Exploring the Magnetic Phases Through the Ising Model of Magnetization

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Magnetic materials can be found everywhere in our daily lives. However, we often think of magnetic materials to be any material that has some magnetization, i.e. a magnet. What we often do not consider is that magnetic materials can exist in two different phases, the ferromagnetic phase and the paramagnetic phase. The ferromagnetic phase is a consequence of the alignment of magnetic spins that generate a net magnetization, while the paramagnetic phase is a result of spins being randomly oriented, resulting in a zero magnetization due to the random nature of the spin configuration. Here we prove through computer simulations that the Ising model can be used to show the existence of the two magnetic phases. We show that in the one-dimensional Ising model there is no phase transition, while in the two-dimensional case there exists a transition around the critical temperature of 2.4 J/k_B.

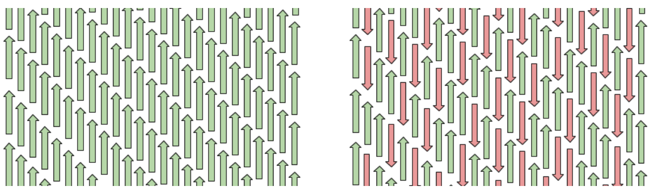

FIG. 1: A system in a ferromagnetic phase (left) and a system in a paramagnetic phase (right). The arrows represent magnetic spins, where the green arrows represent UP spins and the red arrows represent DOWN spins.

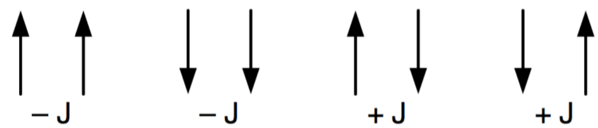

FIG. 2: Energetic contributions of neighboring spins in the Ising model of magnetization

INTRODUCTION

In nature there exist some materials that are sensitive to external magnetic fields. These materials are called magnetic materials. In this paper we focus on such materials and we explore the different physical phases that the materials go through and the transition among such phases when exposed to different sets of parameters, such as external magnetic fields and temperature baths.

In the theory of magnetism, the magnetization of a system is a measurement of its density of magnetic dipoles that exist within the material (1). These magnetic dipoles can be due to the the the electron movement in atoms or the intrinsic magnetic spin of particles. Nevertheless, it is because of these magnetic dipoles that we can observe magnetization of objects, which as consequence exert magnetic forces.

We are interested in two different physical phases: the *paramagnetic* and the *ferromagnetic* phase. Both phases are illustrated in Figure 2. On the left we have a system in a ferromagnetic phase, where there is a net magnetic moment. On the left, however, we have a system in a paramagnetic phase, where the net magnetic moment averages to zero as a consequence of the random nature of the system, since all spins are oriented randomly.

We are interested in the conditions under which the system is ferromagnetic and under which other conditions a system is paramagnetic. We will be exploring the parameter space to identify phase transitions. We will also explore systems with non-interacting magnetic spins and will compare them with systems where magnetic spins experience short-range interactions.

We will be interested in determining the average energy of the system and its magnetization as functions of the applied magnetic field and the temperature of the system.

THE ISING MODEL

First we consider a system of non-interacting particles. In the absence of an external magnetic field, the system's dipoles are oriented randomly. This results in an average zero magnetization of the system. However, when a magnetic field is applied to the system the dipoles align with the external field, resulting in a non-zero magnetization. A system of non-interacting particles is intuitive. We experience a phase transition from a paramagnetic to a ferromagnetic phase when an external magnetic field is applied.

However, a system where particles have short-range interactions is not as intuitive and much more interesting. In order to explore the system's behavior we use the Ising Model of Magnetism and computer simulations to explore the system at equilibrium under different sets of parameters.

