PHYS 905 - Project 3

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PUT ABSTRACT HERE

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1 Introduction

Certain materials exhibit a behavior where the spins of unpaired electrons in the material align in some region of the material. This is called a domain and had a "macroscopic" spacial extent on the order of mm [1]. This behavior is called Ferromagnetism and Iron, Nickel, and Cobalt are the most common elements which display this behavior. When an external magnetic field is applied, the domains which are already in aligned with the field grow, taking over the misaligned domains. Ferromagnetic materials can remain magnetized, even after that external field is removed.

At the same time, these alignments are fighting against thermal excitations which tend to randomize any ordering at the atomic level. However, at the Curie temperature, magnetic materials undergo a sharp change in their magnetic properties. This is the temperature at which random thermal nudges overcome the domain's order and spins are forced out of alignment [2]. This temperature

can vary from well below room temperature for rare earth metals like Dysprosium, all the way to almost 1400 K for Cobalt.

In this project we are going to study one of the simplest and most common models for ferromagnetic materials, the Ising model. This model, although very basic, has proven very useful in understanding, not only ferromagnetic materials, but also antiferromagnetic materials, where neighboring spins anti align with one another, leading to no overall magnetization. The Ising model has even been applied outside of the physical sciences to model a wide variety of situations. Some of these include modeling people's opinions about the future of the economy, urban segregation, and how languages change over time [3]. We will us the Ising model in two dimensions to explore properties of a materials phase transition from a magnetic to a nonmagnetic material. We will employ a Monte Carlo method in this study and, eventually, extract the Curie temperature which can be compared to exact results.

This report will begin with an introduction to the Ising model, beginning with the simple case of a 2 by 2 lattice. We will explain the model and use it to derive important quantities relevant for statistical mechanics. Then we will implement this system using Monte Carlo methods. We will then expand the lattice to a larger size and explore aspects of the Monte Carlo simulation, as well as the phase transition. Finally, we will extract the critical, Curie temperature from our study and compare it with exact results.

2 Methods

2.1 Introduction to the Ising Model

The Ising model in two dimensions has a simple expression for the energy between two neighboring spins which can be expressed as

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l.$$

In this expression, N is the total number of spins, $s_k = \pm$ corresponding to electrons that are spin up or spin down, and the symbol $\langle kl \rangle$ implies that the sum only runs over nearest neighbors. This sum does not include spins which are diagonal from one another. In this framework, J is taken to be a positive value and it is taken as the coupling constant expressing the strength of the spin interaction.

In this work, we will not apply an an external field to the system, although that is a simple extension of the energy expression which gives us

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l - \mathcal{B} \sum_{k}^{N} s_k$$

where $\mathcal{B}$ is the strength of the external magnetic field. Now we can use this energy to develop expressions for relevant quantities from statistical mechanics.

2.2 The Ising Model on a 2 by 2 Lattice

We will begin this development by studying the case of a 2 by 2 lattice (4 spins) where each spin can be either up for down. If we enumerate all possible configurations, there are 16, pictured below.

$$\begin{matrix}- & - \\ - & -\end{matrix} \quad \begin{matrix}+ & - \\ - & -\end{matrix} \quad \begin{matrix}- & - \\ - & +\end{matrix} \quad \begin{matrix}+ & + \\ - & -\end{matrix} \quad \begin{matrix}+ & - \\ + & -\end{matrix} \quad \begin{matrix}+ & - \\ - & +\end{matrix} \quad \begin{matrix}+ & + \\ + & -\end{matrix} \quad \begin{matrix}+ & - \\ + & +\end{matrix}$$

$$\begin{matrix}+ & + \\ + & +\end{matrix} \quad \begin{matrix}- & + \\ - & -\end{matrix} \quad \begin{matrix}- & - \\ + & -\end{matrix} \quad \begin{matrix}- & - \\ + & +\end{matrix} \quad \begin{matrix}- & + \\ - & +\end{matrix} \quad \begin{matrix}- & + \\ + & -\end{matrix} \quad \begin{matrix}+ & + \\ - & +\end{matrix} \quad \begin{matrix}- & + \\ + & +\end{matrix}$$

We can enumerate the energy and the magnetization for each of these configurations where the energy is defined above and the magnetization is defined as

$$\mathcal{M}_i = \sum_{j=1}^{N} s_j$$

where the sum runs over all spins for a given configuration i. These quantites are in the table below.

