

A Simple Model of Ferromagnetism

Recall way back in lecture 4 we discussed a magnetic spin system. In our discussion, we assumed spin 1/2 magnets with an energy $\pm E$ when anti-aligned or aligned with the magnetic field. We had a total of N spins and we let $2s$ be the “spin excess,” the number of aligned minus the number of anti-aligned magnets. We assumed that the magnets were weakly interacting with a thermal reservoir and with each other. We found that

$$\frac{2s}{N} = \tanh \frac{E}{\tau},$$

which gives small net alignment if $E \ll \tau$ and essentially perfect alignment if $E \gg \tau$.

It’s customary to speak of the magnetization which is the magnetic moment per unit volume, and we denote magnetic moment, not the chemical potential, by μ in this section. Then the magnetization is

$$M = \frac{N}{V} \mu \tanh \frac{\mu B}{\tau} = n \mu \tanh \frac{\mu B}{\tau},$$

where n is the concentration of elementary magnets and B is the magnetic field. Previously, we assumed that B was externally supplied. But of course, if the system has a net magnetization, it generates a magnetic field. We assume that when the magnetization is M , there is an effective field acting on each magnetic dipole proportional to the magnetization

$$B_{\text{eff}} = \lambda M,$$

where λ is a proportionality constant. This is essentially an application of the mean field approximation to get B_{eff} . In the crystal structure of a ferromagnet (or any material for that matter), the electric and magnetic fields must be quite complicated, changing by substantial amounts on the scales of atoms. We are encapsulating all our ignorance about what’s really going on in the constant λ . In any case, we now assume there is no external magnetic field, and we have

$$M = n \mu \tanh \frac{\mu \lambda M}{\tau},$$

We can rewrite this in dimensionless form with the following definitions:

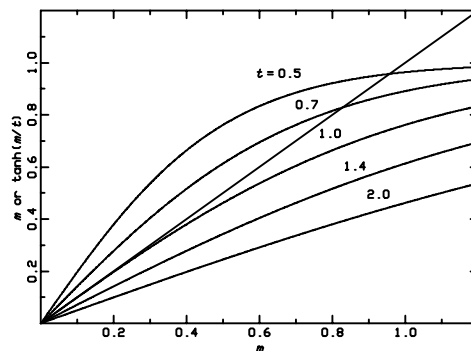
$$m = \frac{M}{n\mu}, \quad \tau_c = n\mu^2\lambda, \quad t = \frac{\tau}{\tau_c},$$

where τ_c is called the Curie temperature. With these definitions, our equation becomes

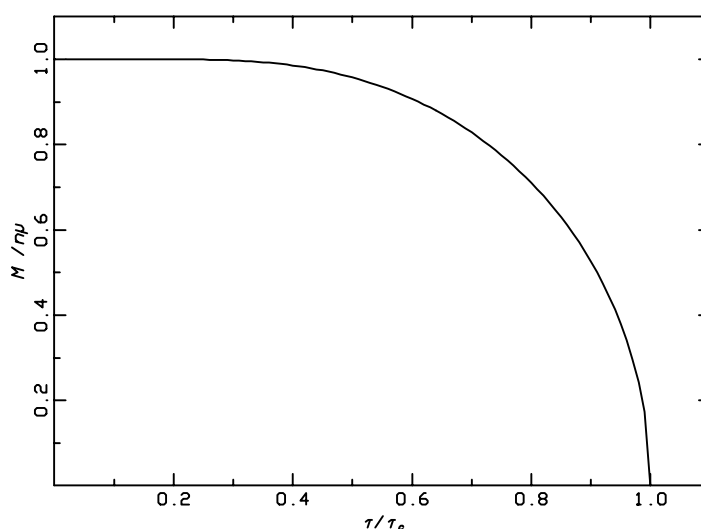
$$m = \tanh \frac{m}{t},$$

which is actually kind of remarkable. It says that at any given temperature, a magnetization occurs spontaneously.

In order to determine the spontaneous magnetization, we must solve this transcendental equation for m . The figure shows a plot of the left hand side (the straight line) and several plots of the right hand side for various values of t . At $t = 1$, the right hand side is tangent to the left hand side at $m = 0$. For $t > 1$, the curves intersect at $m = 0$. So there is no spontaneous magnetization when the temperature is greater than the Curie temperature. For $t < 1$, there is an intersection at a non-zero m which moves to larger m as t gets smaller, approaching $m = 1$ at $\tau = 0$.



