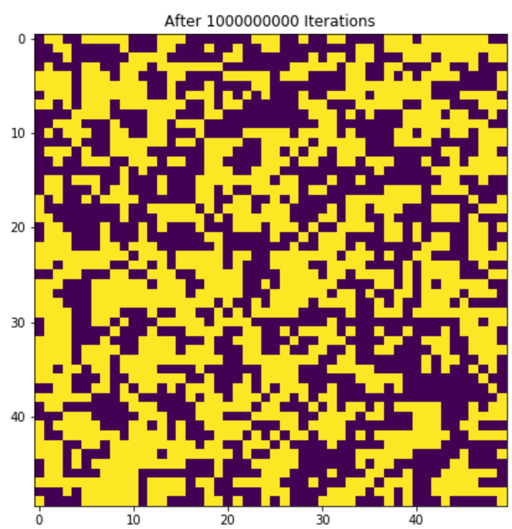
Each of the following plots are after $1,000,000,000$ iterations. I used quite and large number of iterations because with smaller iterations, the system does not converge and it is hard to depict the properties given different variables.

4.1.1 $J = 2, T < T_c$



From the above figure, we can see that at temperatures lower than critical temperature, the system aligns the spins with each neighbor, thus we can observe magnetization.

4.1.2 $J = 2, T > T_c$

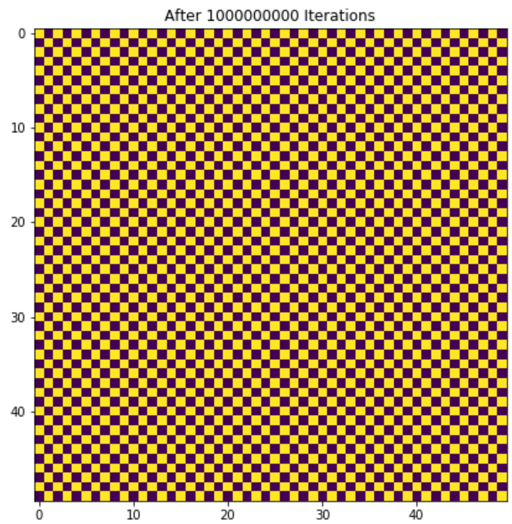


With temperature higher than critical temperature, the spins will be randomized, thus we will not observe its magnetization.

From the above two figures, we can assume that at certain temperature, the spins starts to be randomized. In the following section, we will calculate the observe quantities and compare it to Onsager's exact solutions.

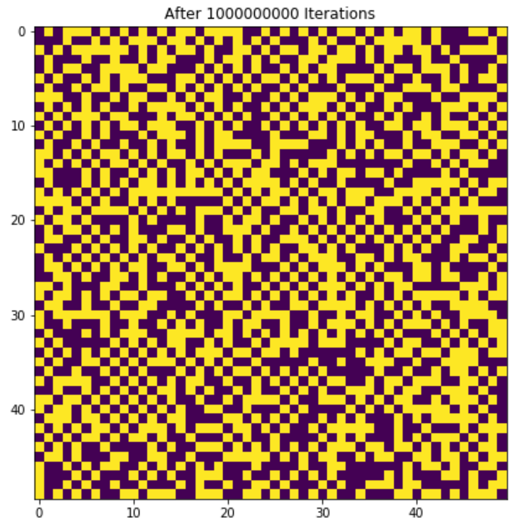
Before we explore the observable quantities, it is worth to explore some properties as we change the parameters.

4.1.3 $J = -2, T < T_c$



Imposing a negative coupling interaction between the neighbor sites will cause the above pattern in the system. This opposite alignment of the spins can be viewed as an *antiferromagnet*. We will explore *antiferromagnet* in section 7 when examine the properties of a Hexagonal lattice shape.

