Phase Transition in Ferromagnetic simulation and experiment

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Abstract

A program is written that implements a 3-dimensional Ising model and the Metropolis algorithm to simulate the phase transition of a ferromagnet to a paramagnet. Vanishing magnetization and a discontinuity in the average energy for simulated data is observed at the Curie temperature. Simulated data compared to experimental measurements of CoNiFeCB magnetization as a function of temperature shows that the simulation approaches the Curie temperature quicker. The Curie temperature for CoNiFeCB is measured to be approximately 600 °C.

1 Introduction

Ferromagnetic materials posses a spontaneous magnetic moment which arises from the regular arrangement of their electron spins. In a ferromagnet the unpaired electrons arrange their alignments parallel to one another within domains separated by so-called Bloch walls. The most well known ferromagnetic materials are iron, nickel and cobalt. Upon application of a magnetic field to a ferromagnetic sample, the domains will align and the material is said to be magnetized. Curiously, if a ferromagnetic sample is heated above a certain critical temperature, the sample's magnetization disappears; this temperature is the Curie temperature. The phase transition that takes place at the Curie temperature is from spin aligned ferromagnetism to disordered paramagnetism. [1][2]

An interesting application for ferromagnetic materials may be found in electronics such as in ferroelectric random access memory for computers (FeRAM). [3] From these points of interest, we aim to understand and model the phase transition at the Curie temperature that characterize ferromagnetic samples. In this study we simulate the thermodynamic effects on spin in a ferromagnet and compare the simulation to data collected from a CoNiFeCB sample consisting of measurements of magnetization as a function of temperature.

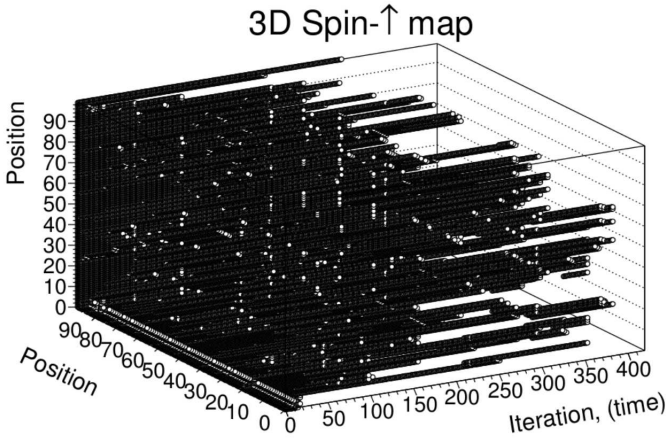


Figure 1: A 3D lattice of 100 spins initially aligned spin-up. Spin up states are denoted with circles and down states are shown as blank areas. Domains begin to form as the system equilibrates. [2]

2 Description of simulation & algorithm

2.1 Ising model

The mathematical model of ferromagnetism we use is the Ising model which takes a Z dimensional lattice and statically represents an atomic spin at each vertex. We will use a 3-dimensional model. Since the particles are fixed at each vertex, we need not be concerned with the Pauli exclusion principle implying the antisymmetry of the wave function since no particles may be exchanged in this system. A particle's initial state is denoted s_i and may be either spin-up or spin-down as shown by the following relation.[2]

$$s_i \equiv s_{z,i} = \pm\frac{1}{2} \tag{1}$$

Were s is spin, z just denotes the axis that the spin is directed along, and $\frac{1}{2}$ is the value of the electron spin. If there are N particles in this system, the total number of possible states is 2^N. Thus, the ket vector for this system is

$$|s_j\rangle = |s_1, s_2, s_3, ..., s_N\rangle\,,\ j = 1, 2^N. \tag{2}$$

Furthermore, we may model the spin-spin interaction as a dipole-dipole interaction as known from quantum mechanics. From solid state physics we know that spins interact with their immediate neighbor, with the exchange field, and the external magnetic field. Thus we have the following potential

$$V_i = -J\vec{s_i}\cdot\vec{s}_{i+1} - g\mu_b\vec{s_i}\cdot\vec{B} \tag{3}$$

Here, V is the potential for some state i, J is the exchange energy which is the strength of spin-spin interaction, g and μ_b is the gyromagnetic ratio constant and the Bohr magneton respectively, and s denotes, as usual, spin.