The Ising Model assumes all magnetic spins to be either up or down, and we represent such orientations as +1 and -1 respectively. Due to the short-range nature of the system, we consider only an interaction energy between neighboring spins. If two spins are parallel to each other we consider them to contribute -J, and if they are antiparallel to each other we consider them to contribure $+J$, where J comes as a quantum mechanical consequence of identical particles, and is known as the *exchange constant*. The Ising model then considers all the interactions among particles as

$$E = -J \sum_{i \in nn(i)}^{N} s_i s_j \tag{1}$$

where s is the spin of a particle with its repsective value of ± 1. However, equation 1 is incomplete since we also need to consider the magnetic field in the system. For that we define a new field

$$\vec{H} = \frac{1}{\mu_0}\vec{B} - \frac{M}{V} \tag{2}$$

where $\vec{B}$ is the external magnetic field and M is the induced magnetization in the system, which we also need to take into account to determine the energy of the system. The resulting equation represents the complete Ising model.

$$E = -J \sum_{i \in nn(i)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i \tag{3}$$

Equation 3 can then be used to calculate relevant physical quantities of a magnetic system with interacting particles.

QUANTITIES OF INTEREST

As we expressed before, we are interested in the energy of the system and the magnetization of the system as functions of the magnetic field and the temperature bath being applied. For these two quantities we can easily calculate their value if we know the spin of every magnetic moment. These quantities are discrete and can be expressed as

$$E = -J \sum_{i \in nn(i)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i \tag{4}$$

and

$$M = \frac{dm}{dv} = \frac{1}{N} \sum_{i=1}^{N} s_i \tag{5}$$

We are also interested in the rate of change of the system's energy as a function of the temperature (the heat capacity) and the change in the magnetization as a consequence of the external magnetic field (susceptibility).

The heat capacity (at a constant magnetic field) is defined as

$$C = \left(\frac{dE}{dT}\right)_B \tag{6}$$

which is not a discrete quantity. However, we can calculate the heat capacity of a system by considering the partition function.

$$Z = \sum_{states\ s} e^{-\beta E(s)} \tag{7}$$

and use the fact that

$$\frac{1}{Z}\frac{dZ}{d\beta} = -\sum_{states\ s} E(s) e^{-\beta E(s)} = -\langle E \rangle \tag{8}$$

and

$$\frac{1}{Z}\frac{d^2 Z}{d\beta^2} = -\sum_{states\ s} E^2(s) e^{-\beta E(s)} = \langle E^2 \rangle \tag{9}$$

to obtain

$$C = \frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right) \tag{10}$$

In a similar fashion, we can use the partition function to derive an expression for the susceptibility of the system.

$$\chi = \frac{1}{k_B T}\left(\langle M^2 \rangle - \langle M \rangle^2\right) \tag{11}$$

We can then use the spin configuration of the system to calculate numerically the energy, magnetization, heat capacity, and susceptibility of the system.

COMPUTATIONAL METHODS

In order to calculate energy, magnetization, heat capacity, and susceptibility of the system, we use a variation of the Monte Carlo algorithm that examines the system at equilibrium and at a constant temperature bath T. In our computer simulations we use a Metropolis algorithm, which steps are:

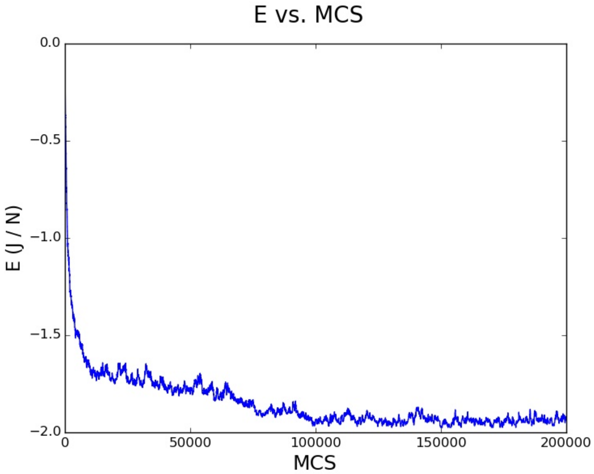

FIG. 3: Energy of the system as a function of Monte Carlo Steps.