Number of Spin Ups	Number of Configurations	Energy	Magnetization
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

Note that there are two kinds of configurations with 2 spin ups. This configuration results in 0 energy if the spin up points are adjacent to one another, but has a positive energy if they are diagonal from one another.

Now we have the energies, we can compute the partition function, which is defined as

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}$$

where the sum is over all microstates M and $\beta = 1/(kT)$. In the case of the two dimensional lattice, Z is equal to

$$\begin{aligned} Z &= 2e^{-8J\beta} + e^{8J\beta} + e^{8J\beta} + 12e^{0} \\ &= 2e^{-8J\beta} + 2e^{8J\beta} + 12 \\ &= 4(3 + cosh(8J\beta)). \end{aligned}$$

We can define a probability distribution using the partition function

$$P_i(\beta) = \frac{e^{i\beta E_i}}{Z}$$

And the mean value of some quantity of interest is

$$\langle X \rangle = \sum_{i=1}^{M} X_i P_i.$$

Using this, the expectation value of the energy is

$$\begin{aligned}\langle E \rangle &= \frac{-8Je^{8J\beta} + 8Je^{-8J\beta} - 8Je^{8J\beta} + 8Je^{-8J\beta}}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} \\ &= \frac{8Jsinh(8\beta J)}{3 + cosh(8\beta J)}.\end{aligned}$$

The mean magnetization is

$$\begin{aligned}\langle |M| \rangle &= \frac{4e^{8J\beta} + (4+4)2e^{0} + 4e^{8J\beta}}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} \\ &= \frac{8e^{8J\beta} + 16}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} \\ &= \frac{2(2 + e^{8J\beta})}{3 + cosh(8\beta J)}.\end{aligned}$$

The specific heat can be defined as

$$C_V = \frac{1}{T^2}(\langle E^2 \rangle - \langle E \rangle^2).$$

We can easily find $\langle E^2 \rangle$ in the same way as before, giving us

$$\begin{aligned}\langle E^2 \rangle &= \frac{64J^2e^{8J\beta} + 64J^2e^{-8J\beta} + 64J^2e^{8J\beta} + 64J^2e^{-8J\beta}}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} \\ &= \frac{64J^2cosh(8\beta J)}{3 + cosh(8\beta J)}.\end{aligned}$$

This leaves us with a final expression for the heat capacity

$$\begin{aligned}C_V &= \frac{1}{T^2}\Big(\frac{64J^2cosh(8\beta J)}{3 + cosh(8\beta J)} - \Big(\frac{8Jsinh(8\beta J)}{3 + cosh(8\beta J)}\Big)^2\Big) \\ &= \frac{64J^2}{T^2}\frac{1 + 3cosh(8J\beta)}{(3 + cosh(8J\beta))^2}.\end{aligned}$$

There is a very similar expression for the magnetic susceptibility

$$\chi = \frac{1}{T}(\langle M^2 \rangle - \langle |M| \rangle^2).$$

The value of $\langle M^2 \rangle$ is given by

$$\begin{aligned}\langle M^2 \rangle &= \frac{16e^{8J\beta} + (4+4)4e^0 + 16e^{8J\beta}}{12 + 2e^{-8J\beta} + 2e^{8J\beta}} \\ &= \frac{8(e^{8J\beta}+1)}{3 + cosh(8\beta J)},\end{aligned}$$

so the susceptibility can be written as

$$\begin{aligned}\chi &= \frac{1}{T}\Big(\frac{8(e^{8J\beta}+1)}{3+cosh(8\beta J)} - \Big(\frac{2(2+e^{8J\beta})}{3+cosh(8\beta J)}\Big)^2\Big) \\ &= \frac{4}{T}\frac{3 + 4cosh(8J\beta) + 2sinh(8J\beta)}{(3+cosh(8J\beta))^2}.\end{aligned}$$

2.3 The Metropolis Algorithm and Detailed Balance

In order to perform our calculations, we need the partition function that describes the physical situation. For the case of the 2 by 2 lattice, it is simple to write this function explicitly, but as the size of the grid grows to large values, the partition function becomes intractable to write explicitly. This is true in almost every physical application. Therefore, we need some methodology which avoids calculating the partition function explicitly. This is where the Metropolis algorithm and detailed balance come in.

