Lecture 32 - Ising model

What's Important:

- Ising model in 3D

Text: Reif

Ising model

In the previous lecture, we considered the effects of dimensionality on the existence of phase transitions, using a spin system as an example. Let's now examine the properties of this system, which is called the Ising model, in three dimensions.

Comments:

- The Ising model in two dimensions has been solved exactly by Onsager, although the proof is difficult.
- Reif also considers systems subject to magnetic fields, and extends the results here for spin - 1/2 to systems with general spin S.

One form often used to represent the interaction energy between two objects with spin vectors $\mathbf{S}_j$ and $\mathbf{S}_k$ is the so-called **Heisenberg** model

$$[energy] \quad -2J\, \mathbf{S}_j \bullet \mathbf{S}_k \qquad \text{(Heisenberg)} \qquad (32.1)$$

where

- $J > 0$ makes the interaction attractive
- the factor of 2 is chosen to ease the normalization later.

This form also appears for systems where the energy is proportional to the sum of spin vectors, via the identity

$$(\mathbf{S}_j+\mathbf{S}_k)^2 = 2S^2 + 2\mathbf{S}_j \bullet \mathbf{S}_k.$$

The restricted form of Eq. (32.1) is called the **Ising** model, which depends only on the z-components of the spin vectors:

$$[energy] \quad -2J\, S_{jz} \bullet S_{kz} \qquad \text{(Ising)} \qquad (32.2)$$

The Hamiltonian for an Ising system is thus

$$\begin{aligned} H &= \frac{1}{2}\left(-2J\sum_{j=1}^{N}\sum_{k=1}^{n} S_{jz}S_{kz}\right) \\ &= -J\sum_{j=1}^{N}\sum_{k=1}^{n} S_{jz}S_{kz} \end{aligned} \qquad \text{(Ising)} \qquad (32.3)$$

where:

- N is the total number of particles
- n is the number of interacting neighbours, usually restricted to nearest neighbours
- the first factor of 1/2 arises because of double-counting in the summations.

To solve this problem, we invoke the mean field approximation (or molecular field approximation) which assumes that each spin experiences an environment equal to the average of the system as a whole:

↑↓↑↑
↑↑↓↑ = (↑ • average)$_1$ + (↓ • average)$_2$ + (↑ • average)$_3$ +... (N particles)
↓↑↑↓

The energy of particle j is then

$$\begin{aligned} H_j &= -2JS_{jz}\sum_{k=1}^{n} S_{kz} \\ &= -2nJS_{jz}\bar{S}_z \end{aligned} \qquad (32.4)$$

where the average spin in the z-direction, averaged across the whole system is

$$\bar{S}_z = \frac{1}{N}\sum_{k=1}^{N} S_{kz} \,. \qquad (32.5)$$

The factor of n in Eq. (32.4) arises because there are n interactions for particle j.

The average spin is determined by self-consistency, as we now demonstrate for a spin-1/2 system.

Spin - 1/2 Ising model

Under the mean field approximation Eq. (32.4) gives the energy experienced by particle j according to its spin orientation. But we can use statistical mechanics to calculate the mean spin from the Boltzmann weight. That is

$$\bar{S}_z = \frac{\frac{1}{2}e^{-ßH_+} - \frac{1}{2}e^{-ßH_-}}{e^{-ßH_+} + e^{-ßH_-}} \qquad (32.6)$$

where

$$\begin{aligned} H_+ &= -2nJ\bar{S}_z\left(+\tfrac{1}{2}\right) = -nJ\bar{S}_z \\ H_- &= -2nJ\bar{S}_z\left(-\tfrac{1}{2}\right) = +nJ\bar{S}_z \end{aligned} \qquad (32.7)$$

In other words, $\bar{S}_z$ depends on H_+ and H_- according to Eq. (32.6), but H_+ and H_- also depend on $\bar{S}_z$ according to Eq. (32.7). This provides the self-consistency condition for determining $\bar{S}_z$.

To simplify the notation, we define

$$\eta \equiv 2ßnJ\,\bar{S}_z$$

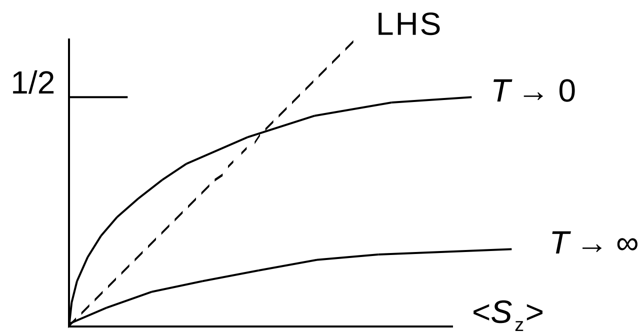
so that

$$ßH_+ = -\eta\bar{S}_z/2 \qquad\qquad ßH_- = +\eta\bar{S}_z/2,$$

from which

$$\bar{S}_z = \frac{\frac{1}{2}e^{\eta/2} - \frac{1}{2}e^{-\eta/2}}{e^{\eta/2}+e^{-\eta/2}} = \frac{1}{2}\cdot\frac{2\sinh(\eta/2)}{2\cosh(\eta/2)} = \frac{1}{2}\tanh(\eta/2) \qquad (32.8)$$

We resort to a graphical method to determine the solution to this equation by plotting both the left hand side and right hand side as a function of $\bar{S}_z$



The left hand side is pretty simple - it's just the dashed line at 45°. In contrast, the right hand side is temperature-dependent (or η dependent)

asymptotic limit for all temperatures at large η : $\tanh\theta \rightarrow 1$
RHS = (1/2)tanhη/2 $\rightarrow$ 1/2

initial slope of RHS at small η: $\tanh\theta \rightarrow \theta$
RHS = (1/2)tanhη/2 $\rightarrow$ (1/2)•(η/2) = $(nJ\beta/2)\bar{S}_z$
slope = $nJ / (2k_B T)$
large at small temperature
small at large temperature.

The behavior of the RHS is now easy to see.

- Low temperature: initial slope is large, RHS intersects LHS at finite $\bar{S}_z$, system is partially ordered
- High temperature: initial slope is small, RHS intersects LHS only at $\bar{S}_z = 0$, system is disordered.

The critical temperature for the onset of disordering occurs when the initial slope is unity, or

$$nJ / (2k_B T) = 1$$

or

$$k_B T = nJ/2.$$

General solution for spin-S Same method as spin-1/2 leading to

$$k_B T_c = \frac{2nJS(S+1)}{3},$$

as shown in Reif.