The 2D Ising Model and Ferromagnetism

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1 Abstract

The 2D Ising model is remarkable in that it can replicate the phase transition in ferromagnetic materials at the Curie temperature while having a very simple formulation and implementation with the Metropolis algorithm. In this project a code was written to implement the 2D Ising model with the Metropolis algorithm, and simulations were subsequently run to determine the Curie point and simulate the behavior and phase transition of a ferromagnetic material.

2 Introduction

The Ising model, along with associated computational Monte-Carlo methods, can be used to simulate the behavior of simple thermodynamic systems and particularly the behavior of ferromagnetic materials. A ferromagnet is a material (such as iron) with areas/volumes in which all of the atoms' magnetic moments are aligned, and this usually occurs below a certain point, called the Curie point [1]. These regions generate magnetic fields from the sum total of all of the magnetic moments of the atoms, from their electrons, which are in turn generated by the electrons' spins [1]. This is because an particle's (electron's) magnetic dipole-dipole interaction is equivalent to its spin-spin interaction, from the theory of quantum mechanics [1]. If an external magnetic field is applied to a larger domain in the ferromagnet, the aligned regions will align with it, and the ferromagnet becomes magnetized [1].

However, this behavior of aligning magnetic moments is only exhibited below the Curie point or temperature, T_c, after which the thermal energy of the system is too high, and the magnetic moments are no longer aligned across ferromagnetic regions [1]. Above this temperature, the total magnetization of the ferromagnet will thermodynamically fluctuate around a point closer to zero [1]. This behavior is a particularly interesting phase transition that is seen in many metals. As it is stated in Landau et al., "Below the Curie temperature the system is in a quantum state with macroscopic order; above the Curie temperature there is only short-range order extending over atomic dimensions" [1].

3 Thermodynamic Background

The behavior of a ferromagnet below and above the Curie temperature is explained/modeled by statistical physics and the Boltzmann distribution [1]. Below the Curie point, alignment is energetically favored for materials of particular properties. But a system's kinetic energy is proportional to it's temperature, so as a ferromagnet's temperature increases, so do its atoms' kinetic energies [1]. This increase in kinetic energy provides an opposing mechanism to the atoms being aligned as before, but only above the Curie point.

Let's begin discussing the relevant quantities and physics required to describe this ferromagnetic system. Since this project is about the 2D Ising model, let's also consider our ferromagnet to be a 2D lattice of particles, with each particle having a spin up or down:

$$s_i = \uparrow or \downarrow \tag{1}$$

Firstly, a material's total magnetization, as previously described, can be defined by how many of it's spins are aligned. This leads us to define the Magnetization of a material (or lattice) with N particles (or spin sites) as:

$$M = \sum_{i=1}^{N} s_i \tag{2}$$

Where we mainly consider the absolute value of the magnetization, or Abs(M). Secondly, each particle (or spin site), s_i, has an interaction with each of its neighboring atoms, or "nearest neighbors", s_j (left,right,top,bottom for a 2D spin lattice). This interaction, with the addition of an exchange energy J_i (with units of Joules) which depends on the properties of the material, is responsible for the total energy of the system in the absence of an external magnetic field B [1]. This energy is given by:

$$E_{spin-interaction} = -\sum_{i=1,j}^{i=N} J_i s_i s_j \tag{3}$$

where $\sum_j s_j$ runs over the four nearest neighbors s_j. The sign of the exchange energy of a material determines its behavior; for J $>$ 0 a material exhibits ferromagnetic behavior, and for J $<$ 0 antiferromagnetic behavior is exhibited where domains of a material have strictly anti-aligned spins [1]. This is because for J $>$ 0, aligned spins will give a more negative value for $E_{spin-interaction}$, a more negative energy for the system overall, and thus will be energetically favored. The opposite is true for J $<$ 0, where unaligned spins are favored. For this project, the exchange energy is assumed to be positive, so that we are considering ferromagnetic behavior.

