## Monte Carlo Simulation of Phase Transitions

1   Magnetic Phase Transition

Iron, a *ferromagnetic* material, is magnetic at room temperature. This is because the iron atoms, which have an atomic magnetic moment $\vec{\mu}$, will mutually align their magnetic moments even when there is no externally applied magnetic field. Adding up 10^{23} of these aligned magnetic moments leads to a magnetization that is noticeable on the everyday scale. However, if you heat iron enough, the magnetic moments will become randomly oriented, and so 10^{23} of them added together mostly cancel out and leave no net magnetization. The transition from a magnetic to a non-magnetic material is an example of a *phase transition*. The fundamental question of interest is how a temperature change can so dramatically affect the group behavior of the atoms, from a state where they influence each other to all align to a state where their mutual influence is unable to spread across the whole sample.

2   The Ising Model

We will study a simplified model of magnetism called the Ising model. Normally an atomic magnetic moment $\vec{\mu}$ can point in any direction in three-dimensional space. Instead we will allow only one of two possible directions: up ($+\hat{\mathbf{z}}$ direction) and down ($-\hat{\mathbf{z}}$). We make this assumption mainly for simplicity, but it does describe certain materials in which the $\vec{\mu}$ have a preference to align along a single axis. Furthermore, we will call these magnetic moment vectors *spins* (which is much easier to say) and the two possible orientations are called *spin up* and *spin down*. We will assume the atoms' positions form a regular lattice, such as the 3×3 square lattice below which shows a typical set of spins.
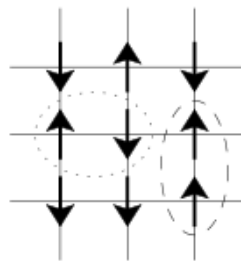
2.1   Exchange Interaction

Due to a quantum mechanical effect called the *exchange interaction*, neighboring spins in ferromagnetic materials prefer to be aligned. In the image, the dashed line circles a pair of

aligned, lower energy spins. The dotted line circles a pair of unaligned, higher energy spins.

In order to have a simple expression for the total energy of this spin configuration, we label each lattice site with a pair of integer indices, i and j, which represent the column and row number, and we introduce at each site a spin variable $s_{i,j}$ that is either $+1$ (spin up) or -1 (spin down). Then the energy of a neighboring pair of spins, say $s_{i,j}$ and $s_{i+1,j}$ can be written $E_{\text{pair}} = -Js_{i,j}s_{i+1,j}$. Here J is just some constant with units of energy that depends on the specific material we might study. Notice that when the spins are aligned $E_{\text{pair}} = -J$ and when the spins are unaligned $E_{\text{pair}} = +J$, so this simple choice for E_{pair} captures the basic ingredients of the QM exchange interaction.

In our model, interactions only occur vertically or horizontally, so each atom interacts with its 4 nearest neighbors. For the purposes of this project, you will need to calculate the total energy of the four interactions for an atom at location (i, j):

$$E_{ij} = \sum_{\text{4 neighbors}} E_{pair} \tag{1}$$

Do these questions with your lab partner, recording your work in your lab notebook:

1. While there are many possible arrangements for the spin at location (i, j) and its 4 neighboring spins, there are only 5 possible values for E_{ij}. Draw a number of distinct possible arrangements for the spin at (i, j) and its 4 neighbors – each drawing should have 5 spins in it arranged in a plus shape.

2. Write the value of E_{ij} for each drawing (i.e., -4J). What are the 5 possible energy values? Make additional drawings if needed to get all 5 energy values.

3. In your drawings, envision flipping the spin s_{ij} of the single atom in the center. For each of the 5 energy values, what is the energy change $\Delta E = E_{ij,final} - E_{ij,initial}$ caused flipping that one spin? Write a formula for ΔE in terms of $E_{ij,initial}$. Explain qualitatively why this formula makes sense.

2.2 Global Properties: System Energy & Magnetization

A given spin configuration, that is, a specified set of $s_{i,j}$ values over the whole lattice, is called a *microstate*, a state in which *all* the micro- (atomic) information is specified. To calculate the total energy of the system for a given microstate, we must sum over all pairs of nearest neighbors in the system, which we write as

$$E_{\text{sys}} = \sum_{\text{n.n.}} E_{\text{pair}} = -J \sum_{\text{n.n.}} s_{i,j}s_{i',j'} \tag{2}$$

Having spin variables which take on the values $s_{i,j} = \pm 1$, arranging them on a lattice, and using Eq. (2) to give the total energy is precisely what defines the Ising model.

