

## Project 8.2 Modeling ferromagnetism

The *Ising model* is a model of a ferromagnet at a microscopic scale. Each atom in the magnet has an individual polarity, known as spin up (+1) or spin down (−1). When the spins are random, the material is not magnetic on its own; rather, it is paramagnetic, only becoming magnetic in the presence of an external magnetic field. On the other hand, when the spins all point in the same direction, the material becomes ferromagnetic, with its own magnetic field. Each spin is influenced by neighboring spins and the ambient temperature. At lower temperatures, the spins are more likely to “organize,” pointing in the same direction, causing the material to become ferromagnetic.

This situation can be modeled on a grid in which each cell has the value 1 or −1. At each time step, a cell may change its spin, depending on the spins of its four neighbors and the temperature. (To avoid inconvenient boundary conditions, treat your grid as if it wraps around side to side and bottom to top. In other words, use modular arithmetic when determining neighbors.)

Over time, the material will seek the lowest energy state. Therefore, at each step, we will want the spin of an atom to flip if doing so puts the system in a lower energy state. However, we will sometimes also flip the spin even if doing so results in a higher energy state; the probability of doing so will depend on the energy and the ambient temperature. We will model the energy associated with each spin as the number of neighbors with opposing spins. So if the spin of a particular atom is +1 and its neighbors have spins −1, −1, +1, and −1, then the energy is 3. Obviously the lowest energy state results when an atom and all of its neighbors have the same spin.

The most common technique used to decide whether a spin should flip is called the *Metropolis algorithm*. Here is how it works. For a particular particle, let  $E_{\text{old}}$  denote the energy with the particle’s current spin and let  $E_{\text{new}}$  denote the energy that would result if the particle flipped its spin. If  $E_{\text{new}} < E_{\text{old}}$ , then we flip the spin. Otherwise, we flip the spin with probability

$$e^{-(E_{\text{new}} - E_{\text{old}}) / T}$$

where  $e$  is Euler’s number, the base of the natural logarithm, and  $T$  is the temperature. Implement this simulation and visualize it using the turtle graphics functions provided for the Game of Life. Initialize the system with particles pointing in random directions. Once you have it working, try varying the temperature  $T$  between 0.1 and 10.0. (The temperature here is in energy units, not Celsius or Kelvin.)

**Question 8.2.1** *At what temperature (roughly) does the system reach equilibrium, i.e., settle into a consistent state that no longer changes frequently?*

**Question 8.2.2** *As you vary the temperature, does the system change its behavior gradually? Or is the change sudden? In other words, do you observe a “phase transition” or “tipping point?”*

**Question 8.2.3** *In the Ising model, there is no centralized agent controlling which atoms change their polarity and when. Rather, all of the changes occur entirely based on an atom’s*

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*local environment. Therefore, the global property of ferromagnetism occurs as a result of many local changes. Can you think of other examples of this so-called emergent phenomenon?*