Now there is a final term in the energy which is given by each spin's interaction of an external, uniform magnetic field B, if present. This interaction energy

is given by:

$$E_B = -\mu_b g \sum_{i=1}^{N} B \cdot s_i$$
$$\mu_b = \frac{e\hbar}{2m_e c} \tag{4}$$

Where e is the electron charge, m_e is the electron's mass, c is the speed of light, and g is the gyromagnetic ratio which gives the relationship between a particle's magnetic moment and angular momentum [1]. Finally the total energy is given by:

$$E = E_{spin-interaction} + E_B \tag{5}$$

Now that we have determined how to calculate the total energy and magnetization of our system of N spins, we can move on to the remaining quantities: heat capacity C_v, which gives a measure of how much a system's energy changes given a change in temperature, and magnetic susceptibility χ, which gives a measure of how likely it is for a spin to flip in a system with a change in the external magnetic field [1]. These can be written in terms of statistical fluctuations in the ensemble's energy and magnetization:

$$C_v = \frac{\partial < E >}{\partial T} = \frac{1}{(k_B T)^2} \left(< E^2 > - < E >^2 \right) \tag{6}$$

$$\chi = \lim_{B \to 0} \frac{d < M >}{dB} = \frac{1}{k_B T} \left(< M^2 > - < M >^2 \right) \tag{7}$$

4 2D Ising Model

All of the computational methods used in the project came from the "Computational Physics - Problem Solving with Python" text written by Landau, Paez, and Bordeianu [1], combined with my own programming experience plus trial and error.

The Ising model consists of a 2D square lattice where each point is assigned a spin of either 1 (up) or -1 (down). Each length of the lattice is labeled with L, and the total number of sites is LxL = N. To program this, one can generate a N length array of 1's and -1's which can be included in some Ising model function, or class/object (the latter was done for this project). As outlined in (2), the magnetization M of the Ising model is given by the sum of all spins, +1 or -1, with the absolute value of M giving a measure of how much alignment there is in the system. The energy is given by (3), (4), and (5), with some simplifications. Firstly, the exchange constant J_i in (3) is assumed to be constant at all sites, and it is set equal to unity for simplification. The model will allow for J to be changed, but J will be hard-coded as constant for all sites. In addition, in (4) the dot product $B \cdot s_i$ can be evaluated to Bs_i, and the values $\mu_b, g, \text{and} B$ can be combined into one variable "h", which has units of Joules.

$$J_i = J = 1 \quad \forall i$$
$$E_{spin-int} = -J \sum_{i=1,j}^{i=N} s_i s_j = -\sum_{i=1,j}^{i=N} s_i s_j \tag{8}$$

$$B \cdot s_i = B s_i \quad \text{and} \quad \mu_b g B = h$$
$$E_B = -h \sum_{i=1}^{N} s_i = -hM \tag{9}$$

Finally, we have the simplified form of the total energy as given by (5):

$$E = -\sum_{i=1,j}^{i=N} J_i s_i s_j - \mu_b g \sum_{i=1}^{N} B \cdot s_i = -\sum_{i=1,j}^{i=N} s_i s_j - hM \tag{10}$$

So now we have generated our lattice and can find the energy and magnetization, as well as C_v and χ as given by (6) and (7). We can initialize our lattice in any number of ways; with all spins up, all spins down, or a random configuration. Given enough iterations of the Metropolis algorithm (outlined below), all initial states should lead to the same equilibrium physics. For this project a random configuration was generated automatically whenever the Ising model object is called. This is accomplished by generating a uniform random number at each site, and if it is less than 0.5 the spin will be down (-1) and otherwise spin up (+1). In order to simulate the thermodynamics and physics of the Ising model we need to bring in an algorithm, which in this case is the Metropolis algorithm. This algorithm uses Monte-Carlo methods combined with simple statistical physics to simulate the Ising model as a thermodynamic system from its initial configuration to equilibrium.

5 Metropolis Algorithm

The Metropolis algorithm accurately simulates spin change fluctuations during thermal equilibrium such that a system's distribution of energies follows the Boltzmann distribution; it is more likely that our system will be found in a lower energy state as opposed to a higher energy state [1]. This algorithm is at the heart of simulating the physics of ferromagnetism described above. The algorithm starts from an initial spin configuration at a certain temperature and proceeds by generating spin flips when they are either energetically favored, or probabilistically determined with Monte-Carlo methods, until equilibrium is reached. Then, the algorithm starts over at the initial configuration with a different temperature, evolves as before, and finds the new thermodynamic quantities. These newly calculated quantities can be compared with the old to determine their temperature dependence. The algorithm evolves as follows:

1. Generate an initial spin system across a 2D lattice of dimension L by L. The lattice will have periodic boundary conditions. Random numbers are generated for each lattice point to determine with equal probability if the spin is up or down. One iteration of the algorithm then runs through the following steps N times:

2. Pick a random lattice point and flip the spin. Then calculate the energy change from the initial to trial spin:

$$\Delta E_i = E_{trial} - E_{initial} \tag{11}$$

3. If the energy change is less than or equal to zero, the flip is energetically favored, and we accept the spin flip.

4. If the new energy is greater than zero, generate a uniformly distributed random number, r_i, and calculate the Boltzmann distribution factors for each state without the weighted sum, which will cancel when we consider the relative probability of the initial and trial states:

$$P_i = Exp(-\frac{E_i}{k_B T}) \tag{12}$$

   We then consider the relative probability of the trial state vs the initial state:

$$RP = P_{trial}/P_{initial} = Exp(-\frac{E_{trial} + E_{initial}}{k_B T}) = Exp(-\frac{\Delta E_i}{k_B T}) \tag{13}$$

   If $RP \geq r_i$, we also accept the new configuration.

   Else, reject the new configuration and repeat from 2 until the algorithm has been run N times [1].

6 Additional Computational Methods

First, the 2D Ising model class was created to define a lattice and each lattice point's nearest neighbors. All relevant quantities are defined; energy (E), magnetization (M), exchange constant (J), and finally the independent variable KbT, where the Boltzmann constant Kb is thought of as set to 1 and KbT is then measured in Joules. Then the spins are defined at each lattice point (and can be either 1 (up), or -1 (down)) and randomly chosen to be up or down with equal probability by default. The method "ThermE" is defined which plays two roles: it can re-define the thermal energy KbT for a 2D Ising object without regenerating it, and secondly it calculates and stores all possible spin-flip energy changes and relative Boltzmann probabilities for said value of KbT; this way we don't have to recalculate them each time the Metropolis algorithm is rerun at the same KbT. Finally, the Metropolis algorithm is defined as outlined above and is the last method to the 2D Ising model class.

Second, the 2D Ising model code was used to simulate a system with L = 20 and LxL = 400 spins (J = 1 Joules, h = 0). The system was set to run over a range of KbT, from 0.05 to 10 Joules in increments of 0.05. At each temperature, the Metropolis algorithm was run N times an iteration for 4,000 iterations (Landau states that 10N should be enough for convergence, which is also what I found over many trials. Here 10N = 4,000 [1]). For each of these iterations, I ran the Metropolis algorithm 3 additional times, and only stored the quantities of the system after the 3rd run for each overall iteration. This ensures that each stored state is decorrelated from one another, which is important; when averaging over ensembles each sample is supposed to be independent from the previous. All quantities, Energy, Magnetization, C_v, and χ, are considered after being averaged over the ensemble and total algorithm iterations. Thus:

$$\begin{aligned} &\text{“}Energy\text{”} =< E >= \text{“} < E > /N\text{”} = E/(N_{sites} \cdot N_{Iterations}) \\ &\text{“}Abs(M)\text{”} =< Abs(M) >= \text{“} < M > /N\text{”} = Abs(M)/(N_{sites} \cdot N_{Iterations}) \end{aligned} \tag{14}$$

Then C_v and χ are formed by the right-most equation in (6) and (7) where the terms $< E >^2$,$< E^2 >$,$< M >^2$, and $< M^2 >$ have been averaged over the total iterations and lattice points. In some figures and at parts of the code, $< E > /N$ and $< M > /N$ are written rather than simply $< E >$ and $< M >$ to emphasize that this is the energy averaged over the ensemble.

Finally, the Ising code was use to simulate 10x10 lattices for different nonzero values of h over a range of KbT, from 0.2 to 10 Joules in increments of 0.2, to investigate what happens when an external magnetic field is added. More details about the computational methods used in this project can be found in the comments of the code itself.

7 Results

Once the simulations were conducted, plots were created of the following quantities averaged over the total number of spin sites (full ensemble) and iterations: energy, magnetization, heat capacity, and magnetic susceptibility. In the following plots, one can clearly see the ferromagnetic phase transition. Looking first at Fig 1, the phase transition occurs from KbT = 2-4 Joules, after which the magnetization transitions from fluctuating around 1 to near 0. This gives us the first hint of where the Curie point occurs. One sees the same trend in the energy in Fig 2, where it increases dramatically after the phase transition, and in general the energy increases as KbT increases, as it should.

