Mean field theory and perturbation schemes

Of the wide variety of models of interest to the critical point theorist, the majority have shown themselves intractable to direct analytic (pen and paper) assault. In a very limited number of instances models have been solved exactly, yielding the phase coexistence parameters, critical exponents and the critical temperature. The 2-d spin-$\frac{1}{2}$ Ising model is certainly the most celebrated such example, its principal critical exponents are found to be $\beta = \frac{1}{8}, \nu = 1, \gamma = \frac{7}{4}$. Its critical temperature is $-2J/\ln(\sqrt{2} - 1) \approx 2.269J$. Unfortunately such solutions rarely afford deep insight to the general framework of criticality although they do act as an invaluable test-bed for new and existing theories.

The inability to solve many models exactly often means that one must resort to approximations. One such approximation scheme is mean field theory.

Mean field solution of the Ising model

Let us look for a mean field expression for the free energy of the Ising model whose Hamiltonian is given in **?@eq-ising** . Write

$$s_i = \langle s_i \rangle + (s_i - \langle s_i \rangle) = m + (s_i - m) = m + \delta s_i$$

Then

$$
\begin{aligned}
H_I = & -J \sum_{<i,j>} [m + (s_i - m)][m + (s_j - m)] - H \sum_i s_i \\
= & -J \sum_{<i,j>} [m^2 + m(s_i - m) + m(s_j - m) + \delta s_i \delta s_j] - H \sum_i s_i \\
= & -J \sum_i (qms_i - qm^2/2) - H \sum_i s_i - J \sum_{<i,j>} \delta s_i \delta s_j
\end{aligned}
$$

where in the last line we have used the fact that when for each site i we perform the sum $\sum_{<i,j>}$ over bonds of a quantity which is independent of s_j, then the result is just the number of bonds per site times that quantity. Since the number of bonds on a lattice of N sites of coordination q is $Nq/2$ (because each bond is shared between two sites), there are therefore $q/2$ bonds per site.

Now the mean field approximation is to ignore the last term in the last line of Equation **??** giving the configurational energy as

$$H_{mf} = -\sum_i H_{mf}s_i + NqJm^2/2$$

with $H_{mf} \equiv qJm + H$ the "mean field" seen by spin s_i. As all the spins are decoupled (independent) in this approximation we can write down the partition function, which follows

by taking the partition function for a single spin (by summing the Boltzmann factor for $s_i = \pm 1$) and raising to the power N to find

$$Z = e^{-\beta q J m^2 N/2}[2\cosh(\beta(qJm + H))]^N$$

The free energy follows as

$$F(m) = NJqm^2/2 - Nk_BT\ln[2\cosh(\beta(qJm + H))]\,.$$

and the magnetisation as

$$m = -\frac{1}{N}\frac{\partial F}{\partial H} = \tanh(\beta(qJm + H))$$

This is a self consistent equation because m appears on both the left and the right hand sides. To find $m(H,T)$, we must numerically solve this last equation-self consistently. You will meet such an equation again later when you learn about mean field theories for liquid crystals.

> 🔥 Why self-consistent?
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> In mean-field theory, the many-body interaction is replaced by an effective one-body problem in which each degree of freedom experiences an average field generated by all the others. The quantity that characterises the ordered phase—the order parameter— is precisely this average. Because the effective (mean-field) Hamiltonian is constructed using a *presumed* value of that average, internal consistency requires that the order parameter obtained by solving the effective problem *match* the value assumed to define it. Enforcing this equality yields a self-consistency condition for the order parameter. In practice: choose the effective field determined by the putative order parameter, compute the corresponding thermal average, and require that the two coincide.

Note that we can obtain m in a different way. Consider some arbitary spin, s_i say. Then this spin has an energy $H_{mf}(s_i)$. Considering this energy for both cases $s_i = \pm 1$ and the probability $p(s_i) = e^{-\beta H_{mf}(s_i)}/Z$ of each, we have that

$$\langle s_i \rangle = \sum_{s_i = \pm 1} s_i p(s_i)$$

but for consistancy, $\langle s_i \rangle = m$. Thus

$$m = \sum_{s_i = \pm 1} s_i p(s_i)$$

$$= \frac{e^{\beta(qJm+H)} - e^{\beta(qJm+H)}}{e^{\beta(qJm+H)} + e^{-\beta(qJm+H)}}$$

$$= \tanh(\beta(qJm + H))$$

as before.

