

PHYS 905 - Project 3

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In this report, we study the 2D Ising model using a Monte Carlo simulation that employs the Metropolis Algorithm for its sampling rule. The code is able to reproduce exact results for the case of a 2 by 2 lattice. We conducted a series of investigations of the average energy, average magnetization, susceptibility, and heat capacity, exploring the second order phase transition as a function of lattice size and temperature. As the lattice size increases, we approach the physical limit where the lattice is infinite. We deduced a critical temperature of 2.242 which differs from the exact solution of 2.269 by about 1% relative error.

Contents

1	Introduction	1
2	Methods	2
2.1	Introduction to the Ising Model	2
2.2	The Ising Model on a 2 by 2 Lattice	3
2.3	The Metropolis Algorithm and Detailed Balance	5
2.4	Phase Transitions in the Ising Model	8
3	Code and Implementation	8
3.1	General Algorithm for Code	9
4	Results and Discussion	10
4.1	Comparing Results to Analytic 2 by 2 System	10
4.2	Equilibrium Time	11
4.3	Probability Distributions	14
4.4	Numerical Studies of the Phase Transition	16
5	Conclusions	21
	References	21

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 it

has a "macroscopic" spacial extent on the order of mm [1]. This phenomenon 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 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 critical 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 use the Ising model in two dimensions to explore properties of a material's 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, $s_k = \pm 1$ 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 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. 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 or down. If we enumerate all possible configurations, there are 16, pictured below.

$$\begin{array}{cccccccc} \begin{array}{c} + - \\ - - \end{array} & \begin{array}{c} + - \\ - - \end{array} & \begin{array}{c} - - \\ - + \end{array} & \begin{array}{c} + + \\ - - \end{array} & \begin{array}{c} + - \\ + - \end{array} & \begin{array}{c} + - \\ - + \end{array} & \begin{array}{c} + + \\ + - \end{array} & \begin{array}{c} + - \\ + + \end{array} \\ \\ \begin{array}{c} + + \\ + + \end{array} & \begin{array}{c} - + \\ - - \end{array} & \begin{array}{c} - - \\ + - \end{array} & \begin{array}{c} - - \\ + + \end{array} & \begin{array}{c} - + \\ - + \end{array} & \begin{array}{c} - + \\ + - \end{array} & \begin{array}{c} + + \\ - + \end{array} & \begin{array}{c} - + \\ + + \end{array} \end{array}$$

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 quantities 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 spins up. 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 micro states 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

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

Using this, the expectation value of the energy is

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

The mean absolute value of 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 $\langle E^2 \rangle$ by substituting $X = E^2$ in Equation 1 giving us.

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

This leaves us with a final expression for the heat capacity

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

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

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

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. Monte Carlo methods are useful in situations, such as these, where the physical process cannot be easily described analytically. Monte Carlo methods require a sampling rule to decide whether or not to accept a simulated move. Here we will use the Metropolis algorithm, which depends on the condition of detailed balance.

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

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

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 probability as

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

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.

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

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

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

We can rearrange this expression as

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

This is very similar to the Master equation given by

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

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 transitions from j to i . In equilibrium, this should be equal to 0. That allows us to write

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

We recognize 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

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

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

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

such that, at equilibrium, we have

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

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

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

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

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

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

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

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 algorithm must encode transitions to lower energies after many transitions, but also allow for many paths which include higher energy states. One way to encode this is

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

where a transition 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 sampling rule is the Metropolis algorithm and we will use it in our calculations.

2.4 Phase Transitions in the Ising Model

Near the critical temperature, many physical properties are modeled using a simple power law. For example, the magnetization, heat capacity, and susceptibility are modeled as

$$\langle M(T) \rangle \sim (T - T_C)^\beta,$$

$$C_V(T) \sim |T_C - T|^\alpha,$$

$$\chi(T) \sim |T_C - T|^\gamma,$$

with the critical exponents $\beta = 1/8$, $\alpha = 0$, and $\gamma = 7/4$, respectively.

We can also think about the correlation length of a system undergoing phase transition. When a material is high above the critical temperature, we expect the correlation length to be on the order of lattice spacing. As the temperature decreases and approaches T_C , we expect the correlation length to increase. This behavior can be modeled as

$$\xi(T) \sim |T_C - T|^{-\nu}.$$

where $\nu = 1$.

A second-order phase transition is characterized by a correlation length which is on the order of the size of the system. Since our model is confined to a finite lattice, ξ will be proportional with the size of the lattice. it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. That relation is

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \quad (2)$$

where a a constant and ν was defined above. At $T = T_C$, we can use this relationship to define the mean magnetization, heat capacity and susceptibility as

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta \rightarrow L^{-\beta/\nu},$$

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu},$$

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}.$$

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.

