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Statistical Mechanics: Lecture A1

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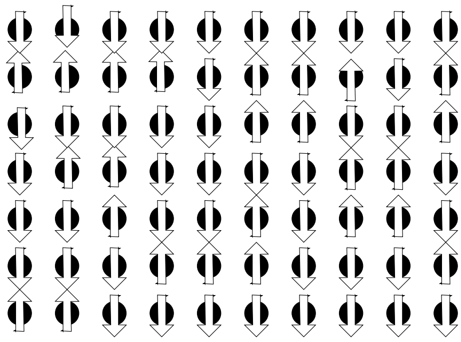
The Ising Model

One of the most interesting phenomena in the physics of the solid state is ferromagnetism. In some metals, e.g., Fe and Ni, a finite fraction of the spins of the atoms align spontaneously in the same direction to give a macroscopic magnetic field. This, however, happens only when the temperature is lower than a characteristic temperature known as Curie temperature. Above the Curie temperature the spins are oriented at random, producing no net magnetic field. Another feature associated with the is phenomenon is that as the Curie temperature is approached either from above, or from below, the *specific heat* of the metal approaches infinity.

The Ising model is a crude attempt to simulate the physics of a ferromagnetic substance. Its main virtue lies in the fact that the two dimensional Ising model yield to an exact treatment in statistical mechanics. It is the only nontrivial example of a phase transition that can be worked out with mathematical rigour.



In the Ising model the system considered is an array of N fixed sites form a periodic lattice which could be 1-, 2- or 3-dimensional. The geometric structure of the lattice could be anything, cubic, hexagonal or whatever one may want. Each lattice site has a spin variable denoted by S_i, which is a *number* that is either +1 or -1. If one is more inquisitive, this variable could represent the eigenvalue of the z-component of a spin$-\frac{1}{2}$. If $S_i = +1$, the spin is said to be *up*, and if it is $S_i = -1$, the spin is said to be down. A given set of numbers $\{S_i\}$ specifies a configuration of the whole system. The energy of the system in the configuration specified by $\{S_i\}$ is defined to be

$$E\{S_i\} = -\frac{1}{2}\sum_{i\neq j} J_{ij} S_i S_j - B\sum_{i=1}^{N} S_i \tag{1}$$

where J_{ij} denotes the strength of interaction between the i'th and the j'th spin, B denotes an external magnetic field, which could be present. The factor of $1/2$ is introduced to account for double-counting in unrestricted sum over i and j (i=3,j=8 and i=8,j=3 both represent the interaction between the 3rd and 8th spin). The quantity J_{ij} is actually the *exchange interaction* between the two magnetic atoms. The magnetic interaction between the two magnetic atoms is too weak to give rise to ferromagnetism.

A simpler version of Ising model is generally used, where all J_{ij}s are assumed to be equal, and each spin interacts only with its nearest neighbours

$$E\{S_i\} = -\frac{J}{2}\sum_{<ij>} S_i S_j - B\sum_{i=1}^{N} S_i \tag{2}$$

where $<ij>$ represents a sum over only the *nearest-neigbours*, One can easily see that the macroscopic magnetic moment for the whole system, for a particular spin configuration, will be given by

$$M\{S_i\} = \sum_{i=1}^{N} S_i \tag{3}$$

Statistical Mechanics of Ising Model

Our aim is to calculate various macroscopic thermodynamic quantities using statistical mechanics. Statistical mechanics is what connects microscopic physics to theromdynamics. The canonical partition function can be written as

$$Z = \sum_{S_1,S_2,...S_N} \exp(-\beta E\{S_i\}), \tag{4}$$

where the summation $\sum_{S_1,S_2,...S_N}$ denotes sum over all *microstates*, which happen to be all possible values all the spins. The canonical density matrix can also be written easily:

$$\rho\{S_i\} = \frac{1}{Z}\exp(-\beta E\{S_i\}) \tag{5}$$

The average value of a quantity, say, $A\{S_i\}$ associated with the Ising system can then be calculated as

$$\begin{aligned}\langle A\rangle &= \sum_{S_1,S_2,...S_N} \rho\{S_i\}A\{S_i\}) \\ &= \frac{1}{Z}\sum_{S_1,S_2,...S_N} A\{S_i\}\exp(-\beta E\{S_i\}),\end{aligned} \tag{6}$$

Let us use this equation to write some average quantities of interest. Average energy of the system is given by

$$\langle E\rangle = \frac{1}{Z}\sum_{S_1,S_2,...S_N} E\{S_i\}\exp(-\beta E\{S_i\}), \tag{7}$$

