

Statistical Physics

Section 10: Mean-Field Theory of the Ising Model

Unfortunately one cannot solve exactly the Ising model (or many other interesting models) on a three dimensional lattice. Therefore one has to resort to approximations. In this section we will go through in detail a mean field approximation which is always the first recourse in trying to construct a theory. Actually there are many possible mean field theories, but they all share the same spirit. Here we present the simplest version which is known as Weiss mean field theory.

10. 1. The mean-field approximation

Recall that the Ising configurational energy is

$$E(\{S_i\}) = -h \sum_i S_i - J \sum_{\langle ij \rangle} S_i S_j \quad (1)$$

Consider all contributions involving spin j

$$\epsilon(S_j) = -h S_j - J S_j \sum_k^{n.n.} S_k \quad (2)$$

where the sum is over nearest neighbours (n.n.) k of site j .

We now *approximate* this contribution by replacing the S_k by their mean value

$$\epsilon_{mf}(S_j) = -h S_j - J S_j \sum_k^{n.n.} \langle S_k \rangle = -h_{mf} S_j \quad (3)$$

where

$$h_{mf} = h + J z m \quad (4)$$

and m , the magnetisation per spin, is just the mean value of any given spin

$$m = \frac{1}{N} \sum_i \langle S_i \rangle = \langle S_k \rangle \quad \forall k \quad (5)$$

Thus the mean field approximation is to replace the configurational energy (1) by the energy of a non-interacting system of spins each experiencing a field h_{mf} . For this problem we can write down the single-spin Boltzmann distribution straightaway

$$p(S_j) = \frac{e^{-\beta \epsilon_{mf}(S_j)}}{\sum_{S_j=\pm 1} e^{-\beta \epsilon_{mf}(S_j)}} = \frac{e^{\beta h_{mf} S_j}}{e^{\beta h_{mf}} + e^{-\beta h_{mf}}} \quad (6)$$

However, we still have a *consistency* condition to fulfil: the value of the magnetisation m predicted by (6) should be equal to the value of m used in the expression for h_{mf} (4). Thus we require

$$\begin{aligned} m &= \sum_{S_j=\pm 1} p(S_j) S_j \\ &= \frac{e^{\beta h_{mf}} - e^{-\beta h_{mf}}}{e^{\beta h_{mf}} + e^{-\beta h_{mf}}} = \tanh(\beta h_{mf}) \end{aligned} \quad (7)$$

and we arrive at the mean-field equation for the magnetisation

$$m = \tanh(\beta h + \beta J z m) \quad (8)$$

First we will consider the case $h = 0$ (zero applied field). The solutions of

$$m = \tanh(\beta J z m) \quad (9)$$

are best understood graphically. We see that for low β (high T) the only solution is $m = 0$

Figure 1: Picture of $\tanh(\beta J z m)$ versus m and the straight line m versus m . The intersections give the solutions of (9)

whereas for high β (low T) there are three possible solutions $m = 0$ and $m = \pm|m|$. The solutions with $|m| > 0$ appear when the the slope of the tanh function at the origin is greater than one

$$\left. \frac{d}{dm} \tanh(\beta J z m) \right|_{m=0} > 1 \quad (10)$$

Using the expansion of tanh for small argument

$$\tanh x \simeq x - \frac{x^3}{3} \quad (11)$$

(actually we only need the first term at this point), we find the condition (10) is

$$\beta J z > 1$$

which gives, remembering $\beta = 1/kT$,

$$T_c = \frac{zJ}{k} \quad (12)$$

Thus for $T > T_c$ only the paramagnetic $m = 0$ solution is available, whereas for $T < T_c$ we also have the ferromagnetic solutions $\pm|m|$. These are the physical solutions for $T < T_c$ as we shall see in the next subsection.