3.1 General Algorithm for Code

The heart of this process is the Metropolis algorithm which is shown in Figure 3.1

```
subroutine Metropolis(NumSpins, idum, SpinMatrix, E, M, w)
  implicit none

  integer::NumSpins,x,y,ix,iy,deltaE,right,left,up,down,idum
  integer, dimension(NumSpins,NumSpins)::SpinMatrix
  real(8)::E,M
  real(8)::w(-8:8)
  do y=1,NumSpins
    do x=1,NumSpins
      ix=int(rand()*NumSpins)+1
      iy=int(rand()*NumSpins)+1
      right = ix+1
      if (ix == numspins) then
        right = 1
      end if
      left = ix-1
      if (ix == 1) then
        left = numspins
      end if
      up = iy+1
      if (iy == numspins) then
        up = 1
      end if
      down = iy-1
      if (iy == 1) then
        down = numspins
      end if
      deltae = 2*spinmatrix(ix,iy)*(spinmatrix(right,iy)+&
        spinmatrix(left,iy)+spinmatrix(ix,up)+ &
        spinmatrix(ix,down) )
      if ( rand() <= w(deltae) ) then
        spinmatrix(ix,iy) = -spinmatrix(ix,iy)
        M = M+2*spinmatrix(ix,iy)
        E = E+deltaE
      end if
    end do
  end do
end subroutine Metropolis
```

Figure 1: The implementation of the Metropolis algorithm used in the Monte Carlo simulation of the Ising Model

Below is a general overview of the algorithm for our Monte Carlo code for solving the Ising model

1. Using a random number generator, choose a random position on the lattice and compute the energy of that state.

2. Flip only one spin in that configuration and compute the new energy of the state.
3. Calculate the energy difference between these two state.
4. If the energy difference is less than 0, we accept the transition.
5. If the energy difference is greater than 0, we calculate $w = e^{-\beta\Delta E}$
6. We generate a random number between 0 and 1. If that number is less than w , we accept the change. If not, we keep the old configuration.
7. Update expectation values for various quantities.
8. Repeat these steps for each desired Monte Carlo iteration at every desired energy.

4 Results and Discussion

4.1 Comparing Results to Analytic 2 by 2 System

The first test of our code is to compare our results from our Monte Carlo simulations to the analytic results we achieved for the 2 by 2 case. All results for our code will be normalized to the size of lattice so that we can compare across calculations. Therefore, all of the results we obtained before should be divided by four. In this comparison, we will study the behavior at $T=1.0$ in units of kT/J . Here, our or calculations started with a configuration where all spins are aligned, which is the configuration that we expect at low temperature.

The table below gives the results of the calculations, including the relative error when comparing to the analytical values. For $T = 1$, the exact results yield $\langle E \rangle = -1.99598$, $\langle |M| \rangle = 0.998661$, $C_V = 0.0320823$, and $\chi = 0.00401074$ respectively.

Cycles	E/N	ϵ	$ M /N$	ϵ	C_V/N	ϵ	χ/N	ϵ
10	-1.8182	0.0891	0.9091	0.0869	1.3223	40.2163	0.3306	81.4232
50	-1.9608	0.0176	0.9894	0.0183	0.3076	8.5870	0.0769	18.1719
100	-1.9208	0.0377	0.9703	0.0284	0.6086	17.9689	0.0955	22.8063
500	-1.9521	0.0290	0.9820	0.0166	0.3741	10.6592	0.0586	13.6080
1000	-1.9740	0.0110	0.9905	0.0082	0.2051	5.3927	0.3061	6.6317
5000	-1.9908	2.5953E-3	0.9966	2.0625E-2	0.0732	1.2831	0.0112	1.7804
10000	-1.9928	1.5939E-3	0.9974	1.3123E-3	0.0574	0.7887	8.6711E-3	1.1620
50000	-1.9945	7.5256E-4	0.9981	5.8151E-4	0.0440	0.3726	5.9893E-3	0.4923
100000	-1.9955	2.6162E-4	0.9985	2.0301E-4	0.0363	0.1305	4.721E-3	0.17697
500000	-1.9961	7.9066E-5	0.9987	4.9233E-5	0.0308	0.0393	3.8735E-3	0.0342
1000000	-1.9961	4.9031E-5	0.9987	2.4270E-5	0.0313	0.0244	3.9692E-3	0.01036

From this table, we can see that we can reach good agreement for the energy and magnetism very quickly, although this is not surprising because we began the simulation in a configuration that is highly favored at low temperature. It took much longer, however, to reach good agreement with the heat capacity and susceptibility. It took about a million Monte Carlo cycles to reach agreement on the order of a couple percent.