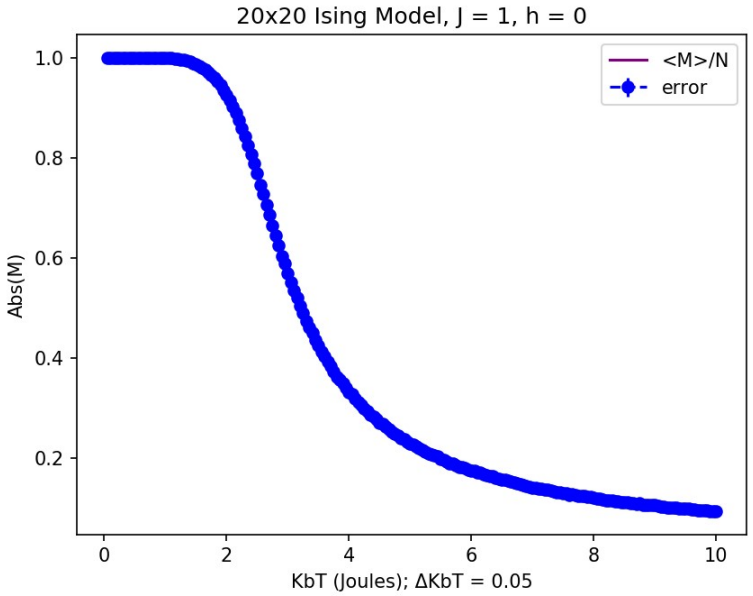

Figure 1: $\frac{<M>}{N}$ as a function of KbT for J = 1, h = 0

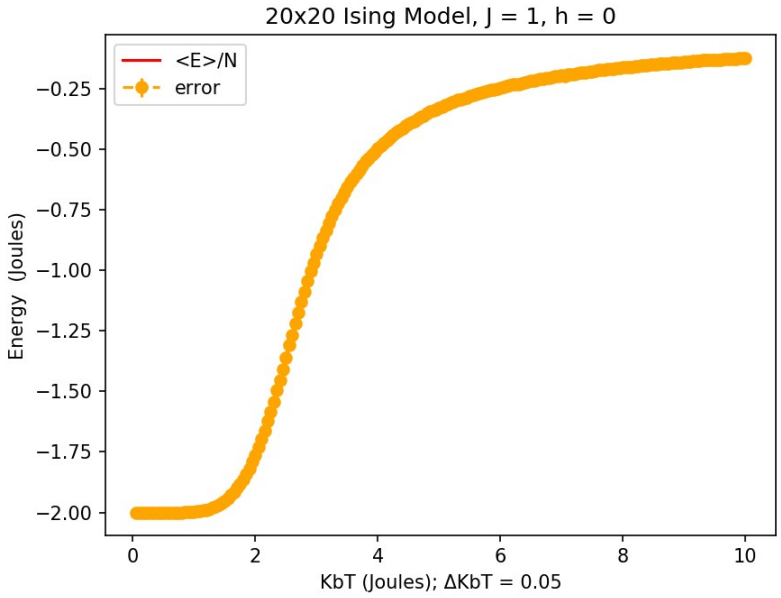

Figure 2: $\frac{<E>}{N}$ as a function of KbT for J = 1, h = 0

Finally, consider C_v and χ in Figures 3 and 4. Here, we can clearly see a phase transition as C_v and χ increase up to a point, peak, and start to decrease down exponentially. The Curie point is the peak of C_v, because in moving away from that point the system will have the greatest change of energy, as the system undergoes the ferromagnetic phase transition. χ decreases more gradually after the peak and is not as accurate when determining the Curie point. The peak of C_v was then found to occur at $KbTc = 2.5 \pm 0.05$ Joules. This gives a 10.1% error when compared with the theoretical value, KbTc = 2.27 Joules, as predicted by the analytical solution to the 2D Ising model, derived by Yang in 1952 [2][1].