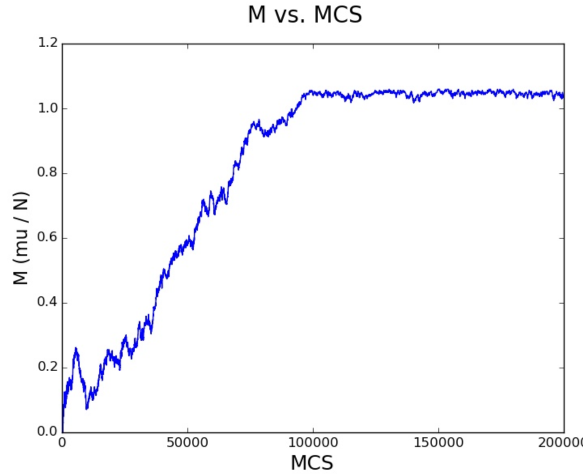

FIG. 4: Magnetization of the system as a function of Monte Carlo Steps.

1. Choose the initial state of the system (lattice of spins).

2. Loop at this step: choose a random spin and calculate the potential energy change that would result from flipping the spin. If $\Delta E < 0$ we accept the change, if not we accept the change with a probability of $p = e^{-\beta \Delta E}$.

3. Compute averages of quantities of interest after the system has reached equilibrium.

With such an algorithm is easy to compute the changes in energy since we only need to check the new relationships between the targeted spin and its neighbors.

Moreover, in order to make relevant measurements of the system's state at equilibrium we need to find a useful criteria to determine whether a system has reached equilibrium or not. For any particular lattice size we run the simulation (the Metropolis algorithm) and measure some observable at a constant temperature and a constant magnetic field.

We then determine after how many Monte Carlo steps (number of times we loop in the algorithm) the system presents minimum fluctuation. It is at this point that we consider the system to be at equilibrium. For a lattice of 10 by 10 spins, equilibrium is reached after 1,000,000 Monte Carlo steps as seen in Figure 3 and Figure 4.

THE ONE-DIMENSIONAL CASE

We consider a magnetic system in one dimension and in two dimensions and explore their dependency on temperature and external magnetic field. For the one-dimensional case, we consider an Ising chain that consists of 100 interacting spins. We initialize the system by

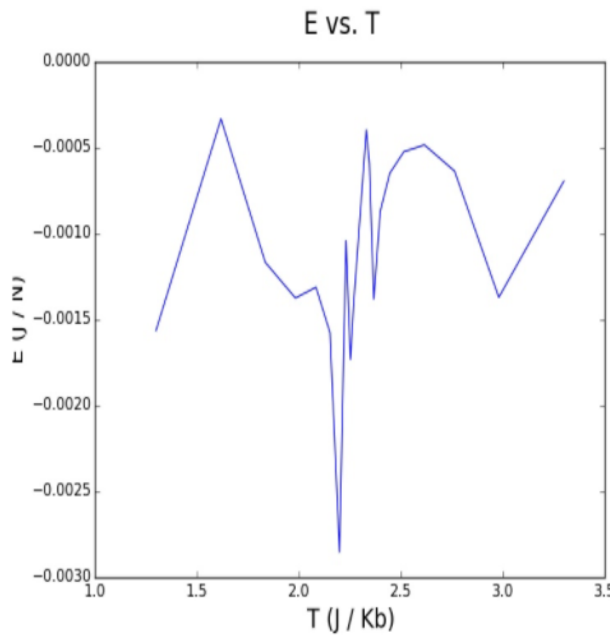

FIG. 5: Dimensionless energy as a function of dimensionless temperature.

setting every spin randomly to an up or down orientation (+1 or -1). We then run the Metropolis algorithm until the system has reached equilibrium and take measurements of the system's energy, magnetization, heat capacity, and susceptibility. The results are shown in Figures 5 through 8.