4.2 Equilibrium Time

We can ask ourselves how long it takes for our spin system to settle on its most likely state. In a sense, the number of Monte Carlo cycles represents the passing of time, so we can examine how many cycles it takes for the calculation to reach equilibrium. Here we studied this by looking at both the energy and the magnetization as a function of the number of Monte Carlo cycles (time). We performed this calculation on a 20 by 20 lattice at two different temperatures, $T=1$ and $T=2.4$. For both cases we began the calculation from two different orientations: an ordered, spin up configuration, and a random configuration. Those results are shown below.

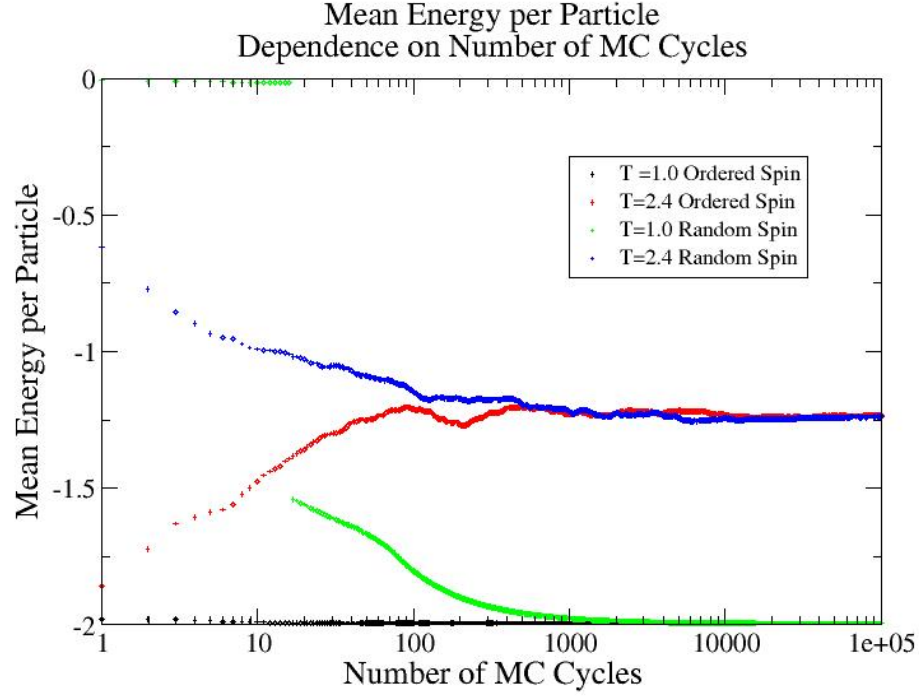


Figure 2: The mean energy of the 20 by 20 system as a function of the number of Monte Carlo Cycles. The calculation is repeated at $T=1$ and $T=2.4$. For each case, the calculation is performed with an initial spin configuration that is random and an initial spin configuration that is ordered, with all spins pointing up.

For all four cases, the energy levels out, indicating the system seems to come to equilibrium, by about 1,000 Monte Carlo cycles. Conservatively, waiting until 10,000 cycles eliminates almost all further variation. It is worth noting that the case of $T=1$ with an ordered configuration comes to equilibrium much faster, but this is because the beginning configuration is already very close to the equilibrium state.