Suppose we have some PDF, $w(t)$ that evolves via a transition probability W such that

$$w_i(t = \epsilon) = W(j \to i)w_j(t = 0),$$

then we can write the action of W as

$$w_i(t+1) = \sum_j W_{ij} w_j(t).$$

In the case of the Ising model, w depends on the partition function, which we often cannot write explicitly, additionally, we do not have an analytic form for the transition probability, W. Therefore, we can choose to model the transition probability as the product of two probabilities, one probability for accepting a move from i to j (A) and one that makes the transition to i from j (T). We can now express the prbability as

$$W(j \to i) = T(j \to i)A(j \to i).$$

W, w, A, and T are all probabilities and, therefore, must be between 0 and 1 and their sums over all states must be normalized. Now we can define the

probability of being in state i after some time in terms of our newly defined transition probability.

$$w_i(t+1) = \sum_j [w_j(t) T_{j\to i} A_{j\to i} + w_i(t) T_{i\to j}(1 - A_{i\to j})]$$

Then we can apply the condition that $\sum_j T_{i\to j} = 1$, leaving us with

$$w_i(t+1) = w_i(t) + \sum_j [w_j(t) T_{j\to i} A_{j\to i} - w_i(t) T_{i\to j} A_{i\to j}].$$

We can rearrange this expression as

$$w_i(t+1) - w_i(t) = \sum_j [w_j(t) T_{j\to i} A_{j\to i} - w_i(t) T_{i\to j} A_{i\to j}].$$

This is very similar to the Master equation given by

$$\frac{dw_i(t)}{dt} = \sum_j [W(j\to i) w_j - W(i\to j) w_i].$$

This equation states that the rate that a system moves from state j to state i is balanced by the rate at which the system transtitions from j to i. In equilibrium, this should be equal to 0. That allows us to write

$$\sum_j w_j T_{j\to i} A_{j\to i} = \sum_j w_i T_{i\to j} A_{i\to j}$$

We recongnize the product of the transition probabilities on the right side as W_{ij} and we know that this probability is normalized when we sum over all final states, j. This allows us to rewrite the expression as

$$w_i = \sum_j w_j W_{j\to i}.$$

This condition, however, is not sufficient to guarantee that we arrive at the correct distribution in the system. We just apply the additional condition of detailed balance, which can be written

$$W(j\to i) w_j = W(i\to j) w_i$$

such that, at equilibrium, we have

$$\frac{W(j\to i)}{W(i\to j)} = \frac{w_i}{w_j}.$$

Finally, in terms of A and T, this gives is

$$\frac{T_{j\to i} A_{j\to i}}{T_{i\to j} A_{i\to j}} = \frac{w_i}{w_j}.$$

w_i and w_j both take the form of a Boltzmann distribution, with the partition function, Z, in their denominators so this proportion can be calculated, independent of Z. This can be rearranged to read

$$\frac{A_{j\to i}}{A_{i\to j}} = \frac{T_{i\to j}w_i}{T_{j\to i}w_j}.$$

Detailed balance asumes that $T_{i\to j} = T_{j\to i}$, causing a cancelation. If we insert the expression for the Boltzmann distribution for w, we now have

$$\frac{A(j\to i)}{A(i\to j)} = e^{-\beta(E_i - E_j)}.$$

If we think about an application to a system with many different energy states, we know that the physical system will tend towards the lowest energy state, but our system must also be ergodic, meaning that it must be possible for the system to reach any possible state from any starting position. This means that our aglorithm must encode transitions to lower energies after many transitions, but also allow for many paths which include midpoints that reach higher energy states. One way to encode this is

$$A(j\to i) = \begin{cases} e^{-\beta(E_i - E_j)} & \text{if } E_i - E_j > 0 \\ 1 & \text{else} \end{cases}$$

where a transtition to a lower energy state is always accepted, but a transition to a higher energy state is accepted with some probability depending on the energy difference. This is the algorithm we will us in our calculation.

3 Code and Implementation

All of the programs, results, and benchmarks for this work can be found in my GIT repository (https://github.com/poxonpea/PHYS905). All codes for this project were written in FORTRAN.

4 Results and Discussion

5 Conclusions

References

[1] Hjorth-Jensen, Morten. Computational Physics, Lecture Notes Fall 2015. August 2015.

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[3] Stauffer, D. Social Applications of two-dimensional Ising models. arXiv:0706.3983.