We measure all the observables and plot in dimensionless units. We plot dimensionless energy per spin $E(T,B)/JN$, dimensionless magnetization per spin $M(T,B)/\mu N$, dimensionless specific heat $C(T,B)/k_B$, and dimensionless susceptibility per spin $\chi(T,B)/\mu^2 N$, as functions of dimensionless temperature $K_B T/J$ and

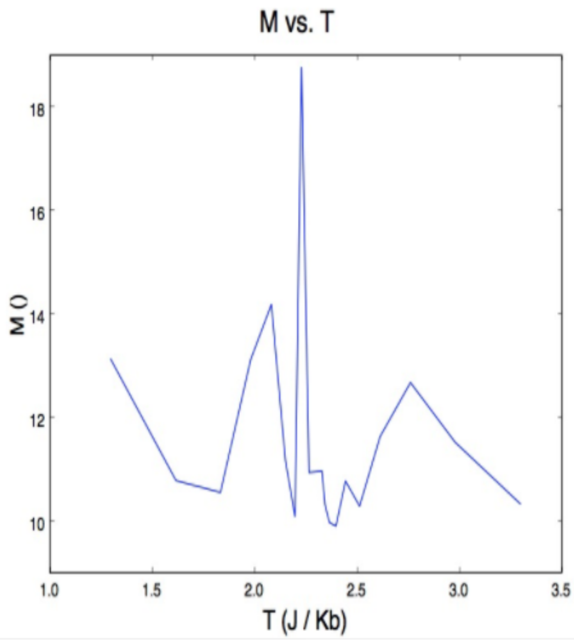

FIG. 6: Dimensionless magnetization as a function of dimensionless temperature.

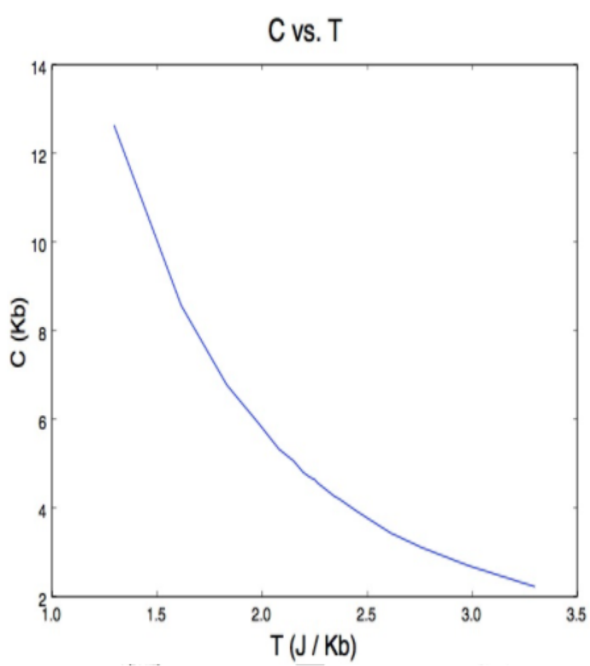

FIG. 7: Dimensionless heat capacity as a function of dimensionless temperature.

dimensionless magnetic field $B\mu/J$.

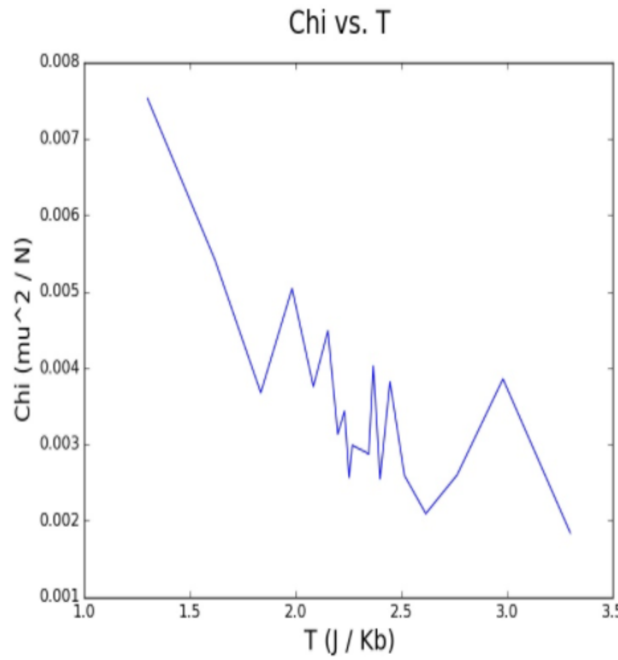

FIG. 8: Dimensionless suscesibility as a function of dimensionless temperature.