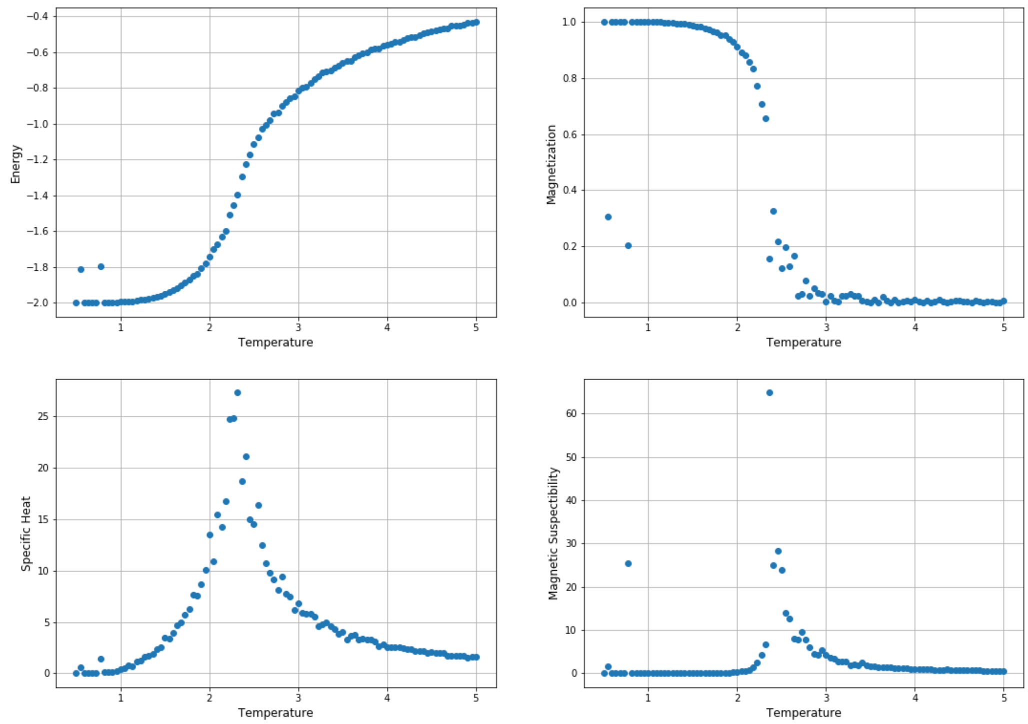
4.1.4 $J = -2, T > T_c$



This figure captures to two properties of each parameters. When J is negative, the neighbor spins tends to be opposite with each other, whereas with high temperature, it tries to randomize all the spins. The above figure is a nice plot depicting both parameters' characteristics.

4.2 Observable Quantities

In this section, I simulate the Ising model using $N = 22$ and $J = 2$ with different temperatures. The following are plots of the calculated observable quantities from our model.