10. 2. Critical Behaviour

Consider again equation (9) which becomes using (12)

$$m = \tanh\left(m \frac{T_c}{T}\right) \quad (13)$$

We wish to analyse the emergence of the ferromagnetic solutions when T is near T_c , that is, in the *critical regime* where $T \simeq T_c$ and $|m| \ll 1$. Using (11) we obtain

$$m = m \frac{T_c}{T} - \frac{m^3}{3} \left(\frac{T_c}{T} \right)^3$$

Thus $m = 0$ or

$$m^2 = 3 \left(\frac{T}{T_c} \right)^3 \left(\frac{T_c}{T} - 1 \right) \quad (14)$$

We now define the *reduced temperature* t by

$$\boxed{t = \frac{T - T_c}{T_c}} \quad (15)$$

which gives

$$\frac{T}{T_c} = 1 + t \quad \frac{T_c}{T} = \frac{1}{1 + t}. \quad (16)$$

The reduced temperature t measures the proximity to the critical point. When t is small (14) becomes (exercise)

$$m^2 = 3(1 + t)^3 \left(1 - \frac{1}{1 + t} \right) \simeq -3t$$

Thus

$$\boxed{\begin{array}{l} T > T_c \quad m = 0 \\ T < T_c \quad m \simeq \pm(3|t|)^{1/2} \end{array}} \quad (17)$$

It is important to understand that what we have done is to identify the *leading* behaviour in t for t small

We now proceed to compute the susceptibility

$$\chi = \left. \frac{\partial m}{\partial h} \right|_{h=0} \quad (18)$$

and we should now expand (8). To capture the leading order behaviour in t, h it suffices to expand to first order in h :

$$m = m \frac{T_c}{T} + \beta h - \frac{m^3}{3} \left(\frac{T_c}{T} \right)^3$$

Taking the derivative w.r.t. h yields

$$\chi = \chi \frac{T_c}{T} + \beta - \chi m^2 \left(\frac{T_c}{T} \right)^3$$

or

$$\chi = \frac{\beta}{\left(1 - \frac{T_c}{T} + m^2 \left(\frac{T_c}{T} \right)^3 \right)} \quad (19)$$

Then we find for t small and using the appropriate expression for m ($m = 0$ or (14))

$$T > T_c \quad \chi = \frac{\beta}{\left(1 - \frac{T_c}{T} \right)} \simeq \frac{\beta}{t} \quad (20)$$

$$T < T_c \quad \chi = \frac{\beta}{\left(1 - \frac{T_c}{T} + 3\left(\frac{T_c}{T} - 1 \right) \right)} \simeq \frac{\beta}{2|t|} \quad (21)$$

Figure 2: Sketch of the critical behaviour of $|m|$ and χ as functions of the reduced temperature t

Again we have just identified the leading behaviour as $t \rightarrow 0$

The critical behaviour is sketched in the figure. Note how $|m| > 0$ emerges in a non analytic way since $\frac{\partial|m|}{\partial t}$ diverges at $t = 0$. Also note the divergence in χ (the response function to the applied field) at $t = 0$.

Finally we note that if we had taken the $m = 0$ solution below T_c in (19) we would have obtained a negative response function which is simply unphysical. Therefore below T_c the ferromagnetic solution is the physical one.

10. 3. Limitations of Mean Field Theory

The essence of the mean field assumption is the neglect of *correlations* between spins i.e. we effectively replace

$$\langle S_i S_j \rangle \simeq \langle S_i \rangle \langle S_j \rangle \quad i \neq j \quad (22)$$

Note we can write the energy (1) in the form

$$E(\{S_i\}) = E_0 - h \sum_j S_j, \quad (23)$$

where $E_0 = -J \sum_{\langle ij \rangle} S_i S_j$, which is the same form as that which we used to discuss the fluctuation response theorem in Section 3 when we identify $f = h$ and $A = \sum_j S_j$. Then we know that

$$\chi_{AA} = \frac{\partial \langle A \rangle}{\partial f} = \beta [\langle A^2 \rangle - \langle A \rangle^2] \quad (24)$$

In our case

$$\chi = \frac{\partial m}{\partial h} = \frac{1}{N} \chi_{AA} = \frac{\beta}{N} \sum_{jk} [\langle S_j S_k \rangle - \langle S_j \rangle \langle S_k \rangle] \quad (25)$$

This equation is exact. But if we now naively insert the mean field approximation (22) then all terms in the sum with $j \neq k$ will vanish and we are left with

$$\chi = \frac{\beta}{N} \sum_j [\langle S_j^2 \rangle - \langle S_j \rangle^2] = \beta [1 - m^2] \quad (26)$$

Clearly (26) does not diverge at T_c so the mean field approximation is inconsistent with regard to χ . The root of the problem lies in the neglect of correlations which become important as the critical point is approached.

