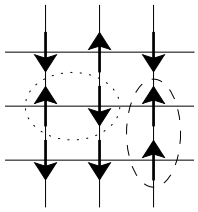
Monte Carlo Simulation of Phase Transitions

1 Magnetic Phase Transition

Iron 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.



Due to a quantum mechanical effect called the *exchange interaction*, neighboring spins prefer to be aligned. 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 an simple expression for the total energy of this spin configuration, we label each lattice site with an integer index i and introduce at each site a spin variable s_i that is either $+1$ (spin up) or -1 (spin down). Then the energy of a neighboring pair of spins s_i and s_j can be written $E_{ij} = -Js_is_j$. Here

J is just some constant that depends on the specific material we might study. Notice that when the spins are aligned $E_{ij} = -J$ and when the spins are unaligned $E_{ij} = +J$, so this simple choice for E_{ij} captures the basic ingredients of the QM exchange interaction.

A given spin configuration, that is, a specified set of s_i 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

$$E = \sum_{n.n.} E_{ij} = -J \sum_{n.n.} s_i s_j \tag{1}$$

Having spin variables which take on the values $s_i = \pm 1$, arranging them on a lattice, and using Eq. (1) 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, $M = \sum_i s_i$. If there are an equal amount of up and down spins, then this will give $M = 0$, while a majority of either up or down spins will give $M \neq 0$. It is convenient to introduce a magnetization per spin, m. For an $L \times L$ lattice we have $m = (1/L^2) \sum_i s_i$.

3 Statistical Mechanics

We have not yet put in 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 $(s_1, s_2, s_3, \dots)$ where, for example, $s_1 = 1$, $s_2 = 1$, $s_3 = -1$, and so on. In other words, $\{s\}$ labels a microstate. Then

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

The $1/Z$ factor is a normalization constant, and $E(\{s\})$ is just the total energy given by Eq. (1) 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:

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

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

$$\langle m(T) \rangle = \frac{1}{Z} \sum_{\{s\}} e^{-E(\{s\})/k_B T} \Big(\frac{1}{L^2} \sum_i s_i \Big) \tag{2}$$

In principle, then, we only need to compute the sums in Eq. (2) 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. (2), even with a computer, is not possible. 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.

So the Metropolis algorithm is powerful and useful. It is also easy. 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 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, then we flip the spin with probability $p = e^{-\Delta E/k_B T}$.

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.