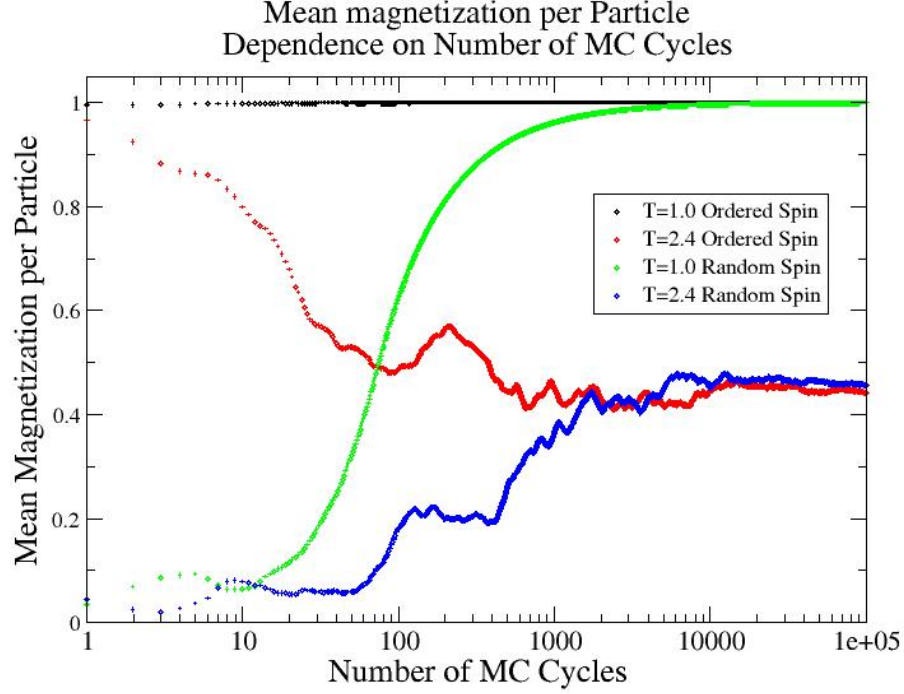


Figure 3: The mean magnetization of the 20 by 20 system as a function of the number of Monte Carlo Cycles. The calculation is repeated at $T=1$ and $T=2.4$. For each case, the calculation is performed with an initial spin configuration that is random and an initial spin configuration that is ordered, with all spins pointing up.

For all four cases, the magnetization levels out, indicating the system seems to come to equilibrium, by about 10,000 Monte Carlo cycles. Again, the case of $T=1$ with an ordered configuration comes to equilibrium much faster, but this is because the beginning configuration is already very close to the equilibrium state. This test seems to indicate that about 10,000 cycles are necessary to get reliable values for $\langle E \rangle$ and $\langle |M| \rangle$.

Finally, we can look at the behavior of the number accepted configuration as a function of the time. The plot below demonstrates this behavior for the 20 by 20 system at three different temperature, $T=1, 3$, and 5 .

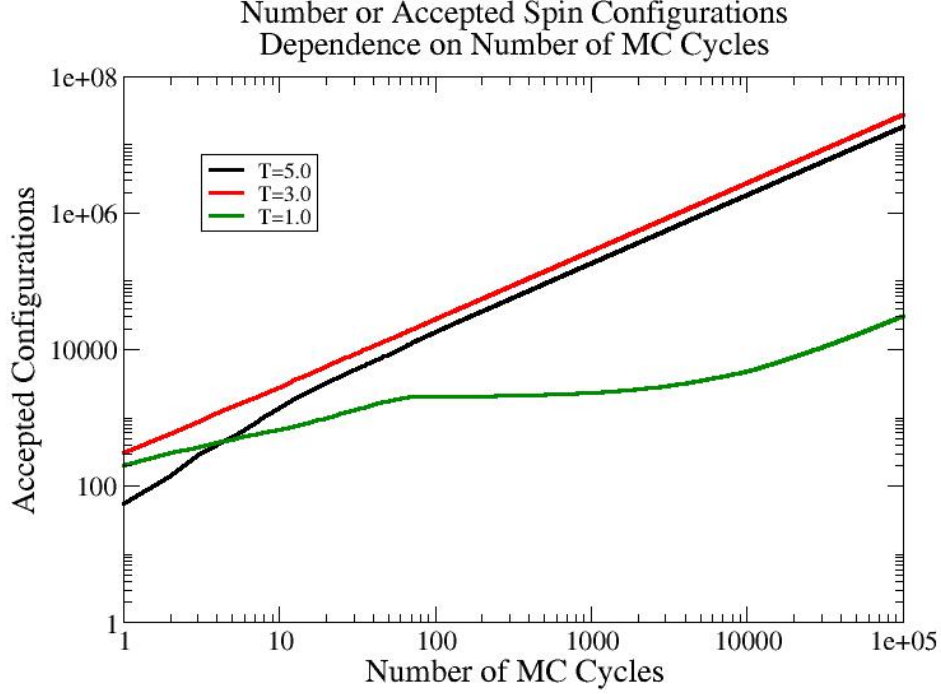


Figure 4: The number of accepted configurations as a function of the number of Monte Carlo Cycles at $T=1, 3$, and 5

The plot is in log-log scale, indicating a strong linear behavior, with the slope increasing with temperature. This makes sense because as the temperature increases, more possible configurations are open to the system, allowing for a higher acceptance rate. As T increase, we expect the slope to approach the total number of configurations.