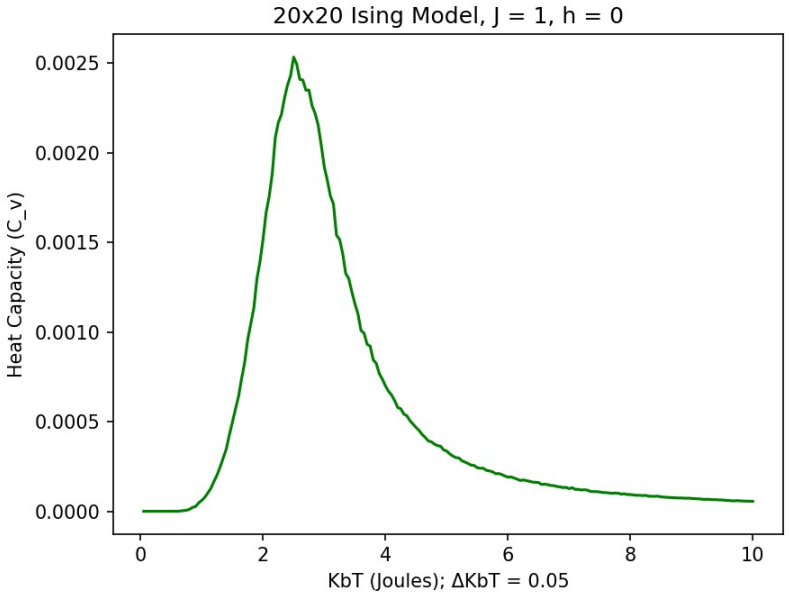

Figure 3: $\frac{1}{(k_B T)^2}\left(< E^2 > - < E >^2\right)$ as a function of KbT for J = 1, h = 0

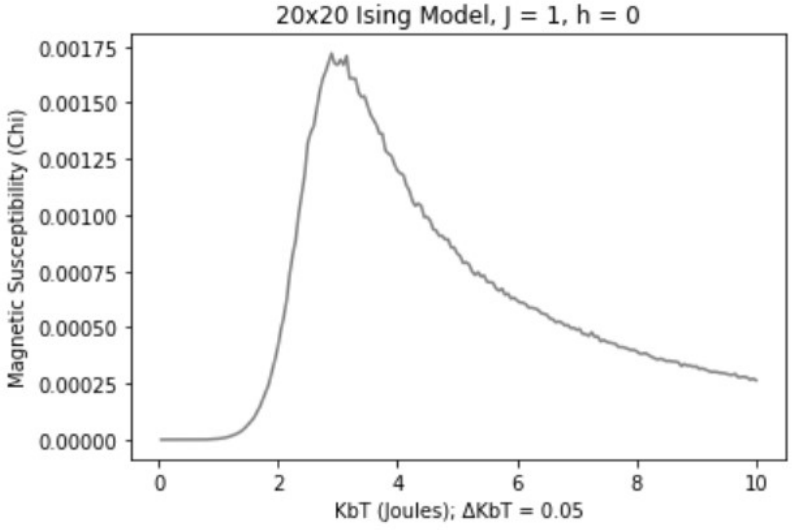

Figure 4: $\frac{1}{k_B T}\left(< M^2 > - < M >^2\right)$ as a function of KbT for J = 1, h = 0

Next, simulations were run for 4,000 iterations and the energy and magnetization for these runs were plotted as a function of iteration at KbT above and below KbTc, as seen in Figures 6 and 5. One can clearly see from Fig 5 that the 2D Ising model exhibits ferromagnetic behavior and fluctuates around Abs(M) = 1 below the Curie point, but fluctuates around Abs(M) = 0.2 above it. From 6 we simply see that the system gains energy when KbT is increased.