Due to the extremely large number of particles in systems such as this, usually given as 10^{23} particles, statistical methods are necessary. The Ising model uses the Boltzmann distribution to obtain the probabilistic energy of the system, and is given in equation (4).

$$P(s_j) = \frac{e^{-E(s_j)/kT}}{\sum\limits_{s_j} e^{-E_j/kT}} \tag{4}$$

Above, P represents probability, E denotes energy, and k and T is Boltzmann's constant and temperature respectively. The Boltzmann distribution says that states with lower energy are more likely to occur, while states with higher energy are possible, yet have less probability to occur. The energy of the system to be applied to equation (4) is given by the expectation value of (3) over all states of the system, which is shown in the following equation. [2] [4]

$$E(s) = \langle s|\sum_i V_i\,|s\rangle = -J\sum_{i=1}^{N-1} s_i s_{i+1} - B\mu_b\sum_{i=1}^{N} s_i \tag{5}$$

An interesting outcome of the Boltzmann distribution which one can see in figure (1) and which we will see more of below, is that there is no single configuration of lowest energy. The statistical nature of the thermodynamics which effect the spin arrangements are constantly randomly exchanging via thermal energy and the exchange field. A written C++ program implements the Ising model in three dimensions by randomly flipping the spin of dipole arrangements in the lattice points of a cube. After a random number generator is seeded with number 94180717 the program is run and a loop randomly determines spin-up or spin-down and calculates the energy based on equation (5). The program determines lowest energy, and a three dimensional map of spin-up states is output.

2.2 Metropolis algorithm

The Metropolis algorithm is similar to Monte Carlo methods, but extends it to essentially be a Markov chain Monte Carlo which allows one to apply it to the Boltzmann distribution. The notion of the Metropolis algorithm is that the

arrangements of the spins which randomly alternate between spin-up and spin-down due to thermodynamics, are processed via the variance reduction method and the von Neumann reduction technique. The variance reduction method reduces computation time by obtaining a minimum variance between functions so that integration may be solved quicker than when considering the set of smaller and larger variances combined. The von Neumann rejection technique generates random points in a probability distribution and counts only those point that fall within the desired weighting function. [2]

The outline of the Metropolis algorithm is the following. First, initial temperature and configuration of all states beginning in spin-up in the 3-dimensional lattice is set and the algorithm runs until the system reaches equilibrium. Next, a particle is chosen randomly and its spin is flipped, this generates a statistically random configuration of which we may calculate thermodynamic quantities such as magnetization and internal energy. After energy is calculated, the following conditionals are the main parts of this algorithm. If $E(s_{trial}) \leq E(s_j)$, then accept and set $s_{j+1} = s_{trial}$. If $E(s_{trial}) > E(s_j)$, then accept with relative probability $P = e^{-\Delta E/kT}$. Within this last step, another random number between 0 and 1 is generated and compared to the probability just obtained. If the random number is less than or equal to the probability, the spin state is accepted and set to s_{j+1}, and if the probability is less than the random number, the state is rejected. The key to the Metropolis algorithm is that states that are not lowest energy are not simply thrown away because that is not how thermodynamic statistical systems work. The states with higher energy are run through the second conditional and determined whether it is accepted to rejected, which shows that higher energy states although less probable are still kept to a statistical degree in the system. [2]

A C++ program written by the author based off of the outline given above implements the Metropolis algorithm and a 3-dimensional Ising model. The source code is freely available upon request. The program is run for various temperatures thereby obtaining the temperature dependence of the spin system.

3 Experiment

This semester the author has been granted an Undergraduate Research Opportunity through the University of Hawaii at Manoa (UROP) for the project: Magnetization characterization of novel multiferroic materials, dependence of particle size, temperature, strength and gradient of magnetic field. A summary of the experimental set up is given here. Measurements of thermo-magnetic properties are conducted using Faraday's balance method in an external non-uniform magnetic field. Direct current power supply provides current for a solenoid which induces a time constant magnetic field. The ferrite sample is placed in the measurement position and lowered into the solenoid by use of a custom-made high temperature resistant dielectric diamagnetic holder. The measurement of the magnetic field is done by a high precision balance, the Sartorius Entris 64-1S.