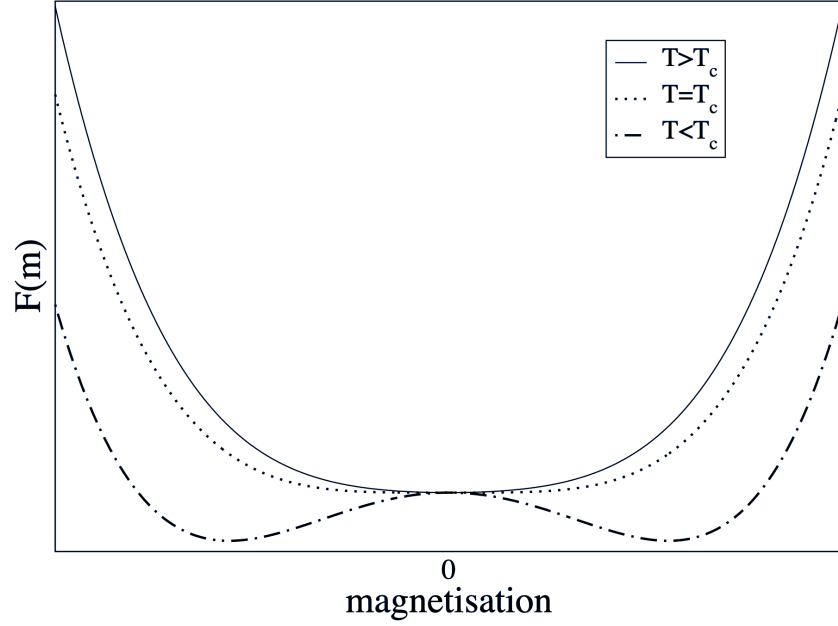## Spontaneous symmetry breaking

Figure 1: Schematic of the form of the free energy for a critical, subcritical and supercritical temperature

This mean field analysis reveals what is happening in the Ising model near the critical temperature T_c. Figure **??** shows sketches for $\beta F(m)/N$ as a function of temperature, where for f simplicity we restrict attention to $H = 0$. In this case $F(m)$ is symmetric in m, Moreover, at high T, the entropy dominates and there is a single minimum in $F(m)$ at $m = 0$. As T is lowered, there comes a point $(T = T_c = qJ/k_B)$ where the curvature of $F(m)$ at the origin changes sign; precisely at this point

$$\frac{\partial^2 F}{\partial m^2} = 0.$$

At lower temperature, there are instead two minima at nonzero $m = \pm m^\star$, where the *equilibrium magnetisation $m^\star$* is the positive root (calculated explicitly below) of

$$m^\star = \tanh(\beta J q m^\star) = \tanh(\frac{m^\star T_c}{T})$$

The point $m = 0$ which remains a root of this equation, is clearly an unstable point for $T < T_c$ (since F has a maximum there).

This is an example of spontaneous symmetry breaking. In the absence of an external field, the Hamiltonian (and therefore the free energy) is symmetric under $m \rightarrow -m$. Accordingly, one might expect the actual state of the system to also show this symmetry. This is true at high temperature, but spontaneously breaks down at low ones. Instead there are a pair of ferromagnetic states (spins mostly up, or spins mostly down) which – by symmetry– have the same free energy, lower than the unmagnetized state.