This can be cleverly recast in the following form.

$$\begin{aligned}\langle E\rangle &= -\frac{1}{Z}\frac{\partial}{\partial\beta}\sum_{S_1,S_2,...S_N} \exp(-\beta E\{S_i\}) \\ &= -\frac{1}{Z}\frac{\partial}{\partial\beta}Z \\ &= -\frac{\partial\log(Z)}{\partial\beta}\end{aligned} \tag{8}$$

Specific heat can then be calculated as

$$C = -\frac{\partial}{\partial T}\frac{\partial\log(Z)}{\partial\beta} \tag{9}$$

Average magnetization of the system is given by

$$\langle M\rangle = \frac{1}{Z}\sum_{S_1,S_2,...S_N} M\{S_i\}\exp(-\beta E\{S_i\}), \tag{10}$$

One look at equation (2) suggests that this can be recast into the form:

$$\begin{aligned}\langle M\rangle &= \frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial B}\sum_{S_1,S_2,\dots S_N}\exp(-\beta E\{S_i\}) \\ &= \frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial B}Z \\ &= \frac{1}{\beta}\frac{\partial\log(Z)}{\partial B}\end{aligned} \tag{11}$$

Remembering that the Helmholtz free energy is given by $F = -k_B T\log(Z)$, the above relation can be written as

$$\langle M\rangle = -\frac{\partial F}{\partial B} \tag{12}$$

Magnetic susceptiblity can then be calculated as

$$\chi = \frac{1}{\beta}\frac{\partial^2\log(Z)}{\partial B^2} \tag{13}$$

One notices that the quantity of central interest is $\log(Z)$. So let us go about calculating it.

$$Z = \sum_{S_1,S_2,\dots S_N}\exp\left(\frac{\beta J}{2}\sum_{<ij>}S_iS_j + \beta B\sum_{i=1}^{N}S_i\right) \tag{14}$$

Evaluating Z is not easy, because the S_iS_j term makes sure that the sums over different S_i and S_j cannot be carried out independently.

A paradox: breakdown of ergodicity

The way magnetization in a configuration is defined by (3), if one flips every spin, it is easy to see that the magnetization will change sign, but its magnitude will not change. So for every value of M, there is another configuration which has magnetization $-M$. Suppose there is no external field ($B = 0$). In that case the expression for energy E, given by (2), tells us that the energy of the system does not change if all the spins are flipped. Of course, if you leave out flipping even one spin, the energy changes. So, for every configuration with a magnetization M and energy E, there is another configuration which has magnetization $-M$ but the same energy E. Since the energy of the two configurations is the same, the probability of the two configurations, $e^{-\beta E}/Z$, is also the same. So when one calculates the average magnetization using (10), the term for every M is exactly canceled by another term with magnetization $-M$. The net result is that average magnetization is zero. We know that at higher temperatures magnetization for all magnetic materials is zero. However, the above argument is independent of temperature, and implies that average magnetization will be zero at all temperatures! However, we do know that ferromagnetic materials show spontaneous magnetization at low enough temperatures. So where is the catch?

What actually happens is that at low enough temperatures, when all spins are (say) up, the system cannot wander off to the configuration where all spins are down, just by random flipping of a few spins. The system is *trapped* in the mode where the spins are predominently up. So, there are configurations which the system never attains, or in other words, there are parts of the phase space which the system never visits. The system is no longer ergodic! So the time-average of any quantity may not be the same as ensemble average. The ensemble average says that the average magnetization is zero, whereas the time-average of magnetization is not zero. This indicates a breakdown of ergodicity. But ergodic hypothesis is a central pillar of statistical mechanics. How does one reconcile the breakdown of ergodicity with using statistical mechanics for studying phase transitions? The answer is that one should tread carefully here, keeping in mind the possible breakdown of ergodicity. For example, if we have a nonzero B, we will not run into the problem of getting zero magnetization at all temperatures. This paradox teaches us about breakdown of ergodicity which is always associated with a phase transtion. A phase transition may not always lead to a breakdown of symmetry, but it will still show breakdown of egodicity.