During the complete duration of measurement while the sample is in the magnetic field, temperature is monitored with a high precision electronic thermometer and using a high temperature resistant thermocouple. Magnetization is measured up to 900K in steps of 20K. The sample is heated in a custom made electric oven where a variable transformer is used to provide power to the oven which enables excellent control over the heating rate. Controlling the heating rate is important since the temperature gradient is one of the parameters which strongly influence the magnetization of the sample.

The goal of the UROP experiment is to measure the magnetic and electric properties of several ferroic materials as a function of temperature and particle size. The aim is to find the optimal compound mixture and thermal prepa-

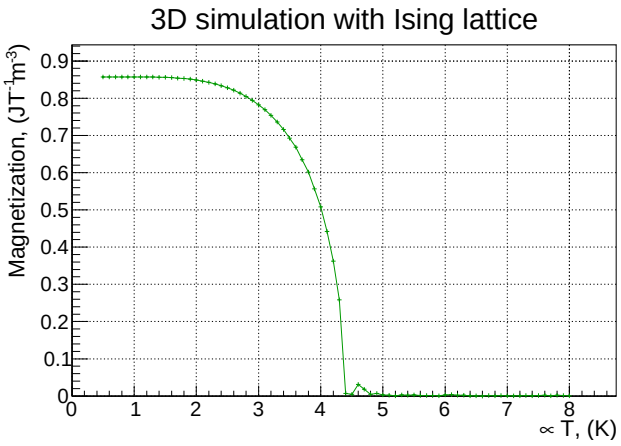
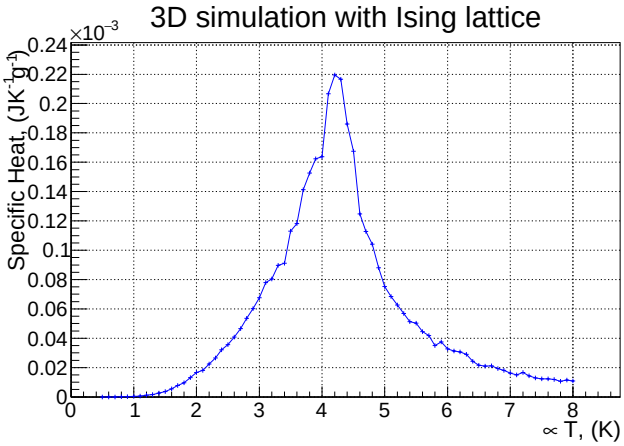
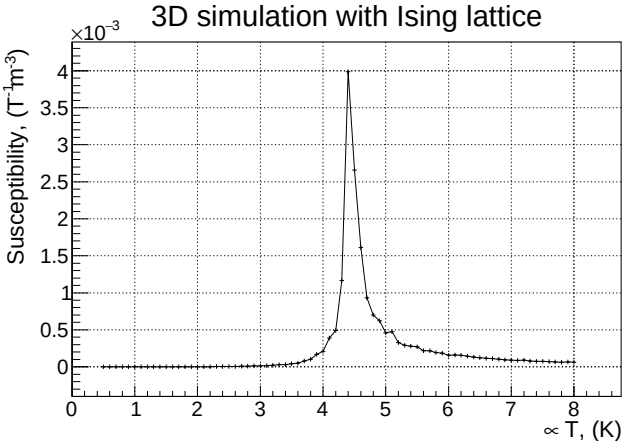


Figure 2: Magnetization as a function of temperature in simulation with the 3D Ising model and the Metropolis algorithm. Note the Curie temperature is observed approximately proportional to 4.5 K, and also relates to the peaks found in figures (3a) and (3b).



(a)



(b)

Figure 3: (a) Specific heat as a function of temperature from simulation results. (b) Susceptibility as a function of temperature.

ration, and to establish the relationship between composition and thermal treatment compared to material performance. The initial compound of CoNiFeCB is measured and discussed in this paper, with more samples to be measured in the Spring of 2017. [5]

4 Discussion

The 3-dimensional model compared to the 1-dimensional case results in less fluctuation of spins due to an increase of couplings to nearest neighbor and thus an increase in thermal inertia.[2] An important aspect of the program is the periodic boundary conditions which are conditionals that keep track of on-going loop summations in the three dimensional array to the boundaries within the cubic structure. The total number of particles, N, applied in the program is 2000.