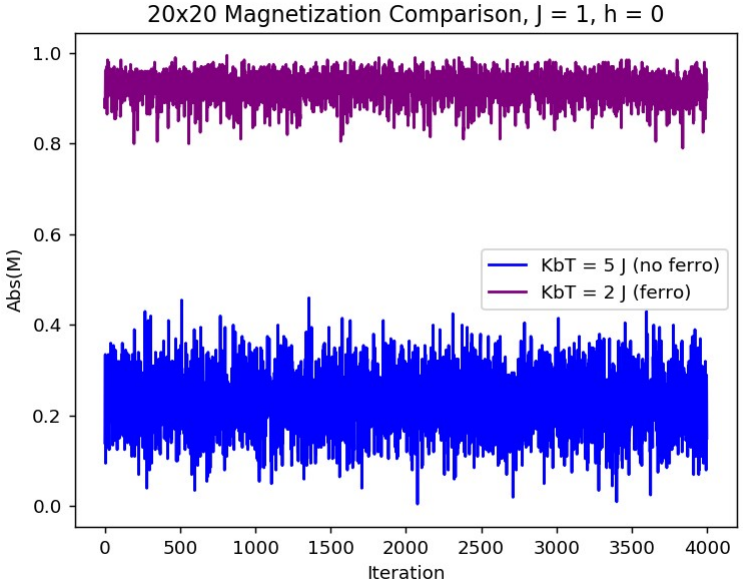

Figure 5: $\frac{<M>}{N}$ as a function of iteration for J = 1, h = 0

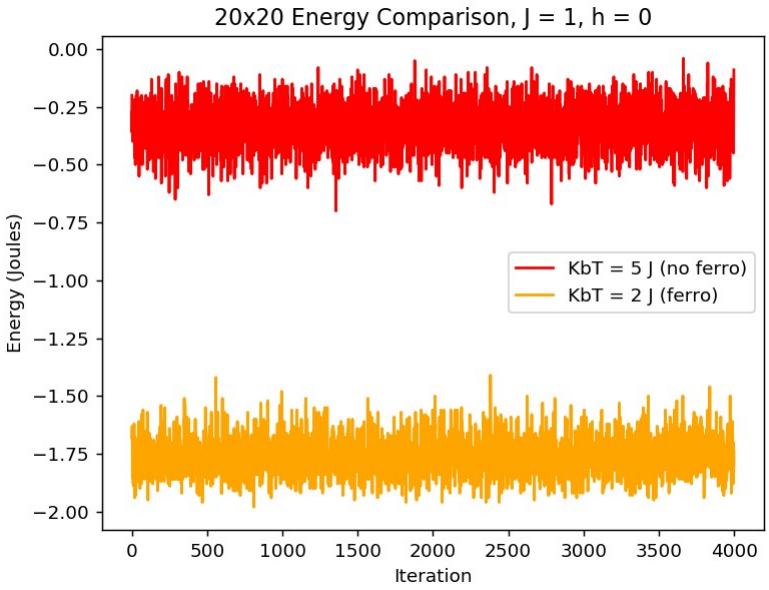

Figure 6: $\frac{<E>}{N}$ as a function of iteration for J = 1, h = 0

Finally we can plot the energy and magnetization as a function of KbT when an external magnetic field is included, controlled by the parameter h (see (9)). These results are for a 10x10 lattice, with 1,000 iterations run for each KbT, with $\Delta KbT = 0.2$. In Fig 7 we can see that as the external magnetic field h is increased, the evidence of a phase transition in the energy disappears and is "smoothed out". As h is increased, the contribution from the magnetization of the system to the energy is more negative, and thus the total energy decreases, as expected. In Fig 8, the phase transition is smoothed out as well as the system's magnetization stays larger for higher KbT. This is because with an external magnetic field added, the spins flipping to be unaligned at larger KbT is no longer as energetically favored as with h = 0 at any given KbT. The spins instead are favored to be aligned with the external magnetic field, and thus with their nearest neighbors as well. Non-magnetized domains will still eventually be favored as KbT is increased and more thermal energy is added to the system, but this occurs at a higher KbT and is not as sharp of a transition as in the case with h = 0.