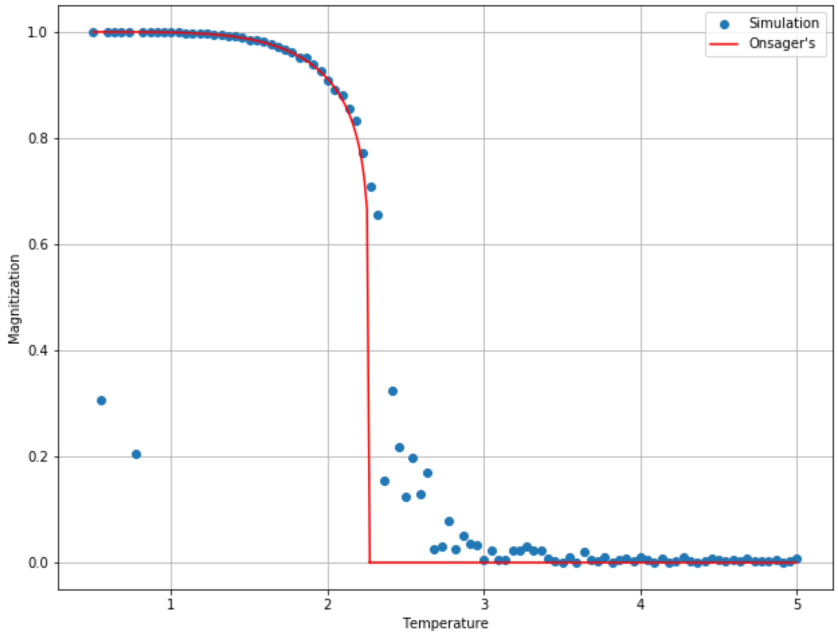


From the above plots, it is clear that at low temperatures, we see a overall magnetization. As we increase the temperature, the system loses it magnetic properties. At the very same temperature where the system lose its magnetization, there is a spike in both specific heat and magnetic suspectibility. Therefore, at T_c we see a *phase transition* of our material. Recalling Onsager's exact solution for critical temperature T_c,

$$T_c = \frac{2J}{k_B \ln(1+\sqrt{2})} \approx 2.269K$$

which is around the temperature is see the changes.

The following a plot of my simulated magnetization with Onsager's exact solutions.



From the comparison, our algorithm behaves as predicted. Some deviance from the exact solution may arise from the randomization process or I calculated variables without letting the system converge.

This simulation uses a tremendous amount of computational resources, roughly 1 hour, even with relatively small grid size ($N = 22$). Thus there is room for improvement in the efficiency of our algorithm.

5 Ising Model with External Magnetic Field

Now that we have a working algorithm, we can start imposing different variations to the model. Let's first start with a simple scalar magnetic field. Recall, to calculate the site's energy, we need to compute

$$H_j = -J \sum_{<ij>} S_i S_j - k \sum_j S_j$$

with $k \neq 0$, this would prevent the sites from flipping.

5.1 Scalar Magnetic Field

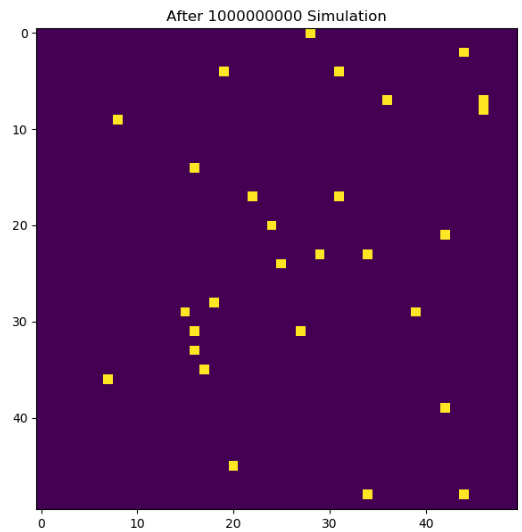


Figure 3: $J = 2, T = 3, k = 6$

From the above plot, when T is greater than T_c, then the system's spins tries to be randomized. However, with a strong external magnetic field applying on the spins at all sites, it forces all the spins to be aligned.

5.2 Vectorized Magnetic Field

To make our Ising model more complex, we can impose vectorized magnetic field $\vec{k}$. The following is a plot of the vectorized magnetic field.

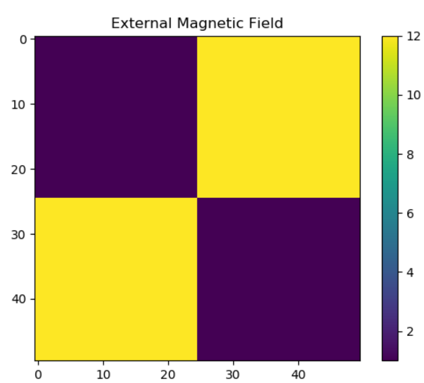


Figure 4: Vectorized Magnetic Field

We can expect after simulating our Ising model with this magnetic field, we will see different regions where spins aligned.

