Ising Ferromagnetism

Original writeup by Dr. Dennis Ugolini (adapted by Dr. Lewis)
Reference: *Introduction to Thermal Physics* by D. Schroeder, chapter 8.

Let's get some physics fundamentals out of the way. First, the mechanics of magnetic dipoles:

- An atom can be treated as a magnetic dipole.
- A magnetic dipole with magnetic moment μ in a magnetic field B will have a potential energy $U = -\mu B \cos\theta$, where θ is the angle between the dipole and the field ($\theta = 0$ means the two are parallel).
- The torque on the dipole will be $F \times r = \mu B \sin\theta$. $F = 0$ at $\theta = 0$ or π (parallel or antiparallel), so the dipole will be stable at these points.
- Thus an atom will tend to have a potential energy of $U = -\mu B$ (parallel, low-energy state) or $U = \mu B$ (antiparallel, high-energy state).

We'll also need the idea of a Boltzmann factor from statistical mechanics – the probability of a system being in a state with energy E is related to $e^{-E/kT}$

In most materials, the magnetic dipole moments of the atoms are scattered in all directions. When a magnetic field is applied, the atoms have a little freedom to move, and try to align with the field, thus resulting in a weak overall magnetic moment. This is paramagnetism.

But in some materials, the magnetic moment of a given atom is affected by the alignment of its neighbors. This will cause large blocks of atoms to all align in the same direction, resulting in a strong magnetic moment even when an external field is not applied. This is ferromagnetism.

We'd like to model this effect, as well as another observed behavior -- above a certain critical temperature, the thermal excitation of the atoms is enough to overcome the coupling to its neighbors, and no overall magnetic moment is present. Can we come up with a simple simulation that shows ferromagnetic behavior, and gives us the critical temperature?

Let's take our ferromagnet to be a two-dimension square grid of atoms, each aligned up (white) or down (black). We will also say that only an atom's four closest neighbors (horizontally and vertically) affect its alignment. This leaves five possibilities for the initial potential energy of our atom (note that I'm using units where $\mu = B = k = 1$):

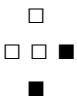
A. All four antiparallel

■
■ □ ■ U = +4 (highest energy state)
■

B. Three antiparallel

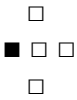
■
■ □ ■ U = +2
□

C. Two parallel



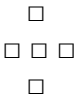
U = 0

D. Three parallel



U = -2

E. All four parallel



U = -4 (lowest energy state)

Let's say we pick one of the dipoles in our grid at random, and flip its alignment over. What will the change in energy be? And what is the Boltzmann factor for this transition?

A. U from +4 to -4	Change = -8	Boltzmann factor = $e^{8/T}$
B. U from +2 to -2	Change = -4	Boltzmann factor = $e^{4/T}$
C. U from 0 to 0	Change = 0	Boltzmann factor = $e^{0/T} = 1$
D. U from -2 to +2	Change = +4	Boltzmann factor = $e^{-4/T}$
E. U from -4 to +4	Change = +8	Boltzmann factor = $e^{-8/T}$

Or in general, if n of the atom's neighbors are aligned parallel to its original state, the Boltzmann factor for a flip in dipole alignment (and thus the probability of that transition) will be $e^{-2n/T}$.

So let's make an assumption. If the Boltzmann factor is greater than or equal to one, we'll say that the atom will happily flip, since it is moving from a higher energy state to a lower (or equal) energy state. If it is less than one, we'll pick a random number from zero to one. If it is less than the Boltzmann factor, the atom will flip; even though it's moving to a higher energy state, random thermal fluctuations are allowing the transition.

To begin this project you will code a model based on this description. Here's how it could be set:

- Randomly initialize each cell in a square grid to "up" or "down" (10x10 runs in a reasonable amount of time).
- Set up a "for" loop from 1 to (large number × grid size). For example, in a 10x10 grid, I might loop from 1 to 10000, so that each cell in the grid will be chosen 100 times.
- Choose a cell at random, and check the alignment of its neighbors.
- If two or more neighbors are antiparallel, flip the cell. If one or none, if a random number is less than the Boltzmann factor, flip it anyway.
- Display the new grid, and iterate the loop.

Make it so that your routine can handle grids of different sizes and play with some larger

grids as well as the 10x10 one that you start with. Make sure that the temperature is also a parameter that you can vary since that it what you will be doing below. You have to take a bit of care in how you deal with the edges. If you pick a cell at the edge, you should compare it to "neighbors" that are wrapped around on the other side.

After you have this working we want to turn to answering the question, "What is the critical temperature at which the spins no longer align?" Your first attempt at this will be done by just running your code with several different values of T to get a rough estimate of the value. Basically, if the fields mostly all align then you are below the critical value and if they don't then you are above it.

Once you have a rough estimate, you will edit your code so that you can get a more accurate measure. Try to do this in two ways. One is by measuring a cluster size. That is, how many cells with the same spin are clustered together on average? Plot that as a function of T to see where the transition is. You can also check to see what fraction of your "flips" actually flip the spin of the atom. Above the critical temperature, most of the checks you do will actually end up in flips. You can plot the number of flips in a certain number of checks as a function of T as another test of the critical temperature.