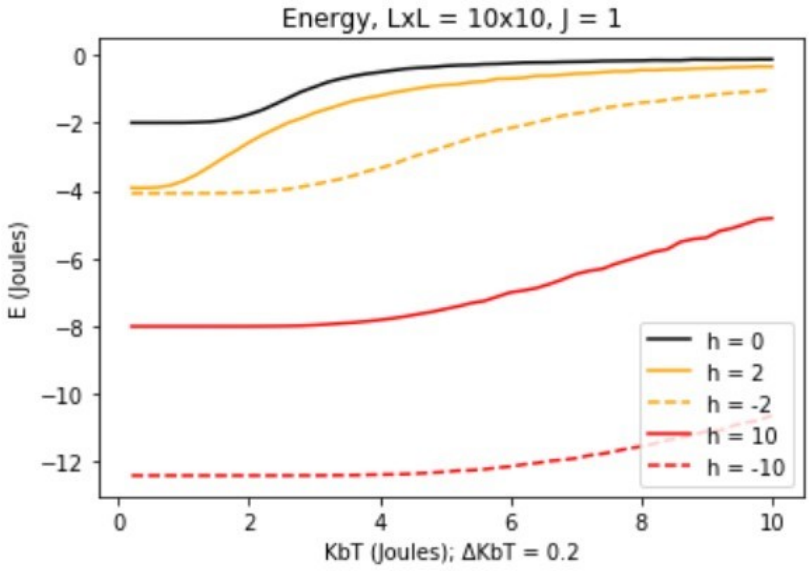

Figure 7: $\frac{<E>}{N}$ as a function of KbT for J = 1, varying h

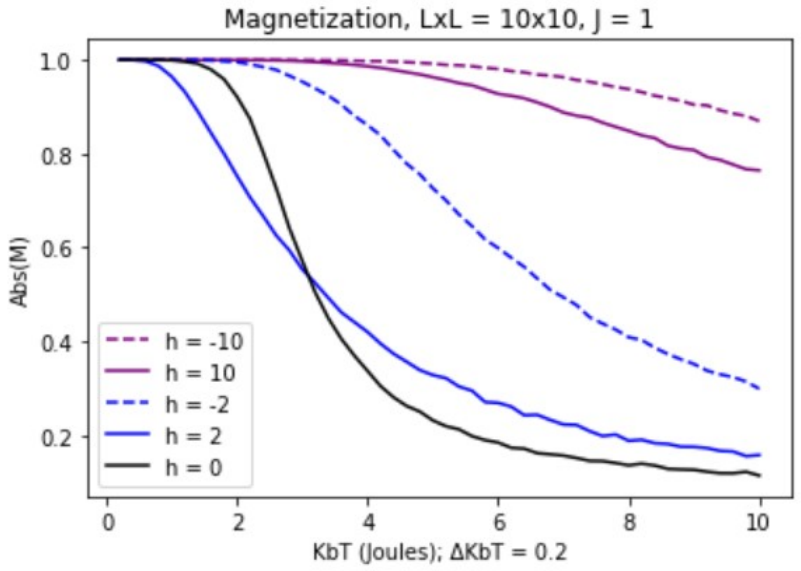

Figure 8: $\frac{<M>}{N}$ as a function of iteration for J = 1, h = 0

8 Conclusion

In conclusion, the 2D Ising model is an excellent sandbox with which to explore phenomenon in thermodynamics and statistical physics, such as ferromagnetism and the Curie point phase transition. Simulations such as have been done in this project show that the physics involved in the strange behavior of ferromagnets and their Curie point phase transitions can be boiled down to simple statistical rules enacted with Monte-Carlo methods. The 2D Ising model accurately shows the behavior of a ferromagnet above and below its Curie point, both with and without an external magnetic field present in the system. Moving forward, there are many more interesting things to explore with the code as it stands. Firstly, one could explore the behavior of the ferromagnetic case with nonzero h more fully, looking more quantitatively and in more detail about how the size of h changes the behavior of the phase transition. In addition, one could simulate higher L Ising models to see how accurate of a Curie point can be achieved, and how this accuracy scales with L. On top of these investigations of ferromagnetism, one could switch the value of J to $J < 0$ and explore the properties of antiferromagnetism with and without the presence of an external magnetic field. One could also see if there is interesting behavior to be found when testing different ratios of J/h.

Moving forward, there are also many ways that the existing model can be improved. One of these ways is with the implementation of Wang-Landau sampling (WLS) rather than the Metropolis algorithm [1]. The Metropolis algorithm focuses on the probabilities of each spin being in a particular state, up or down. The WLS algorithm on the other hand focuses on the probability that the entire system will have a particular energy, using the concept of density of states [1]. This algorithm is found to be much faster than Metropolis, and in addition provides a direct calculations of the density of states, which is useful [1]. Finally, one could move on entirely to constructing the 3D Ising model. Therefore, there are many things still to be investigated with the 2D Ising model formulation as it appears in this project, and many ways to improve this formulation. Still, even a relatively simple implementation of the 2D Ising model, such as was used in this project, gives rise to many interesting investigations of the underlying physics of a wide range of thermodynamic systems.

References

[1] Rubin H. Landau, Manuel J. Paez, and Cristian C. Bordeianu. *Computational Physics - Problem Solving with Python - Third edition.* Wiley-VCH, 2015.

[2] C. N. Yang. The Spontaneous Magnetization of a Two-Dimensional Ising Model. *Physical Review*, 85(5):808–816, March 1952.