The magnetization in the Ising model is given by the sum of all spins, $M = \sum_{i,j} s_{i,j}$. If there is an equal number of up and down spins, then $M = 0$, while if there are an unequal number

$M \neq 0$. It is convenient to introduce a magnetization per spin, m. For an $L \times L$ lattice we have

$$m = \frac{1}{L^2} \sum_{i,j} s_{i,j}. \tag{3}$$

We expect the spins to all be aligned in the low-temperature case, and to be randomized in the high-temperature case. Pause and work on the following problems. Discuss them with your partner, but you should each work on your own iPython notebook:

1. What value would m have if the atoms are all spin up? All spin down? Random (assuming a large number of atoms)?

2. Download the IsingTemplate.ipynb Jupyter notebook from the course web page and work through it. This notebook provides a structure for you to code up the high-temperature case using a Monte Carlo approach. In the high temperature case, there is a large amount of collisions and vibrations because of thermal energy. Any given collision can flip a spin up or down. You will simulate this in a 2D array, starting from a lattice of atoms that are all spin up, then randomly choosing a location in the lattice and flipping its spin. Then you repeat that many times: throw a dart at the board to choose a random (i,j), flip that spin, repeat. After many iterations, your lattice should have changed from all spin up to random. While this is not the most efficient way to generate a random set of spins, it sets up a Monte Carlo approach that will be useful when we start the more complex case of low temperature. **Make sure to document your work in your lab notebook, or in Jupyter then print it for your notebook**: goals, how far you got, main take-away points from results and anything weird or bugs, sketch or print graphs as needed to illustrate points about what you saw.

3 Statistical Mechanics

We have not yet quantified the effect of temperature. For this we need the Boltzmann factor $e^{-E/k_B T}$, where k_B is Boltzmann's constant. What the Boltzmann factor tells us is the probability of the system being found in a particular microstate. Let $\{s\}$ denote a particular set of spin values $(s_{11}, s_{12}, s_{13}, \dots)$ where, for example, $s_{1,1} = 1$, $s_{1,2} = 1$, $s_{1,3} = -1$, and so on. In other words, $\{s\}$ labels a microstate. Then

$$\text{Probability of } \{s\} = \frac{1}{Z} e^{-E_{\text{sys}}(\{s\})/k_B T}. \tag{4}$$

The $1/Z$ factor is a normalization constant, and $E_{\text{sys}}(\{s\})$ is just the total energy given by Eq. (2) for the particular microstate. Since the probability must be normalized (there is a

probability 1 that the system is in *some* microstate) we can use this to determine Z:

$$1 = \sum_{\{s\}} \text{Probability of } \{s\} = \frac{1}{Z} \sum_{\{s\}} e^{-E_{\text{sys}}(\{s\})/k_B T}$$

$$\Rightarrow \quad Z = \sum_{\{s\}} e^{-E_{\text{sys}}(\{s\})/k_B T}. \tag{5}$$

Here the notation $\sum_{\{s\}}$ means to sum over all possible microstates.

Now we can determine the magnetization at a given temperature: we want to average the magnetization for each microstate, weighted by the probability for that corresponding microstate. We will write this average with angle brackets, so

$$\langle m(T) \rangle = \frac{1}{Z} \sum_{\{s\}} \left[e^{-E_{\text{sys}}(\{s\})/k_B T} \left(\frac{1}{L^2} \sum_{i,j} s_{i,j} \right) \right]. \tag{6}$$

In principle, then, we only need to compute the sums in Eq. (6) to discover everything we want to know about how the magnetization depends on temperature.

Question (put your answer in your lab book): what can you say about the probability of various microstates in the limit of $T \to \infty$?

4 Monte Carlo Methods and the Metropolis Algorithm

Unfortunately, performing the sum in Eq. (6) is not possible, even with the best computer we can imagine. To see this, consider a 10×10 lattice and calculate the number of microstates there are (put this calculation in your lab notebook). If a computer could calculate a billion terms of the sum every second, how long would it take to sum over all microstates? Express your answer in terms of years. Notice that we have no hope, even if the computers get a lot faster, especially considering that we want to go to much larger systems like 200×200 and more.

So what do we do? One idea would be to randomly select a manageable number of microstates, say a billion, hope they are a typical set, and just use this reduced set for averaging. This idea of replacing a complete sum with a (hopefully) representative sample is known as the *Monte Carlo* method. (The name comes from the similarity to gambling.) However, our randomly selected microstates won't help us here, because nearly every microstate we pick this way will, according to the Boltzmann factor, be an incredibly improbable state for the actual system at some given temperature. The more probable states that provide the main contribution to $\langle m(T) \rangle$ are such a small fraction of the total number of microstates that our random sampling will not represent them well.