The figure shows the magnetization versus temperature. For temperatures less than about a third of the Curie temperature, the magnetization is essentially complete—all the magnetic moments are lined up. This is the case for iron at room temperature. K&K show a similar plot including data points for nickel. The data points follow the curve reasonably well. Before we get too excited about this theory, we should plug in some numbers. For iron, the Curie point is $T_c = 1043$ K, the saturation magnetic field is about $B_s =$



$21,500$ G, the density is $\rho = 7.88$ g cm $^{-3}$ and the molecular weight is about 56 g mole $^{-1}$. We might also want to know the Bohr magneton, $\mu_B = 9.27 \times 10^{-21}$ G cm 3 . The Bohr magneton is almost exactly the magnetic moment of the electron. If we assume that one electron per atom participates in generating the magnetic field, we have $n = 8.47 \times 10^{22}$ cm $^{-3}$, $M = n\mu_B = 785$ G. Note also that we expect $B = 4\pi M = 9900$ G. So we are in the ballpark. Next, let's calculate T_c . To do this, we have to know λ , which hasn't entered into the calculations so far. If we assume that the smoothed field which we just calculated is the effective field acting on an electron spin, then $\lambda = 4\pi$ and $T_c = 0.66$ K, just a little on the small side! We're off by a factor of 2 in the overall magnetic field and a factor of 2000 in the Curie temperature. Perhaps more than one electron per atom participates in generating the mean field. After all, iron has 26 electrons per atom. If the electrons pair with opposite spins, an even number per atom have to wind up with the same spin. (Of course this ignores the fact that electrons are in the conduction band of the solid.) Also, λ is supposed to characterize the field acting on the aligned electrons. Since it appears that a simple estimate of λ is off by a factor of a thousand or so, there must be some complicated interactions going on in order to get an effective field this strong. These interactions are presumably due to the other electrons in the atom, in nearby atoms, and in the Fermi sea

of electrons in the metal. Without a detailed understanding of what's going at the atomic level, we can't say much more about this model.

Superconductors, the Meissner Effect, and Magnetic Energy

As you know, when some materials are cooled, they become superconductors. All resistance to the flow of electricity disappears. K&K state that superconductivity disappears for temperatures above about 20 K. This is a little out of date. In the last decade or so, high temperature superconductors were discovered (called high T_c) and the record high temperature is around 140 K. (Of course, I might be out of date, too!) The new high T_c superconductors are ceramics with anisotropic superconductivity. The old-style or normal superconductors are metals with isotropic superconductivity.

We will be talking about old-style superconductors. There are two kinds of superconductors, naturally called type I and type II! Type I superconductors completely exclude magnetic fields from their interiors when in a superconducting state. This is called the Meissner effect. Type II superconductors partially exclude magnetic field. Actually what happens is the type II superconductor organizes itself into vortex tubes with normal conductor and magnetic field in the centers of the vortices and superconductor and no magnetic field between the vortices.

We will consider type I superconductors. The Meissner effect is actually quite amazing. You will recall from E&M (or you will learn when you take physics 304) that you can't get a magnetic field inside a perfect conductor. If you try, then by Lenz' law the induced currents create an induced magnetic field opposite to the one you're trying to push into the conductor. In the case of a perfect conductor, the currents are sufficiently large to exclude the field from the interior of the conductor. So if you have a superconductor (in its superconducting state) and you try to move it into a region of magnetic field, you might not be surprised that the magnetic field is excluded. But, suppose you start with a superconductor in its normal state, warm, and you turn on a magnetic field. There is no problem with having a static magnetic field in a good, but not perfect, conductor. Now cool the superconductor until it becomes superconducting. When it makes the transition to the superconducting state, the magnetic field pops out leaving no magnetic field in the interior. This cannot be explained by Lenz' law plus a perfect conductor. It's a property of the superconducting phase.

As you can imagine, it costs energy to expel the magnetic field from the interior of the superconductor. The system is in a superconducting state because the free energy in the superconducting state is lower than the free energy in the normal state. But the energy cost of excluding the magnetic field can make the normal state the minimum energy state. What's actually observed is that at the transition temperature, superconductivity is destroyed by a very small magnetic field. As the temperature is lowered, it takes a larger and larger magnetic field to destroy the superconductivity. The increase in free energy of

a superconductor upon excluding a magnetic field B must just be the energy required to create a field of $-B$ inside the super conductor. This energy is just

$$\Delta U = VB^2/8\pi ,$$

or $B^2/2\mu_0$ if you really want SI units! So the critical field will be determined by

$$\frac{1}{V}(F_N(\tau) - F_S(\tau)) = \frac{B_c^2(\tau)}{8\pi} ,$$

where F_N is the free energy of the normal state (which doesn't change much with a magnetic field present) and F_S is the free energy of the superconducting state in the absence of a magnetic field. For fields larger than B_c , the free energy of the normal state with magnetic field is less than the free energy of the superconducting state with excluded field and the normal state is the equilibrium state. In K&K chapter 8, you'll find some plots of the critical field versus temperature for various superconductors.

The Ising Model

In the mean field theory of ferromagnetism, we attempt to account for the interactions of the magnetic dipoles by considering the "global mean field." Our only allowance for the microscopic structure of the atoms was the proportionality factor λ which related the field acting on a dipole to the mean field.

In the Ising model, we go to the other extreme! We assume that all the interaction comes from nearest neighbors and that far away electrons, atoms, or molecules have no direct effect.