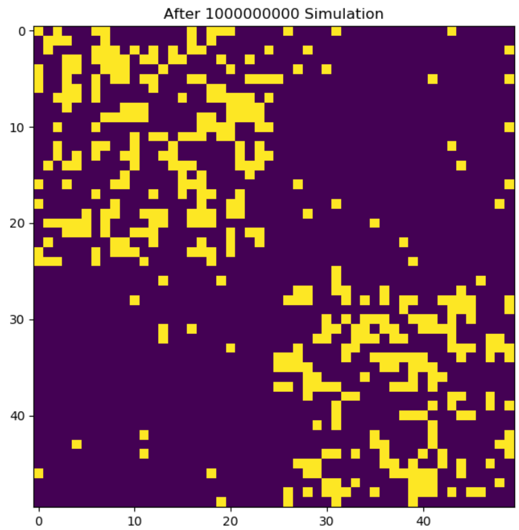


Figure 5: Vectorized Magnetic Field

After imposing $\vec{k}$ on our model, we can definitely different regions being affected by the magnetic field. We get creative with constructing a magnetic field and apply it on the model.

6 Simulation

As a Data Science student, I invested quite a lot in making a simulation of this model because it would be beneficial for my career. All the videos for each simulation can be viewed at https://github.com/nyu-compphys-2018/project-nk2673

7 Hexagonal Lattice

In all our models, we always use a square lattice as our model. We can examine the properties given a different lattice shape. In this section, suggested by Javier, we will explore a Hexagonal configuration of the lattice.

A representation of a Hexagonal lattice is as follows:

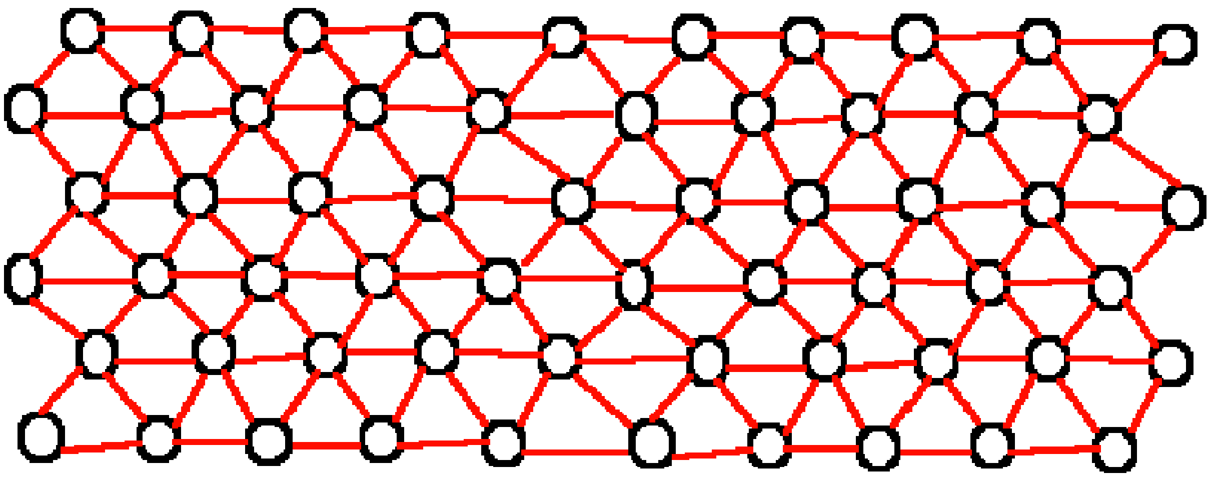


Figure 6: Visualizing Hexagonal Lattice

The main difference between square lattice and hexagonal lattice is the amount of interactions between atoms. In a square lattice, the number of neighbors for an atom is four. However, in a hexagonal lattice, each atoms has two extra atoms interacting with it, thus each site will have six neighbor interacting atoms. The main changes in the code is simply the introduction of new interacting atoms.