We need instead to do *biased* selection that tends to pick microstates that have a high probability of occurring in the physical system. The *Metropolis algorithm* (named after a person, no connection to Superman) is a Monte Carlo method that does this biased selection for us — in fact it ends up selecting microstates based on their Boltzmann probability, that is, their

probability of occurring in the physical system. This will make our life easy for computing the average magnetization, because we only need to average together the magnetization m for the microstates we generate. We don't need to do any extra weighting, such as computing Boltzmann factors — the microstates are a biased set with all the weighting built in.

The Metropolis algorithm is powerful and useful, and it's also easy to implement. We use our previous microstate $\{s\}$ to generate our new microstate $\{s'\}$. The rule for generating the new state is that we randomly select one spin $s_{i,j}$ out of the whole system and then decide whether or not to "flip" the spin (change the sign). The rule for flipping is the following:

- If flipping the spin lowers the energy or leaves it the same, then we flip it.

- If flipping the spin raises the energy an amount ΔE_{sys}, then we flip the spin with probability $p = e^{-\Delta E_{\text{sys}}/k_B T}$.

That's it. We will write a computer program to implement the Metropolis algorithm, and therefore calculate quantities like $\langle m(T) \rangle$ to high accuracy.

5   Defining a dimensionless temperature

In the expression for the average magnetization given in Eq. (6), the temperature dependence is all in the exponent:
$$-\frac{E_{\text{sys}}(\{s\})}{k_B T} = \frac{J}{k_B T} \sum_{\text{n.n.}} s_{i,j} s_{i',j'}. \tag{7}$$

It is clear that we will get the same value of the magnetization for all combinations of J and T in which the ratio J/T is the same, so we shouldn't bother calculating all cases of J and T. One other thing of note about the exponent here is that it contains the constant k_B, which has an extremely small value in SI units.

These observations suggest that we define a dimensionless temperature parameter, T', in the following way
$$T' \equiv \frac{k_B T}{J}, \tag{8}$$
which can be rearranged to give
$$T = T' \frac{J}{k_B}. \tag{9}$$
Inserting this in the expression for the exponent gives
$$-\frac{E_{\text{sys}}(\{s\})}{k_B T} = \frac{1}{T'} \sum_{\text{n.n.}} s_{i,j} s_{i',j'}. \tag{10}$$

How nice — the constants J and k_B have disappeared! And they disappear from all expressions that are ratios of energy to temperature. You should do all of your computer calculations with this dimensionless temperature parameter. In effect, this means set $J = k_B = 1$ in your calculations.

This raises the question of how to relate a calculation done for a dimensionless T' to the "real world." It's simple: use Eq. (9).

6   Steps in this Project

The main goal of this project is to calculate the average magnetization per spin, $\langle m(T) \rangle$, for a range of temperatures, generating a plot of $\langle m(T) \rangle$ vs. T. That plot should demonstrate that a phase transition occurs in the 2D Ising model and show the T_c at which this transition occurs. How can you get there? Pilot the following steps for a smallish lattice ($L \sim 10$) then apply them to a bigger lattice, being careful to make sure you

1. Implement the Monte Carlo model for high (infinite) temperature, generating m vs. time plots. Figure out how to use the m vs. time plot to find $\langle m \rangle$, the average magnetization in the steady state. (Note the distinction between m, an instantaneous value that changes over time, and $\langle m(T) \rangle$, the time average in the steady state!)

2. Add the flip probability to implement the Metropolis algorithm, in order to generate an m vs. time plot for any temperature. Get one value of $\langle m \rangle$ from each m vs. time plot.

3. Determine $\langle m \rangle$ at a wide range of temperatures to generate your $\langle m(T) \rangle$ plot.

If you complete this goal before the end of the project, you should then choose a way to extend your project. You could investigate a question that you came up with during the course of the project, or you could choose another physical property of the system to study in your simulations. Some ideas:

- Figure out how to add uncertainties to each data point on your $\langle m \rangle$ vs. T plot.

- Track E_{sys} in your simulations and study how it varies over time and depends on temperature.

- Study how heat capacity C depends on temperature.

- Characterize the spatial behavior of magnetization near the critical temperature, or how the timescale of fluctuations in m vs. time changes near the critical temperature.