# Physics 127b: Statistical Mechanics

# Second Order Phase Transitions

## The Ising Ferromagnet

Consider a simple $d$-dimensional lattice of $N$ classical "spins" that can point up or down, $s_i = \pm 1$. We suppose there is an interaction $J$ between nearest neighbor spins so that the parallel alignment is favored, with the Hamiltonian

$$H = -\frac{1}{2} J \sum_{i,\delta} s_i s_{i+\delta} - \mu \sum_i s_i B. \tag{1}$$

Here the $i$ sums run over all sites in the lattice, and the $\delta$ sum runs over the $2d$ nearest neighbors. The factor of $1/2$ in the first term is to avoid double counting the interaction, and the second term is the interaction of the moments $\mu s_i$ with an external magnetic field $B$.

The canonical partition function is

$$Q = \sum_{\{s_i\}} e^{-\beta H\{s_i\}} \tag{2}$$

summing the Boltzmann factor over all spin configurations $\{s_i\}$. The enumeration of all configurations cannot be done for $d \geq 3$, and although possible in $d = 2$ is extremely hard there as well (a problem solved by Onsager). We will use an approximate solution technique known as *mean field theory*.

Last term we solved the problem of noninteracting spins in a magnetic field described by the Hamiltonian

$$H_0 = -\sum_i s_i b, \tag{3}$$

writing $b$ for $\mu B$. This is easy to deal with, since the Hamiltonian is the sum over independent spins, unlike Eq. (1) which also has pair interaction terms. For example we can calculate the partition function as the product of single spin partition functions

$$Q_0 = [e^{-\beta b} + e^{\beta b}]^N \tag{4}$$

and the average spin on each site is

$$\langle s_i \rangle = \frac{e^{\beta b} - e^{-\beta b}}{e^{\beta b} + e^{-\beta b}} = \tanh(\beta b). \tag{5}$$

In the mean field approximation we suppose that the $i$th spin sees an *effective field* $b_{eff}$ which is the sum of the external field and the interaction from the neighbors calculated as if each neighboring spin were fixed at its ensemble average value

$$b_{eff} = b + J \sum_\delta \langle s_{i+\delta} \rangle . \tag{6}$$

We now look for a self consistent solution where each $\langle s_i \rangle$ takes on the same value $s$ which is then given in analogy with Eq. (5)

$$s = \tanh[\beta(b + 2Jds)]. \tag{7}$$

Lets first look at $b = 0$. Define $\varepsilon = 2d\beta Js$ so that

$$\varepsilon = 2d\beta J \tanh \varepsilon. \tag{8}$$

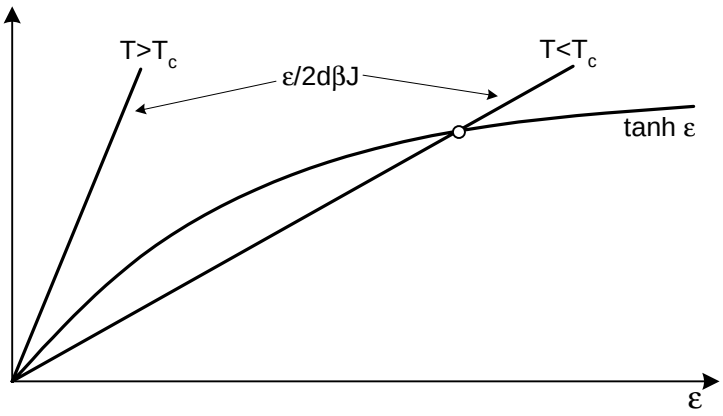


Figure 1: Graphical solution of the self consistency condition.

This is easily solved graphically. For $T > T_c = 2dJ/k_B$ the only solution is $\varepsilon = 0$. For $T < T_c$ two new solutions develop (equal in magnitude but opposite signs) with $|s|$ growing continuously below $T_c$. Near $T_c$ we can get the behavior by expanding $\tanh \varepsilon$ in small $\varepsilon$, so that Eq. (8) becomes

$$\varepsilon = \frac{T_c}{T}(\varepsilon - \frac{1}{3}\varepsilon^3) \tag{9}$$

giving to lowest order is small $(1 - T/T_c)$

$$s = \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2}. \tag{10}$$

Focusing on the *power law* temperature dependence near $T_c$ we introduce the small reduced temperature deviation $t = (T - T_c)/T_c$ and write this for small $t < 0$ as $s \propto |t|^\beta$. This introduces the *order parameter exponent* $\beta = 1/2$ in mean field theory.

We can also calculate the magnetic susceptibility $\chi = ds/db|_{b=0}$. From Eq. (7) we have (writing $s' = ds/db$)

$$s' = \mathrm{sech}^2[\beta(b + 2Jds)](\beta + \frac{T_c}{T}s') \tag{11}$$

so that just above $T_c$

$$\chi = \frac{1}{k_B T_c}\left(\frac{T - T_c}{T_c}\right)^{-1}, \tag{12}$$

giving a *diverging* susceptibility as $T$ approaches $T_c$ from above $\chi \propto |t|^{-\gamma}$ with the susceptibility exponent $\gamma = 1$ in mean field theory. (The usual definition of the susceptibility is $dM/dB = N\mu^2 ds/db$.)

Exactly at $T_c$ there is a *nonlinear* susceptibility easily derived by expanding the tanh function in Eq. (7)

$$s \simeq (\beta_c b + s) - \frac{1}{3}(\beta_c b + s)^3 + \cdots. \tag{13}$$

The terms linear in $s$ cancel, so we must retain the $s^3$ term. On the other hand the lowest order, linear term, in $b$ survives, so we can ignore terms in $b^2$, $bs$ etc. This gives

$$s(T = T_c, B) \simeq \left(\frac{3b}{k_B T_c}\right)^{1/3} + \cdots. \tag{14}$$

The dependence of the order parameter $s$ on the symmetry breaking field $b$ at $T_c$ and for small $b$, i.e. $s \propto b^{1/\delta}$ introduces the exponent $\delta = 3$ in mean field theory.