CONCLUSIONS

After running the simulation in one dimension and obtaining each observable for a variety of temperatures and magnetic fields (while the system has reached equilibrium), we see that in the cases of the energy and the magnetization of the system, the observables fluctuate around a mean value. In the absence of an external field the energy of the system is minimal and the magnetization of system is small (around 12% of maximum possible magnetization). It is important to realize that the data represented in Figures 5 through 8 is zoomed in, but the energy and the magnetization of the system do in fact have minimal fluctuations around their mean value.

From the plotted data we conclude that there does not exist a phase transition from the paramagnetic phase (the starting phase) to the ferromagnetic phase. The system's energy diminishes when more and more domain walls are created, making it favorable for the system to stay in a paramagnetic phase. However, a more *pure* paramagnetic phase could be achieved for larger chains than a hundred spins.

THE TWO-DIMENSIONAL CASE

Now we examine the case of the two-dimensional Ising model. We consider a lattice of 50 spins by 50 spins and initialize the system randomly, by choosing each spin's value at random (either +1 or -1). After choosing our ini-

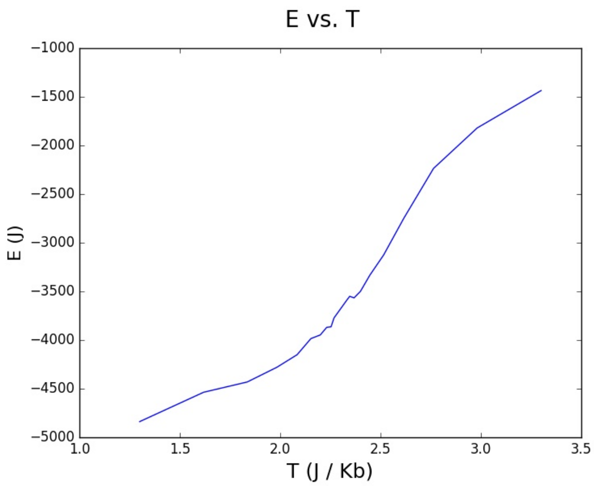

FIG. 9: Dimensionless energy as a function of dimensionless temperature for $H = 0$.

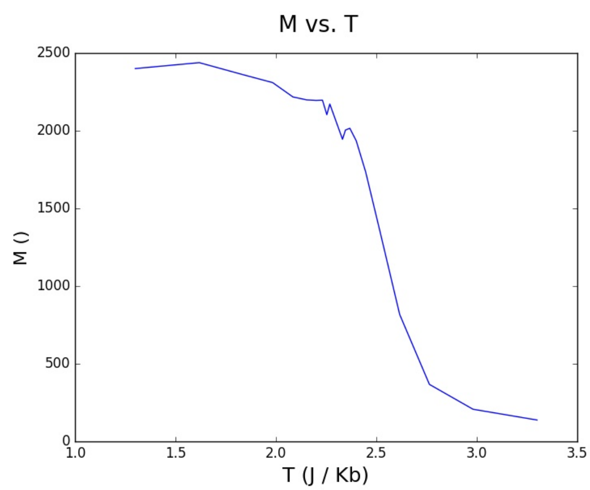

FIG. 10: Dimensionless magnetization as a function of dimensionless temperature for $H = 0$.

tial state we can run the Metropolis algorithm until equilibrium is reached and take measurements of the physical observables we are interested in. However, we need to slightly modify the algorithm. Instead of considering two neighboring spins (as in the one dimensional case) we need to consider all eight surrounding spins when calculating the change of energy resulting in a spin flip.

We consider two cases: the case where the magnetic field is zero, $H = 0$, and the case where the magnetic field is 1, $H = 1$.

We run the simulation for a range of dimensionless temperatures 1.0 J/k_B through 3.5 J/k_B and calculate all dimensionless observables for an equilibrated system.

The results for the simulation for the case where there is not magnetic field applied are shown in Figures 9 through 12. And the results for the simulation for a system with $H = 1$ are shown in Figures 13 through 16.