Mean Field Theory

In the following we will carry out an approximate treatment of the Ising model. Let us rewrite the energy for the Ising model in a suggestive form:

$$E\{S_i\} = -\frac{J}{2}\sum_i S_i \sum_{<j>_i} S_j - B\sum_{i=1}^{N} S_i \tag{15}$$

where we have split the sum over pairs into a sum over all the i sites and the nearest neigbours of i, $<j>_i$. The term $\sum_{<j>_i} S_j$ can be thought to be a *local magnetic field*, because of the neighbouring spins, acting on the spin S_i. Needless to say that this local field varies from site to site, because spin states vary from site to site. It depends on the configuration of nearest neigbour spins of that particular site.
Now we make an approximation that **the local field acting on all the sites is the same**. Mathematically this can be written as

$$\sum_{<j>_i} S_j = \gamma m, \tag{16}$$

where γ is the number of nearest neigbours of spin S_i and m is the average magnetization per spin of the system. It should be emphasized that the quantity m is yet to be calculated from the relation $m = \langle M\rangle/N$. Using this approximation, the energy of the Ising model now assumes the following form.

$$\begin{aligned} E\{S_i\} &= -\frac{Jm\gamma}{2}\sum_{i=1}^{N} S_i - B\sum_{i=1}^{N} S_i \\ &= -(\frac{Jm\gamma}{2} + B)\sum_{i=1}^{N} S_i \end{aligned} \tag{17}$$

Let us calculate the partition function using this simpler form of the energy. Z now assumes the form

$$
\begin{aligned}
Z =& \sum_{S_1, S_2, \ldots S_N} \exp\left(\beta(\frac{Jm\gamma}{2} + B)\sum_{i=1}^{N} S_i\right) \\
=& \sum_{S_1, S_2, \ldots S_N} \prod_{i=1}^{N} \exp\left(\beta(\frac{Jm\gamma}{2} + B)S_i\right) \\
=& \prod_{i=1}^{N} \sum_{S_i=-1}^{+1} e^{\beta(\frac{Jm\gamma}{2}+B)S_i} \\
=& \prod_{i=1}^{N} 2\cosh\left(\beta(\frac{Jm\gamma}{2} + B)\right) \\
=& \left[2\cosh\left(\beta(\frac{Jm\gamma}{2} + B)\right)\right]^N
\end{aligned} \tag{18}
$$

Therefore, $\log(Z)$ is given by

$$
\log(Z) = N\log(2) + N\log\left[\cosh\left(\beta(\frac{Jm\gamma}{2} + B)\right)\right]. \tag{19}
$$

Now we are all set to calculate any quantity. Let us start by evaluating the average magnetization of the system

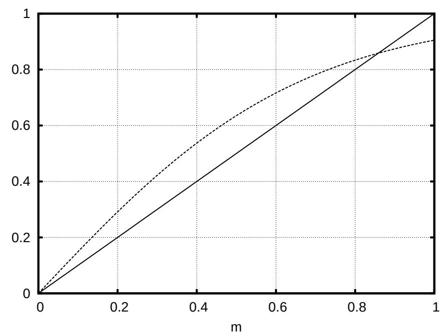
$$
\begin{aligned}
\langle M\rangle =& -\frac{1}{\beta}\frac{\partial\log(Z)}{\partial B} \\
=& N\tanh\left[\beta(\frac{Jm\gamma}{2} + B)\right].
\end{aligned} \tag{20}
$$

But $\langle M\rangle/N = m$, which leads to

$$
m = \tanh\left[\beta(\frac{Jm\gamma}{2} + B)\right]. \tag{21}
$$

This is a trancendental equation, which is not easy to solve. We are looking for spontaneous magnetization, i.e., magnetization without an external magnetic field. For $B = 0$ the equation reduced to

$$
m = \tanh(\beta Jm\gamma/2). \tag{22}
$$



One can look for a solution by plotting the L.H.S. and R.H.S. of this equation on the same graph. The points where the two curves intersect, will be the solutions of the above equation. One such plot is shown in the figure. It is clear that for some values of J, γ, β, a nonzero value of m is a solution. This shows that Ising model yields spontaneous magnetization even in the mean-field approximation.

Let us try to find out an analytical expression for m in some approximation. can have small non-zero value. Expanding $\tanh$ in a series for small argument and for $B = 0$, we obtain,

$$m \approx \beta J m\gamma/2 - (\beta J m\gamma/2)^3/3 \tag{23}$$

Denoting $T_c = J\gamma/2k$, we can rewrite the above equation as

$$m \approx m\left(\frac{T_c}{T}\right) - \left(\frac{T_c}{T}\right)^3 \frac{m^3}{3} \tag{24}$$