4.3 Probability Distributions

We can also examine the energy probability distribution created by our calculation. To do this, we performed the same 20×20 calculation at $T=1$ and $T=2.4$. Once the system has reached equilibrium, we can histogram the number of times a particular energy is produced by the Monte Carlo cycle. To ensure that equilibrium was reached, and to make the amount of data tractable, the following plots show the energy results for every 10th calculation between 200,000 and 1,000,000 Monte Carlo cycles. These plots are shown in Figures 4.3 and 4.3 for $T=1.0$ and $T=2.4$, respectively.

To make the comparison between the two cases transparent, the x axis of both plots cover the same energy difference (0.01) and there are 1000 energy bins in each histogram. It is clear that the $P(E)$ for the $T=1.0$ case is much sharper and narrower. This makes sense because, well below the critical temperature, the spins are going to prefer a low energy, aligned spin configuration.

For $T=2.4$, the distribution becomes much wider. This is because at higher temperatures, more states become energetically accessible. This effect can be understood in terms of the energy variance, which is proportional to the heat capacity. The heat capacities for $T=1$ and $T=2.4$ are about 0.023 and 1.41, respectively. This means the heat capacity for the $T=2.4$ case is about 60 times greater than for the $T=1$ case. If we take a close look at the $P(E)$ s and zoom in on the energy axis, we can see that the $T=2.4$ case is about 50 times wider than its $T=1$ counterpart. This is consistent with the picture of higher temperature leading to a wider energy distribution and larger energy variance.