The idea is that there is an extra interaction energy due to the magnetic dipoles (in addition to whatever else is going on in the material). Furthermore, the dipoles are arranged on a regular lattice. The extra energy is taken to be

$$U = -\frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} J_{ij} \sigma_i \sigma_j - \mu B \sum_i \sigma_i ,$$

where the factor of 1/2 is a double counting correction, $\sigma_i = \pm 1$ is proportional to the spin of the electron, B is an external, constant magnetic field, μ is the electron magnetic moment as we've had before and J_{ij} represents the magnetic interaction between electrons i and j . Note that even at this point, we've already simplified things greatly. In particular, we've taken "scalar spins." Presumably, an exact quantum mechanical treatment would consider $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_j$, that is, a vector treatment of the spins which would also include how the spins are aligned with respect to the line joining them. But, we're going to sweep all that under the rug and just assume that the product of the spins gives ± 1 . Note: a

model in which the interaction energy is proportional to $\sigma_i \cdot \sigma_j$ but still ignoring terms like $\sigma_i \cdot \mathbf{r}_{ij}$, is known as the Heisenberg model.

An additional simplification is the following, In general, we take J_{ij} to be 0 if the dipoles are not nearest neighbors and the single constant J if they are. Thus every pair of nearest neighbor dipoles contributes either $+J$ or $-J$ to the energy. When looking for spontaneous magnetization, we will take $B = 0$. However, a non-zero B can be included if it's desired to see how an external field affects the phase transition.

A bit of history: the Ising model was first proposed in 1920 by Lenz. His PhD student was Ising who in 1925 showed that (what is now called) the Ising model had no phase transition in one dimension. Since the original proposal was motivated by the desire to study a phase transition, this was not a good sign and not much happened for a while. In the 1940s, 50s and 60s, people returned to the model and analytic solutions were obtained for the Ising model on a two dimensional square lattice. It turns out there is a phase transition in this case. The three dimensional Ising model has not been solved analytically. Nor has the 2D model with a non-zero B . However, with computers, it's possible to tackle the Ising model numerically and folks have had a lot of fun playing with the model in the last couple of decades (that is, after K&K was published!).

Ernst Ising died in 1998 and an obituary appeared in *Physics Today*.

Perhaps by now, you've figured out that the Ising model is extremely difficult to solve. What does it mean to solve the Ising model? Answer: we would like to calculate the partition function from which we can calculate the free energy, entropy, specific heat, and so on as a function of temperature. If the model is a good representation of a phase transition, we should be able to see some kind of change in its properties on either side of the critical temperature.

A rather advanced discussion of analytic techniques applied to the Ising model is given in H. S. Robertson, 1993, *Statistical Thermophysics*, (New Jersey: Prentice Hall), chapter 7. The mathematics involved is beyond the scope of this course. However, a couple of results can be quoted. First, the 1D Ising model has no phase transition. Second, the 2D square lattice Ising model (4 nearest neighbors) has a phase transition at $\sinh(2J/\tau_c) = 1$ which gives $\tau_c = 2.269J$. Other results (for example, a plot of the heat capacity) may be found in this reference.

There is also a considerable amount of information about the Ising model on the web. In particular, there are a number of Java applets that do interesting Monte Carlo calculations of a 2D Ising model. Many of these let you set the parameters. Since you know where the critical temperature is, you can set the parameters appropriately if you play with any of these models. A good place to start is

<http://oscar.cacr.caltech.edu/Hrothgar/Ising/index.html> .

What is a Monte Carlo calculation? The basic features involve the following. Set up a 2D lattice (2D array in your code) of spins. Each spin can have the value ± 1 . To start, one might as well choose the values randomly (very hot) or all the same (extremely cold). Pick a value for J . Pick a value for τ . Now make a pass through the lattice. A pass might consist of visiting each spin in turn or it might consist of visiting a number of the spins chosen randomly. As each spin is visited, calculate the difference in energy between having the spin up and having the spin down. Then choose the orientation of the spin randomly so that the probability ratio is a Boltzmann factor:

$$\frac{P(\text{up})}{P(\text{down})} = e^{-(E_{\text{up}} - E_{\text{down}})/\tau} .$$

In other words, each spin is numerically placed in thermal contact with a heat bath at temperature τ . Successive passes correspond to time passing. Since the system is finite (very finite!), relatively large fluctuations in quantities such as the average energy of the system are expected.

If you play with some of the simulations on the net, you will observe the following. At $\tau = 0$, the system is in the ground state—all the spins are either $+1$ or -1 , but in the absence of other influences, either case is equally likely, so there are two ground states. Note that the energy is $U_0 = -2NJ$ if each spin has four nearest neighbors. At very high temperatures, each spin is equally likely to be $+1$ or -1 , so the average energy is 0. Of course you didn't need any simulations to know the preceding—but what happens in the neighborhood of the transition temperature? The simulations show that big patches containing all one orientation of spin form. It's sometimes described as “the system can't make up its mind what it wants to do.” (A rather anthropomorphic statement, don't you think?) In any case, just above the transition temperature, the patches tend to fluctuate but remain the same size (at a given temperature). Below the transition temperature, patches of one orientation tend to win out. This effect becomes stronger as the temperature is lowered.