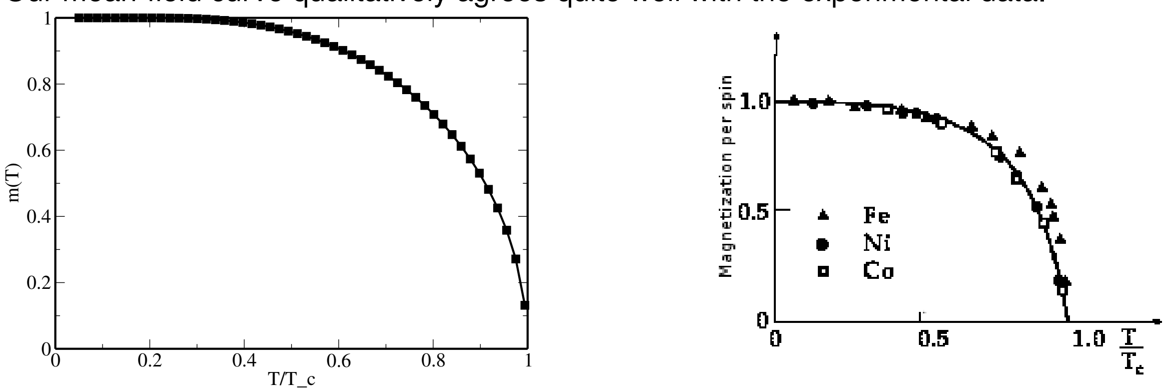
One solution of this equation is $m = 0$, and the other one is

$$m = \pm\sqrt{3}\left(\frac{T}{T_c}\right)\left(1 - \frac{T}{T_c}\right)^{1/2} \tag{25}$$

where $T_c = \gamma J/2k$ can now be identified as a critical temperature. At temperatures close to T_c, we can approximate the above relation as

$$\boxed{m \approx \pm\sqrt{3}\left(1 - \frac{T}{T_c}\right)^{1/2}} \tag{26}$$

This relation implies that at temperature goes below T_c, the magnetization starts from zero, and grows as $(1 - T/T_c)^{1/2}$, even in the absence of an external field. Generally speaking, the order parameter in a phase transition, close to the transition temperature, goes as $\psi = (1 - T/T_c)^\beta$, where β is a critical exponent. Ising model in mean field theory, yields $\beta = 0.5$. Real experiments on ferromagnetic materials show that $\beta \approx 0.33$. So, our simplified model gives a value of β which is not drastically different from the experimental value. This shows that the Ising model, despite its simplicity, captures the essential physics of phase transitions.
We will now attempt at determining the behavior of magnetization m at all temperatures below T_c. Equation (22) can be written as $m = \tanh(mT_c/T)$. We can obtain m by numerically finding the zeros of the function $\tanh(mT_c/T) - m$, for various values of T. This can be done through a simple computer program using bracketing and bisection, and the result is displayed in the figure on the left below. Compare this with the experimental data of three ferromagnets, iron, nickel and cobalt, shown in the figure on the right below. Our mean-field curve qualitatively agrees quite well with the experimental data.



A better agreement is expected if the Ising model is solved without approximations, or with a better approximation.

Magnetic susceptibility

Let us now look at the magnetic susceptibility of the Ising model. To do that we should look at the case $B \neq 0$. Equation (21) can be written as

$$m = \tanh\left(\frac{mT_c}{T} + \frac{B}{kT}\right). \tag{27}$$

Magnetic susceptibility is defined as $\chi = \frac{\partial m}{\partial B}\Big|_{B=0}$. We differentiate both side of the above equation with respect to B

$$\begin{aligned}\frac{\partial m}{\partial B} &= \frac{\partial}{\partial B}\tanh\left(\frac{mT_c}{T} + \frac{B}{kT}\right)\\ &= \left(\frac{\partial m}{\partial B}\frac{T_c}{T} + \frac{1}{kT}\right)\frac{1}{\cosh^2\left(\frac{mT_c}{T} + \frac{B}{kT}\right)}\end{aligned} \tag{28}$$

Putting $B = 0$ on both sides, we get

$$\chi = \left(\chi\frac{T_c}{T} + \frac{1}{kT}\right)\frac{1}{\cosh^2\left(\frac{mT_c}{T}\right)} \tag{29}$$

For $T > T_c$, without any external field, the magnetization m is zero. The above equation then simplifies to yield

$$\boxed{\chi = \frac{1}{k}\cdot\frac{1}{T - T_c}} \tag{30}$$

This is the well-know Curie-Weiss law, which is valid for temperatures above the transition temperature. For $T < T_c$, m has no closed form and hence an analytical expression for χ cannot be obtained.