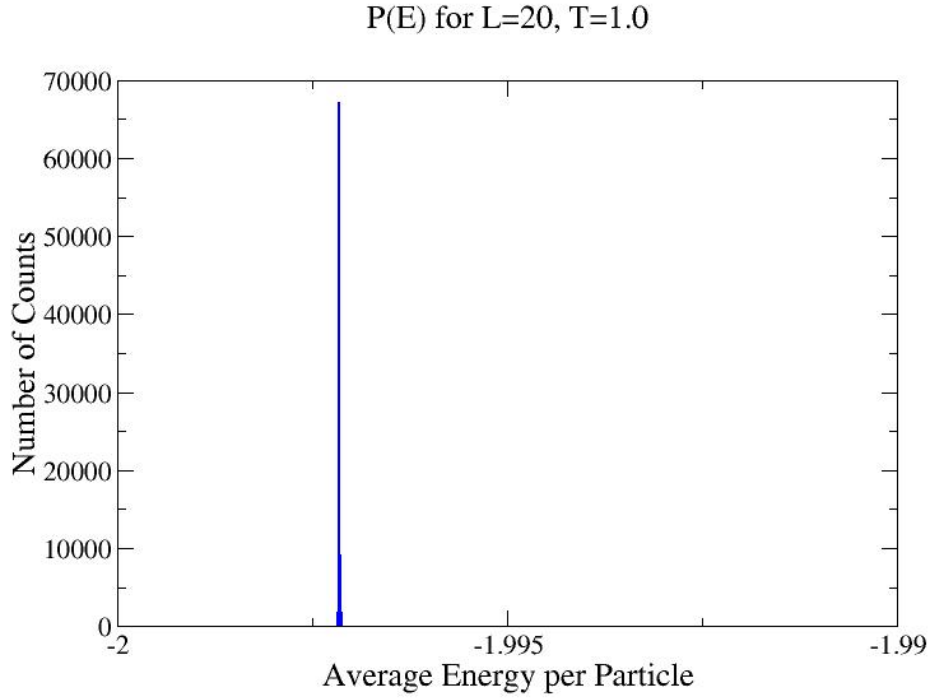


Figure 5: $P(E)$ for the 20 by 20 lattice with $T=1.0$

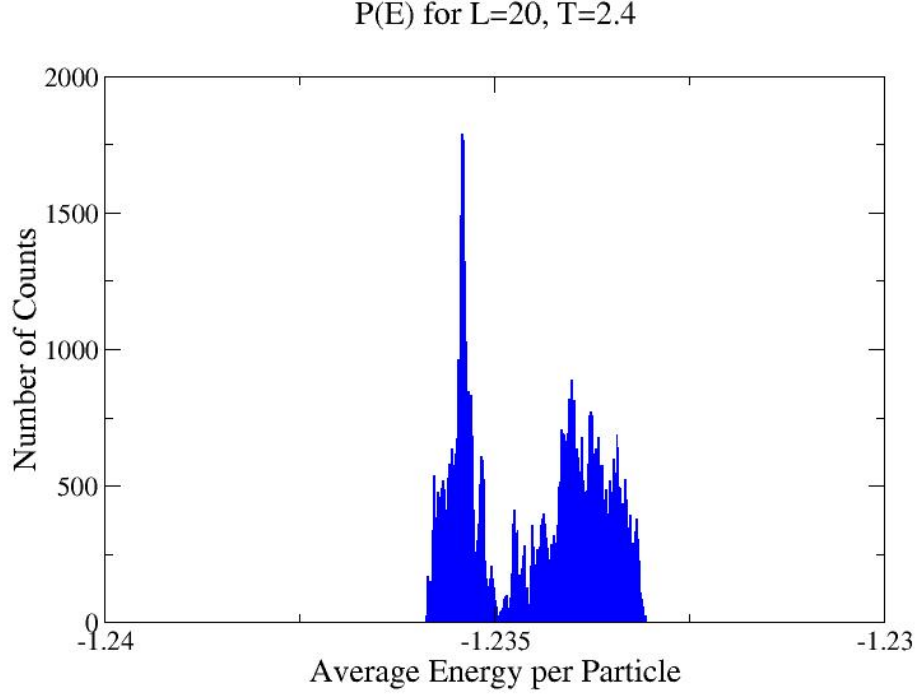


Figure 6: $P(E)$ for the 20 by 20 lattice with $T=2.4$

4.4 Numerical Studies of the Phase Transition

The Ising model displays a second order phase transition where the material loses its magnetic properties at some critical temperature. In these types of transitions, we expect to see a smooth variation in energy when crossing the critical temperature, but a divergence in the heat capacity. To study this effect, we ran Monte Carlo calculations for a range of temperatures that span the phase transition for a number of lattice sizes. As the lattice increases, we begin to approach the more physical approximation of an infinite lattice and these transition effects will approach a physical limit. To get a rough idea of where the critical temperature is, we ran our calculation for temperatures between 2.1 and 2.6, in steps of 0.03. For each temperature value, we ran 100,000 Monte Carlo cycles. The results showing $\langle E \rangle$, $\langle |M| \rangle$, C_V , and χ are shown below.

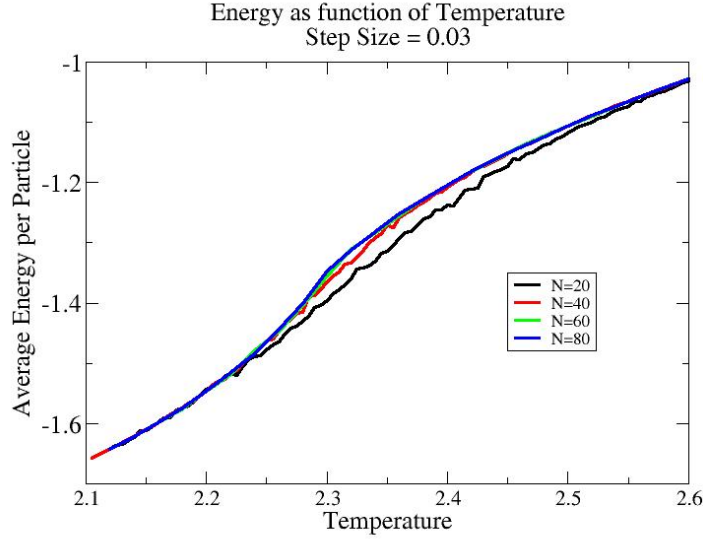


Figure 7: Average energy per particle as a function of temperature

As expected, the energy transition is continuous across the critical temperature, with the rise in energy becoming more pronounced for larger lattices.