Let us call

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \quad (27)$$

$$= \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle \quad (28)$$

Clearly G_{ij} measures the correlations between the *fluctuations* $\Delta S_i = S_i - \langle S_i \rangle$ — a positive G_{ij} implies that the fluctuations of the spins about their mean value are correlated.

We now define the **correlation length**:

Let R_{ij} be the distance between spins i and j . For large R_{ij} we expect

$$G_{ij} \simeq C(R_{ij})e^{-R_{ij}/\xi} \quad (29)$$

where C is some slowly varying function but $e^{-R_{ij}/\xi}$ ‘cuts off’ the correlation function at the correlation length ξ . Thus ξ is the scale at which correlations decrease significantly.

When $T > T_c$ so that $\langle S_i \rangle = 0$ a typical microstate will consist of clusters of up and down spins with the overall magnetisation being zero. Intuitively the correlation length gives a measure of the (linear) size of the largest clusters of correlated spins. See figure for a one dimensional illustration. As the temperature is decreased to the critical temperature the

Figure 3: Sketch of a typical configuration of spins above T_c which consists of clusters of correlated spins but zero overall magnetisation. ξ is the length of the largest clusters

size of the clusters diverge and we expect ξ to diverge.

One can refine mean-field theory to include the calculation of the ‘two-point’ correlation function G_{ij} . This is similar in spirit to the Debye-Hueckel theory but a little too technical than we have time for here. The result is that a correlation length is predicted which grows like

$$\xi \sim |t|^{-1/2} \quad (30)$$

and clearly diverges at T_c .

However the mean field theory is still inconsistent due to the neglect of three-point, four-point and higher order correlations. Basically near criticality correlations and fluctuations on all scales become important!

10. 4. Summary of mean-field picture and comparison with experiment

The mean field theory predicts

- The critical point $T_c = \frac{zJ}{k}$ at $h = 0$
- The singular, critical behaviour is described by

$$m \simeq m_- |t|^{\tilde{\beta}} \quad (T < T_c) \quad (31)$$

$$\chi \simeq c_{\pm} |t|^{-\gamma} \quad (32)$$

$$\xi \simeq \xi_{\pm} |t|^{-\nu} \quad (33)$$

$\tilde{\beta}, \gamma, \nu$ are known as **critical exponents** and take mean-field values $\tilde{\beta} = 1/2$, $\gamma = 1$, $\nu = 1/2$.

N.B. The standard notation for the order parameter (magnetisation) exponent is β and there is an obvious clash with inverse temperature hence we use a tilde to be clear.

Often one sees written, for example,

$$m \sim |t|^{\tilde{\beta}}$$

the precise meaning of which is

$$\lim_{|t| \rightarrow 0} \frac{\ln m}{\ln |t|} = \tilde{\beta} \quad (34)$$

Actually there are even more critical exponents. For example, one can define the zero-field heat capacity

$$C_h = \left. \frac{\partial \bar{E}}{\partial T} \right|_{h=0} \sim |t|^{-\alpha} \quad (35)$$

and near and below T_C one can characterise the discontinuity in the order parameter across the coexistence line by

$$h \sim |m|^{\delta} \text{sign } m \quad (36)$$

In the tutorial you are invited to work out the mean-field values $\alpha = 0$ and $\delta = 3$. The set $\alpha, \tilde{\beta}, \gamma, \delta, \nu$ characterise the critical point. It turns that some of these exponents are implied by the others and in fact there are only three independent exponents which we can take as $\tilde{\beta}, \gamma, \nu$.

Now the experimental data reveals that

- Systems do exhibit such singularities
- but the critical exponents *differ* from the mean field values
- however critical exponents are system independent e.g. for fluids, binary alloys and many magnets it has been found that $\tilde{\beta} = 0.31$, $\gamma = 1.25$, $\nu = 0.64$ in three dimensions. Thus apparently unrelated systems share the same set of critical exponents. This is referred to as *Universality* and remained a mystery for many years.

To summarise, mean-field theory is successful in that it qualitatively describes the critical behaviour but is quantitatively incorrect. Moreover as we shall find next section it is qualitatively incorrect in one dimension. On the other hand as we shall discuss later mean field theory does in fact give the correct critical exponents in high enough space dimension ($d \geq 4$ for the Ising model, which may or may not be reassuring!).