Lecture Notes for PHYS 527 Fall 2007

Deirdre Shoemaker

12 Lecture: Ising Model

Just as electrical current flowing in a loop produces a magnetic field, the motion of electrons around a nucleus can produce a tiny magnetic field. In ordinary matter, these little atomic magnets point in random directions, thus canceling out the overall effect. In some materials, like iron, it is possible for the magnets to line up given a non-zero total magnetic field. Two principles are in play

> Energy Minimization: interactions between atomic-scale magnets (called spins) are such that the lowest energy configurationhas the spins aligned. This would imply that the lowest energy state of a chunk of matter will have aligned spins and thus a huge B.
>
> Energy Maximization: The configuration in which all the spins align is a special case out of a huge number of possible configurations. The sheer number of unaligned configurations will swamp the unique ground state of a macroscopic system. The randomness (entropy) of the system washes out the predicted B from the above energy consideration.

Temperature is the key.

- The existence of any macroscopic magnetic field will depend on the relative importance of the minimization versus maximization.
- Let s denote the particular state of each of N spins.
- We assume that N is very large and is in thermal equilibrium.
- The probability that s is in a particular state is given by the Boltzmann probability distribution function:

  $$P[s] = \frac{e^{-E(s)/kT}}{\sum_A e^{-E(A)/kt}}$$

  where $E(s)$ is the energy of the system when it is in state s. T is the temperature of the system, k is Boltzamnn's constant and $\sum_A$ is the sum over all possible states of the system.

- Consider two different states A and B, with $E(A) < E(B)$. The relative probability that the system is in the two states is

$$\frac{P[A]}{P[B]} = e^{-D/kt}$$

where $D = E(A) - E(B) < 0$. At higher temperatures, $kT > |D|$, the system is equally likely to exist in A or B (entropy wins). At low temperatures, the system is likely to be in the lower energy state.

The Magnet

- Ferromagnetism: aries when a collection of atomic spins align such that their associated magnetic moments all point in the same direction.
- Ferromagnets: Nickel, Iron, Cobalt: they exhibit a permanent magnetization, even in the absence of any external magnetic field, below their Curie temperature.
- At the Curie temperature, they under go a seecond-order phase transition (discontinuous in the second derivative of the energy) and loose their ferromagnetic characteristic.
- Ising Model: simplest theoretical description of ferromagnetism.
- Invented by Wilhelm Lenz in 1920, names after his graduate student (Ernst Ising), did his PhD on it in 1925.
- Ising model is a statistical mechanics theory, and uses a lattice that is evenly spaced in 1, 2 or 3 d.
- Each vertex represents a state of spin-up or spin-down
- The energy at each vertex depends on the spin-state of its nearest neighbors
- This means it is energy-favorable for the spins to be aligned.
- If an external magnetic is introduced, it is favored for the spins to align with its field.

The Model

- evenly space lattice of a 1d line, a 2d square lattice or a 3d cubic lattice
- each particle has spin 1/2 oriented up or down

$$s_i = \{ \begin{array}{cc} 1 & \text{if "up"} \\ -1 & \text{if "down"} \end{array}$$

- We will have N spins, $i = 1, 2, \ldots N$
- If there is an external magnetic field, B, each spin interacts with it

$$E = -B \sum_i s_i$$

- Each pair of neighbors interacts only with its neighbors

  (a) Parallel spins are favored and lower the energy
  (b) Antiparallel spins are discouraged and so raise the energy

  This leads to a total interaction between neighbors

$$E = -\frac{J}{2} \sum_i \sum_j s_i s_j$$

  where J is the coupling constant (we will take $J = 1$). The first sum is over all the particles in the lattice, the second is the sum over the ith particles nearest neighbors.

- As mentioned, the total energy depends on the spin of its neighbors

$$E = \sum_i \left(\sum_j \left(-\frac{J}{2} s_i s_j \right) - B s_i \right)$$

J and B have units of energy.

The Solution

- The Ising model has an analytic solution for the 1d case with no external magnetic field. For a single particle

$$\langle E(T) \rangle = -\frac{1}{4} tanh \left(\frac{J}{4} \beta \right)$$

$$\langle M(T) \rangle = 0$$

  The angle brackets indicate a time average, $\beta \equiv 1/(k_B T)$. This system does not undergo a phase transition.

- In 2d, there is also an analytic soln

$$\langle E(T)\rangle = 2Jtanh(2\beta J) + \frac{K}{2\pi}\frac{dK}{d\beta}\int_0^{\pi} d\phi \frac{sin^2\phi}{\Delta(1+\Delta)} \quad (1)$$

$$\langle M(T)\rangle = (1 - [sinh(1/4\beta J)]^{-4})^{1/8} \text{ for} T \leq T_c \quad (2)$$

otherise $\langle M(T)\rangle = 0$. $K = 2/cosh(2\beta J)coth(2\beta J)$ and $\Delta = \sqrt{1 - K^2 sin^2\phi}$. T_C is the Curie temperature, marking the phase transition, $k_B T_C \approx 0.5672925J$

- The phase transition is econd order, marked by a singluarity in the specific hear $c_v \equiv \frac{dE}{dT}$.

- There are limiting cases to the Ising model
  - High temperature limit: spins should be randomized, there is enough E to flip spins despite neighbors.
  - Low temperature limit: system will eventually reach a state where all spins are aligned - ground state.