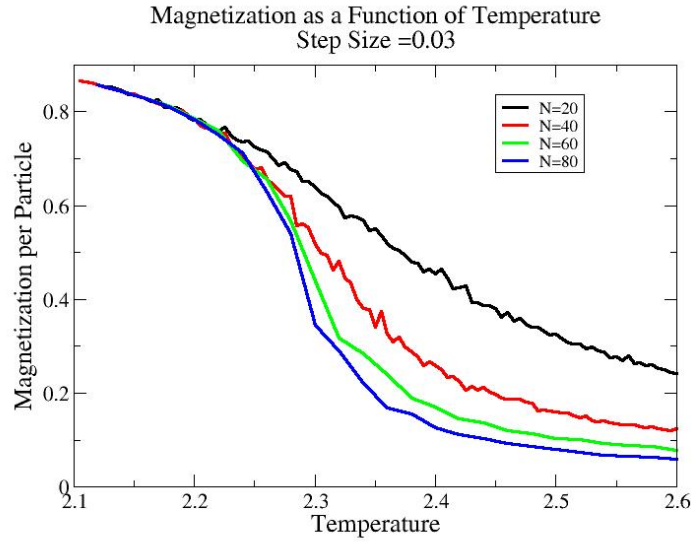


Figure 8: Average magnetization per particle as a function of temperature

The magnetism per particle also exhibits the expected behavior of a phase transition. At low temperature, the magnetism is some positive quantity because the spins tend to be in an aligned orientation. As the temperature increases, more and more spin configurations are allowed until they are, essentially, random. At this critical temperature, the magnetism of all of the spins cancel out, giving an overall 0 magnetism. This is signified by the steep drop to 0 magnetization at the critical temperature. As the lattice size increase, this drop becomes sharper.

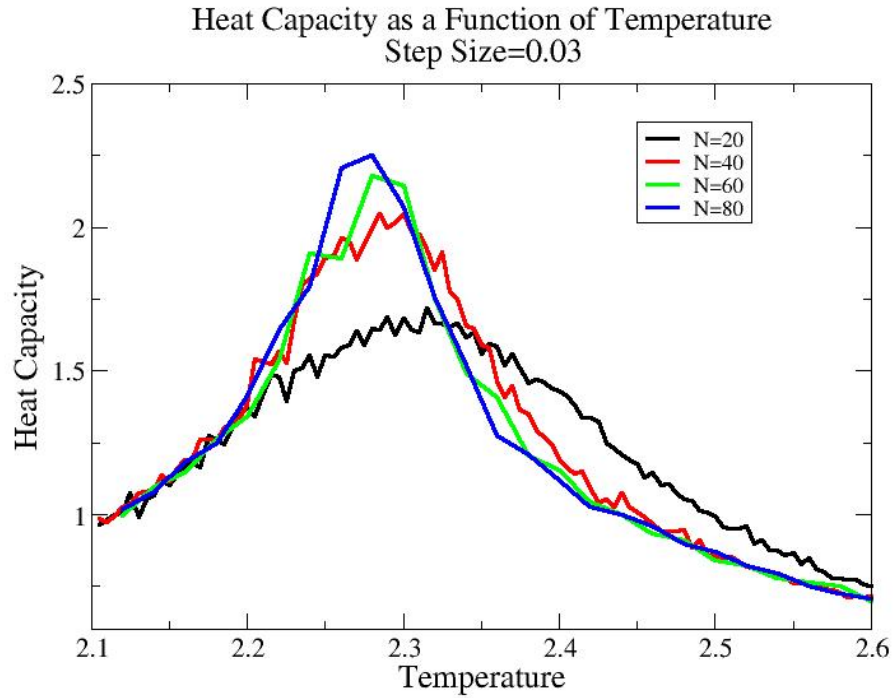


Figure 9: Average heat capacity per particle as a function of temperature

The heat capacity demonstrates a discontinuity at the the critical temperature. Because we are working on a finite lattice, our results will always be finite, but show a clear bump that increases in strength as we move towards a larger, more physical lattice.

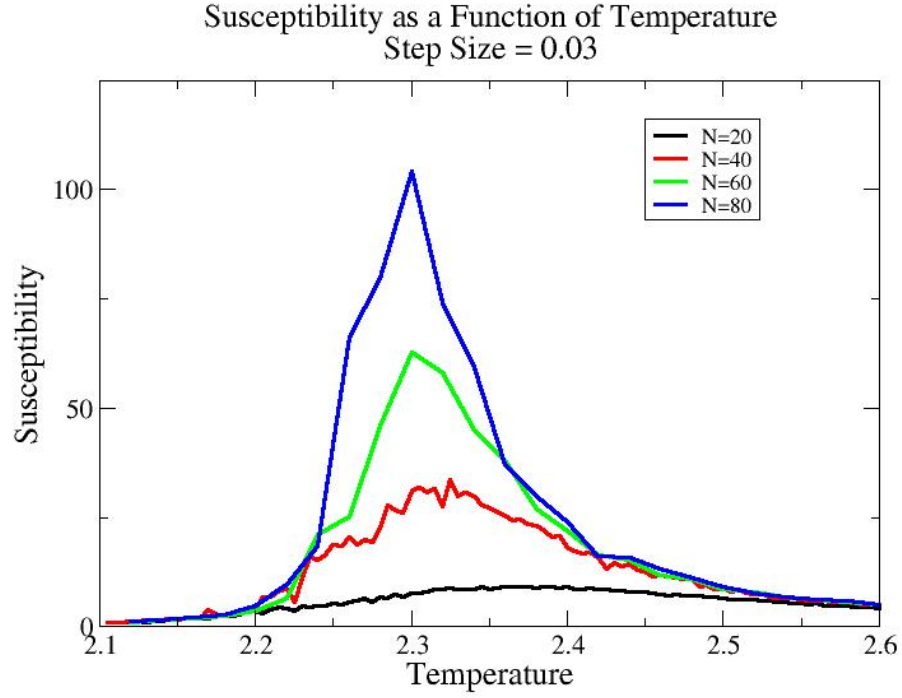


Figure 10: Average magnetic susceptibility per particle as a function of temperature