A paper written by Honecker, Schilenburg, and Richter, studies the magnetization of a hexagonal antiferromagnet. In short, they calculated the magnetization of an antiferromagnet at low temperatures as they increase the strength of the external magnetic field. In this section, I will use my code to recreate results as observed in the paper.

First, let see how the hexagonal antiferromagnet behaves at different temperatures.

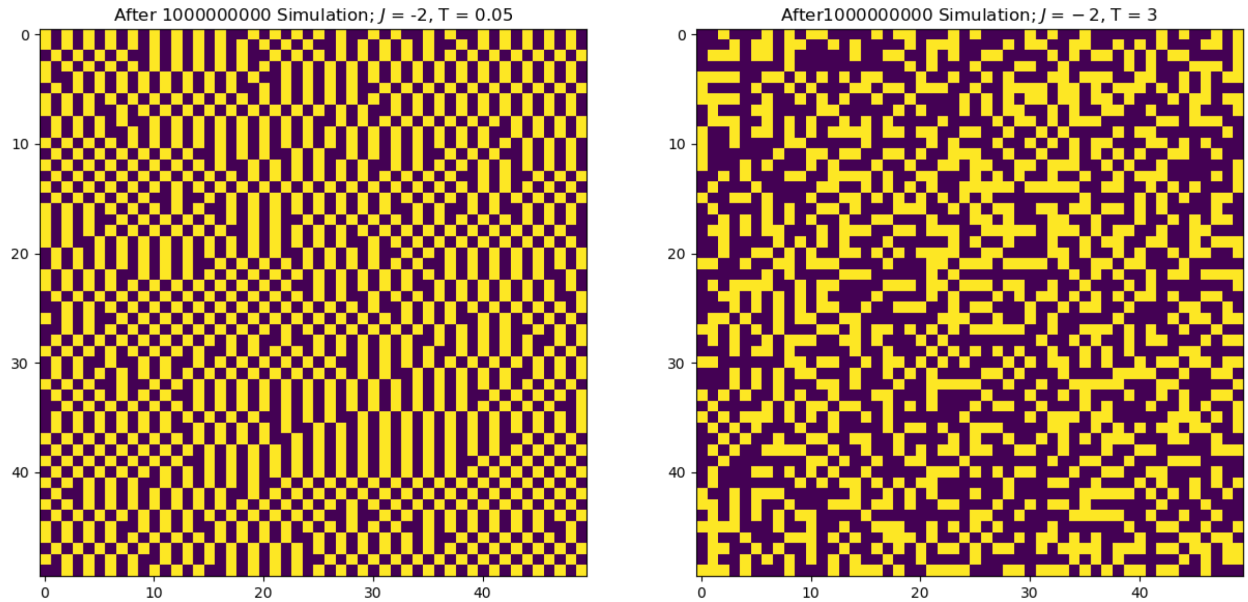


Figure 7: Left: Low Temp Right: Right Temp

At low temperature, a pattern can be seen from the hexagonal model which is not similar to the square model.

The following is a plot of hexagonal antiferromagnet's magnetization against magnitude of magnetic field.