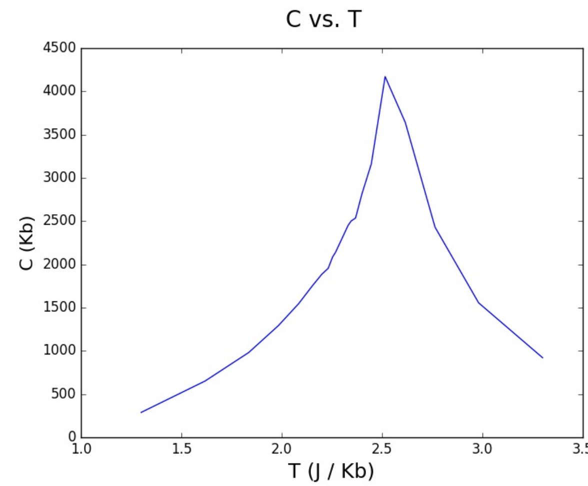

FIG. 11: Dimensionless heat capacity as a function of dimensionless temperature for $H = 0$.

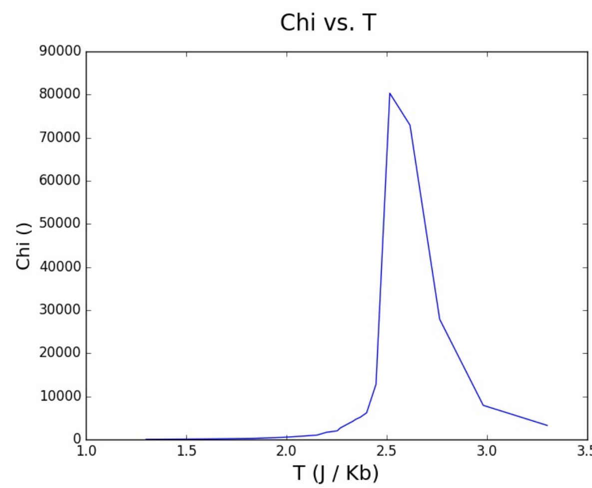

FIG. 12: Dimensionless susceptibility as a function of dimensionless temperature for $H = 0$.

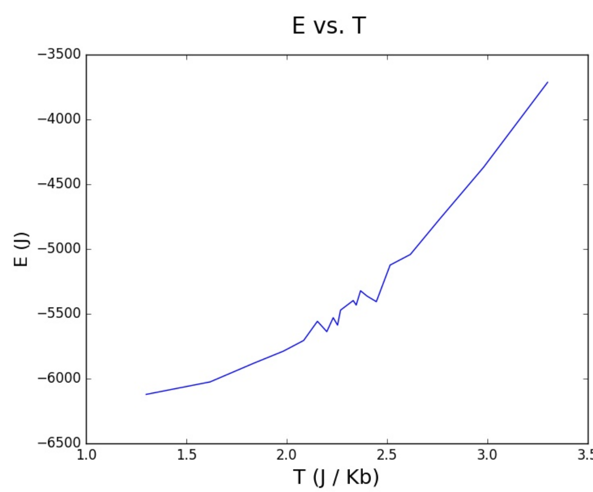

FIG. 13: Dimensionless energy as a function of dimensionless temperature for $H = 1$.

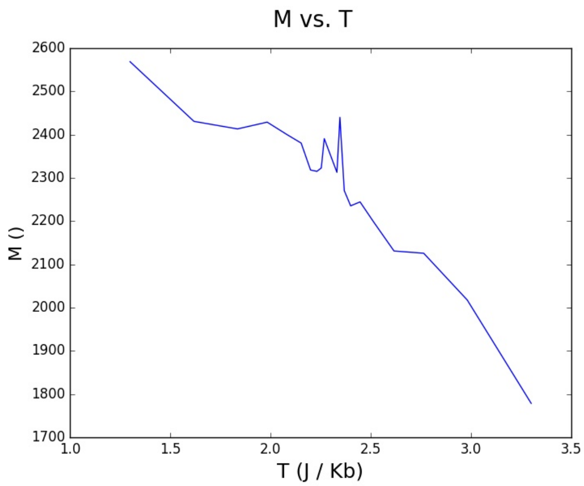

FIG. 14: Dimensionless magnetization as a function of dimensionless temperature for $H = 1$.