Figures (2), (3a), and (3b) show simulation results from the 3-dimensional Ising model and the Metropolis algorithm for magnetization, specific heat, and susceptibility respectively. In thermodynamics, temperature is often expressed as proportional to kT, where k is Boltzmann's constant and T is temperature; in the plots we express kT as $\propto T$.

Phase transition is clearly observed as shown in figure (2) from the ferromagnetic case to paramagnetic. Magnetization vanishes at approximately a temperature proportional to 4.5 K. The specific heat and susceptibility also show peaks at the Curie temperature. Interestingly, specific heat and susceptibility peak for a certain width around the Curie temperature then as temperature increases, the values for the function fall

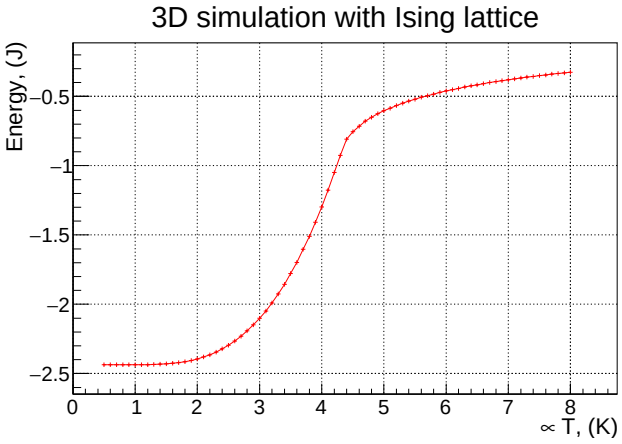


Figure 4: The average energy of the system as a function of temperature from the simulation.

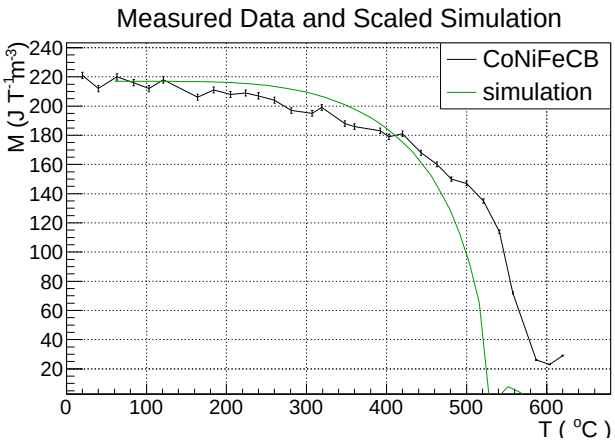


Figure 5: Simulation results compared to experimental data measuring magnetization of CoNiFeCB as a function of temperature.

back down to zero. This shows that when the Curie temperature is met, the configuration of paramagnetic disordered states have a maximum value for specific heat and susceptibility.

Figure (4) plots the average energy of the system. As temperature in the simulation is increased, energy increases with a discontinuity in the increasing slope being observed at approximately a temperature proportional to 4.4 K. This discontinuity also corresponds to the Curie temperature.

Measured magnetization from a CoNiFeCB sample as a function of temperature is plotted in figure (5) and compared to a scaled plot of the simulation results for magnetization. The simulation compared to data have overall a similar shape, although the rate of decrease in magnetization is quicker in the simulation rather than in the CoNiFeCB sample. This may be because the sample we are working with is not a pure ferromagnet. If the sample only included, say Fe, one would expect a better fit between data and simulated results. An interesting point to note is that after magnetization reaches a minimum, in both cases a slight increase in magnetization is observed. Data should be taken in an extended temperature region with the CoNiFeCB sample to see if the slight increase in magnetization after 600 °C reduces back down to minimum.

5 Conclusion

A 3-dimensional Ising model with the Metropolis algorithm is successfully implemented in a C++ program, and simulation of the phase transition of a ferromagnet at high temperature is observed. The Curie temperature is also observed as a discontinuity in the total average energy of the system as temperature increases and as peaks in specific heat and susceptibility in the simulated data. Magnetization simulation is compared to measured data from CoNiFeCB as a function of temperature. Shapes between functions of simulation and data show the simulation approaches the Curie temperature quicker than our experimental measurements. This is most likely because the ferromagnetic sample we are using, CoNiFeCB, is not a pure ferromagnet.

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