Additionally, the susceptibility demonstrates a strong discontinuity at the critical temperature, which behaves very similarly to the heat capacity. We can use this very sharp peak to extract the critical temperature.

Now we have a general idea of where the phase transition occurs, we can zoom in on that region and do a finer search in energy. The plot below shows one such search looking at heat capacity as a function of temperature. We used temperature steps of 0.005 and performed 100,000 Monte Carlo cycles per temperature.

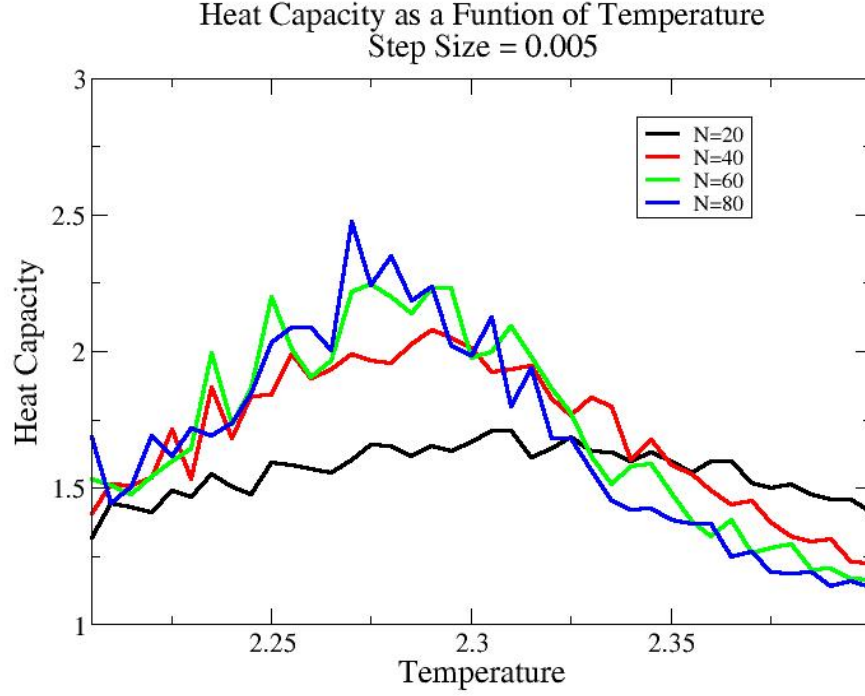


Figure 11: Average heat capacity per particle as a function of temperature on a finer grid.

We can use this result to extract the critical temperature. We recall from before that the critical temperature scales with lattice size as

$$T_C(L) - T_C(L = \infty) = aL^{1/\nu}$$

where $\nu = 1$. Here, we assume a to be 1. We can find T_C for each lattice size by reading the peaks off of Figure 4.4 and multiplying by $1 - \frac{1}{L}$. This can be compared to the exact solution of $2/\ln(1 + \sqrt{2}) \approx 2.269$. The results for different lattice sizes and their relative errors are shown below.

L	T_C	ϵ
20	2.195	0.033
40	2.233	0.016
60	2.237	0.014
80	2.242	0.012

As expected, as L increases, the T_C approaches the value on an infinite lattice.

5 Conclusions

In this project, we modeled magnetic phase transitions using the 2 dimensional Ising model. Our code employs Monte Carlo methods, using the Metropolis Algorithm as the sampling rule. We tested this code by comparing to the exact solutions of the tractable, 2 by 2 lattice. Our code was able to reproduce these results with good accuracy. We explored many aspects of this model, including exploring the energy probability distribution at high and low temperatures, finding that at low temperatures, the system is confined to an aligned spin configuration, but at higher temperatures, the system can access a larger array of spin configurations.

Finally, we conducted a series of investigations exploring the second order phase transition as a function of lattice size and temperature. As the lattice size increases, we approach the physical limit where the lattice is infinite. We deduced a critical temperature of 2.242 which differs from the exact solution of 2.269 by about 1% relative error.

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