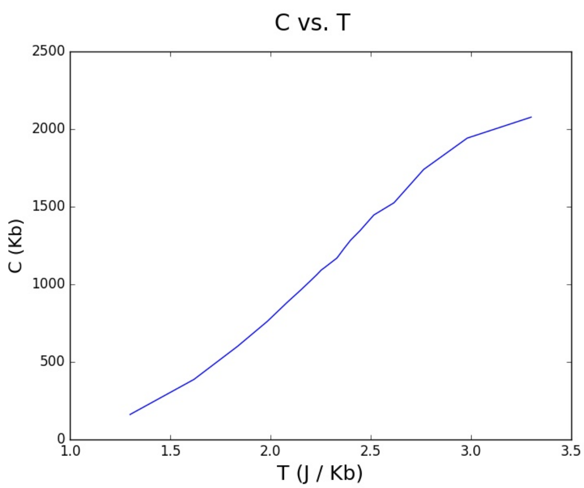

FIG. 15: Dimensionless heat capacity as a function of dimensionless temperature for $H = 1$.

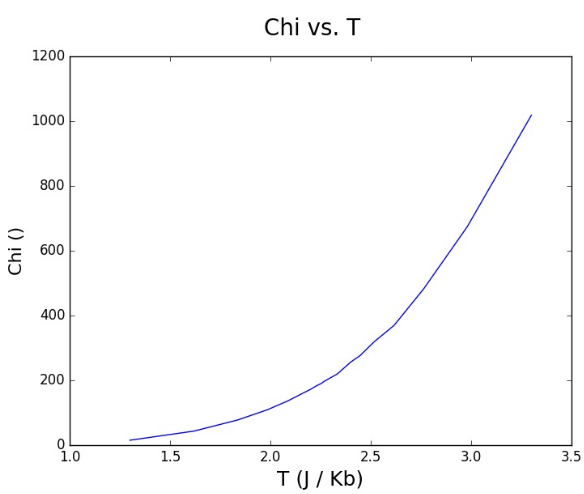

FIG. 16: Dimensionless susceptibility as a function of dimensionless temperature for $H = 1$.

In the case where the magnetic field is zero, $H = 0$, we observe an abrupt transition from the ferromagnetic phase to the paramagnetic phase. With zero magnetic field, the aligment of the spins is due entirely to the short-range interactions of the spins. However, at a critical temperature of approximately 2.4 J/K_B, the short-range interactions stop being significant and the system quickly enters a paramagnetic phase. In order to characterize this transition, we can fit our observables to

$$O(T) \propto \left| \frac{T - T_C}{T_C} \right|^{\alpha} \tag{12}$$

By doing the regression, we obtain a value of 0.38 for the exponent characterizing the specific heat (with a predicted value of 0), and we obtain a value of 1.95 for the exponent characterizing the susceptibility (with a predicted value of 1.75).

For the case where we have a non-zero magnetic field, we can observe a transition between a ferromagnetic phase and a paramagnetic phase. However, in this case the transition is significantly smoother. At very low temperatures the alignment is due to both the interparticle interactions and the applied magnetic field. However, as the temperature rises the short-range interactions stop being so significant and the system starts to transition into the paramagnetic phase. However, it is because of the applied magnetic field that the spins can still algin with each other even after the short-range effects have stopped being significant. This results in a slower transition from one phase to the other.

CONCLUSIONS

We have shown that in the one-dimensional Ising model there exists no transition between ferromagnetic and paramagnetic phases. The system favors a paramagnetic case even for very low temperatures where short-range interactions become significant.

We have seen that in the two-dimensional case we observe an abrupt transition from the ferromagnetic phase to the paramagnetic phase when there is no applied magnetic field. The short-range interactions that are responsible for the ferromagnetic phase at low temperatures stop being significant after the critical temperature of 2.4 J/k_B. The transition is characterized by the exponents extracted from equation 12 and the values for the specific heat and the succesibility are close to the theoretical values. However, in order to obtain more accurate values the simulations could be ran for larger lattices.

We have also seen that in the prescene of magnetic fields, the transition between the ferromagnetic phase and the paramagnetic phase exists, but it is slowed down as a consequence of the external field being applied.

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