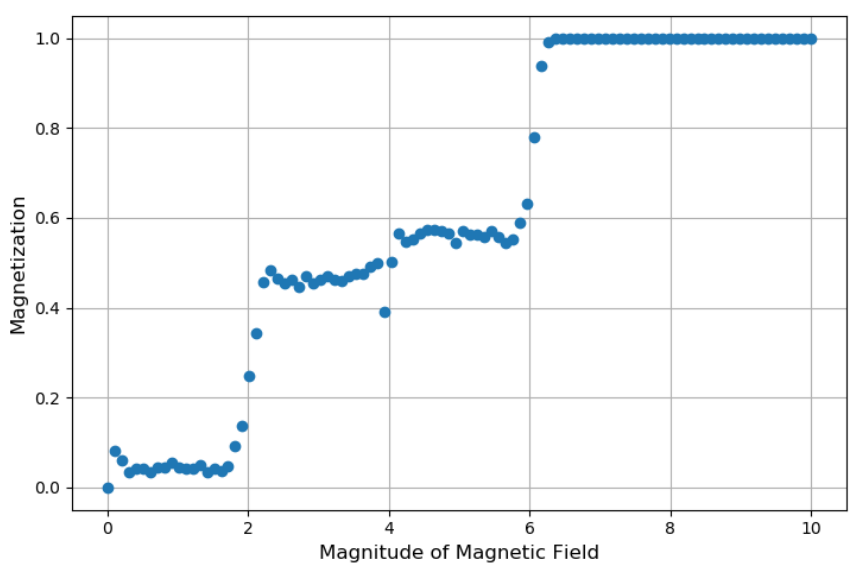


Figure 8: Magnetization vs. Magnitude of Magnetic Field

The result is intriguing because there is a plateau formed around 2 to 6. This result agrees with the result in the paper. With curiosity, I plotted the model around the plateau.

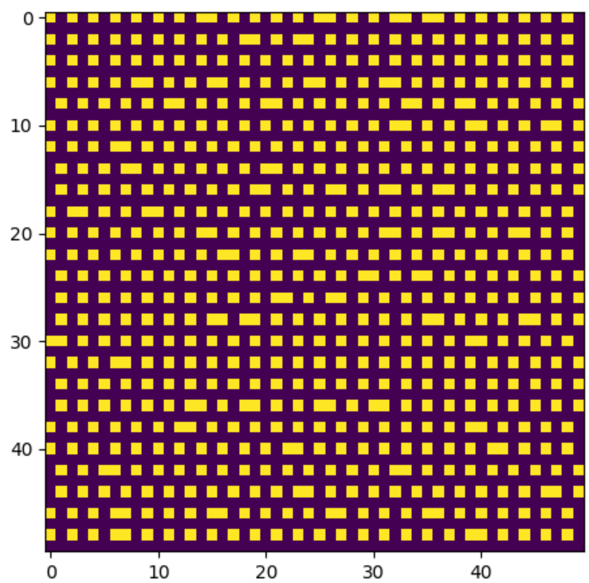


Figure 9: Hexagonal Model with $J = -1$, $T = 0.05$, $k = 3.5$

From this quick test, by varying the shape of the lattice, the model will exhibit different convergence patterns, due to the coupling interactions between the atoms.

8 Conclusions, Reflection, and Future Work

In this paper, we examine the Ising Model by using randomized algorithms, Monte Carlo and Markov Chain, to approximate the behavior of an antiferromagnet and ferromagnet. Once we have a working algorithm to simulate Ising Model, we approximate the model with many variations (different values of J, T, k, lattice shape) and observe its behavior.

There were much hardships while doing this project. A main issue while doing this project was the computational time it takes to calculate and plot the observable quantities. I was not aware that the model has not converged and calculate the observable quantities from it. To overcome that issue, I simply increase the number of iterations for the simulation, and realized that it requires 10^{10} iterations for convergence, which took me around an hour to compute each time.

There are many future work for this project. If one were to continue this project, a much efficient algorithm would be a huge improvement. In addition, the Ising model simulation is limited only to imagination. We can apply a much more complicated magnetic field different configuration lattice and observe its behavior. In Honecker, Schilenburg, and Richter's paper, they observed a series of different interacting patterns and observe how they converge.

This last paragraph is to appreciate professor Andrew MacFadyen for teaching this class. Huge appreciation to Chris Tiede and all my computational physics classmates for providing me feedback and suggested ideas to explore. Finally I would like to acknowledge all the important people that helped build foundations for me to accomplish this project.

References

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