Phase diagram

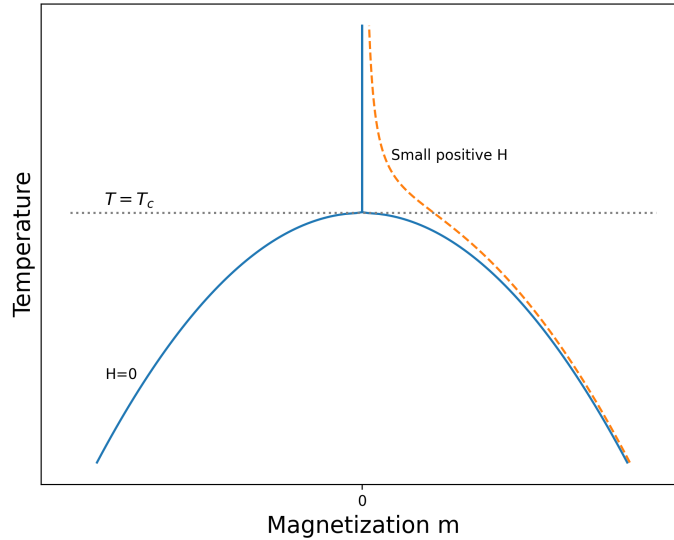The resulting zero-field magnetisation curve $m(T, H = 0)$ looks like Figure **??**.

Figure 2: Phase diagram of a simple magnet in the m-T plane.

This shows the sudden change of behaviour at T_c (phase transition). For $T < T_c$ it is arbitrary which of the two roots $\pm m^\star$ is chosen; typically it will be different in different parts of the sample (giving macroscopic "magnetic domains"). But this behaviour with temperature is

qualitatively modified by the presence of a field H, however small. In that case, there is always a slight magnetization, even far above T_c and the curves becomes smoothed out, as shown. There is no doubt which root will be chosen, and no sudden change of the behaviour (no phase transition). Spontaneous symmetry breaking does not occur, because the symmetry is already broken by H. (The curve $F(m)$ is lopsided, rather than symmetrical about $m = 0$.)

On the other hand, if we sit below T_c in a positive field (say) and gradually reduce H through zero so that it becomes negative, there is a *very* sudden change of behaviour at $h = 0$: the equilibrium state jumps discontinuously from $m = m^\star$ to $m = -m^\star$.
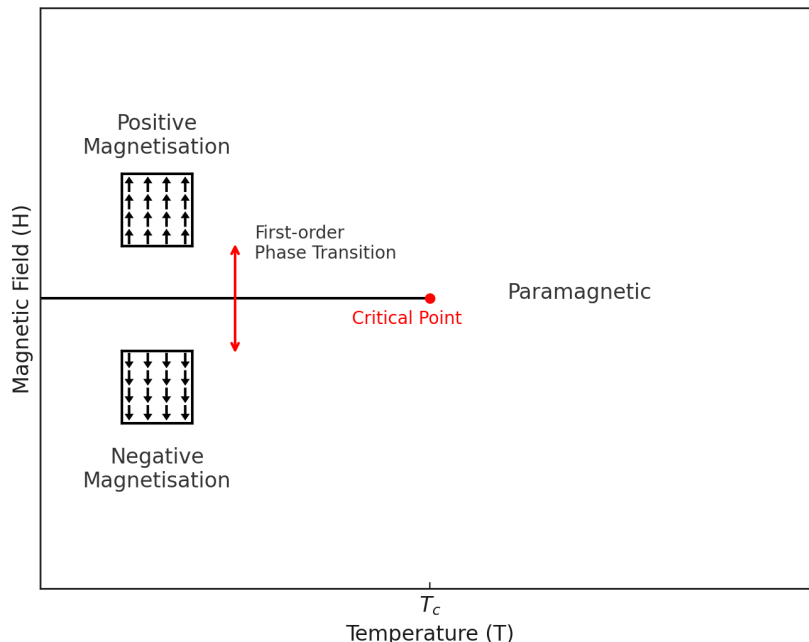

Figure 3: Phase diagram of a simple magnet in the H-T plane.

This is called a first order phase transition as opposed to the "second order" or continuous transition that occurs at T_c in zero field. The definitions are:

First order transition: magnetisation (or similar order parameter) depends discontinuously on a field variable (such as h or T).

Continuous transition: Change of functional form, but no discontinuity in m; typically, however, $(\partial m/\partial T)_h$ (or similar) is either discontinuous, or diverges with an integrable singularity.

In this terminology, we can say that the phase diagram of the magnet in the H, T plane shows a line of first order phase transitions, terminating at a continuous transition, which is the critical point.