With a little more effort we can calculate the internal energy $U$ and other thermodynamic potentials. We will do this in zero magnetic field only. In the mean field approximation $U$ is simply given by $Nd$ "bonds" each with energy $-Js^2$

$$U = -NdJs^2 = -3NdJ\left(\frac{T_c - T}{T_c}\right). \tag{15}$$

We can try to evaluate the free energy from the partition function calculated in analogy with Eq. (4) replacing $\mu B$ there with $\mu B_{eff} = 2Jds$ (remember $B$ is assumed to be zero). This turns out not to be quite right, so we will call the expression $A_I$ ($I$ for independent)

$$A_I = -Nk_BT \ln\left[e^{-(T_c/T)s} + e^{(T_c/T)s}\right] \tag{16}$$

replacing $2dJ/k_B$ by $T_c$. We want to expand this in small $s$ up to $s^4$

$$A_I = -Nk_BT \ln\left[2\left\{1 + \frac{1}{2}\left(\frac{T_c}{T}\right)^2 s^2 + \frac{1}{24}\left(\frac{T_c}{T}\right)^4 s^4 + \cdots\right\}\right] \tag{17a}$$

$$= -Nk_BT \ln 2 - Nk_BT\left[\frac{1}{2}\left(\frac{T_c}{T}\right)^2 s^2 - \frac{1}{12}\left(\frac{T_c}{T}\right)^4 s^4 + \cdots\right]. \tag{17b}$$

The first term is just the free energy of the high temperature phase—in the mean field approximation simply the entropy contribution of free spins. The second term in $s^2$ suggests that the free energy is lowered by a nonzero $s$ for any temperature! Clearly something has gone wrong. The problem is, as often happens in mean field treatments, is that we have double-counted the interaction energy: by adding the free energy of spin 1 in the mean field of its neighbors (including spin 2 say) and the free energy of spin 2 in the mean field of *its* neighbors, including spin 1, we have included the $1-2$ interaction twice. So we need to subtract off a term $U$ to correct for this

$$A = A_I - U = -Nk_BT \ln 2 - NJd\left[\left(\frac{T_c - T}{T}\right)s^2 - \frac{1}{6}\left(\frac{T_c}{T}\right)^3 s^4 \cdots\right]. \tag{18}$$

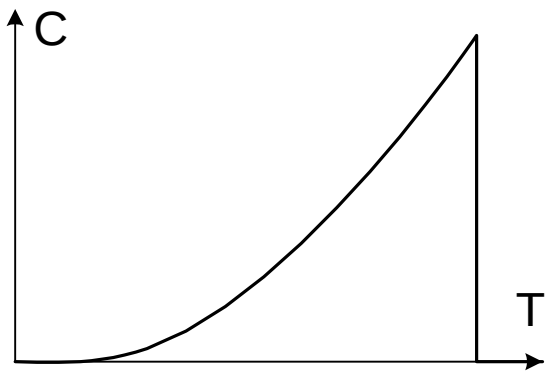


Figure 2: Specific heat of the Ising ferromagnet calculated in the mean field approximation.

Now we see that the free energy is lowered by a nonzero $s$ only for $T < T_c$. Indeed minimizing $A$ with respect to $s$ gives Eq. (10) as before, and then the reduction in $A$ below $T_c$ for nonzero $s$ is

$$\delta A = -\frac{3}{2}NdJ\left(\frac{T_c - T}{T_c}\right)^2 + \cdots. \tag{19}$$

The power law dependence of $\delta A$ near $T_c$ is used to define the *specific heat exponent* $\delta A \propto |t|^{2-\alpha}$ with $\alpha = 0$ in mean field theory.

The specific heat can be derived as $dU/dt$ or $-Td^2A/dT^2$.using the former gives

$$C = -NdJ\,\frac{ds^2}{dT}. \tag{20}$$

This is *zero* above $T_c$, *jumps* to $3Nk_B/2$ at $T_c$, and then decreases to zero as $T \to 0$, see Fig. 2. This is consistent with $C \propto |t|^{-\alpha}$ with $\alpha = 0$.

## General Remarks

The Ising ferromagnet shows a *second order* transition. Features are

1. A new state grows continuously out of the previous one: for $T \to T_c$ the two states become quantitatively the same.

2. As a consequence of (1) the thermodynamic potentials $A, U, S \ldots$ are continuous at $T_c$ but not necessarily smooth (analytic). In mean field theory the changes from the values just above $T_c$ show *power law* behavior in $|1 - T/T_c|$. The *derivatives* of the potentials (specific heat, susceptibility etc.) similarly show power laws (a jump such as in $C$ can be considered a power law 0), and will *diverge* at $T_c$ if the power is negative.

3. For $T < T_c$ equally good (i.e. energetically equal) but macroscopically different states exist. In the Ising ferromagnet these states differ in the macroscopic magnetic moment $M = \pm N\mu\,|s|$. This is a *broken symmetry*—the thermodynamic states do not have the full symmetry of the Hamiltonian (here all $s_i \to -s_i$). Instead the different thermodynamic states below $T_c$ are related by this symmetry operation. Since the states are macroscopically different, once one state is chosen, fluctuations to the other state will not occur in the thermodynamic limit.

4. Because the states are quantitatively similar as $T \to T_c$, fluctuations involving admixtures of other states become important here, so that mean field theory will *not in general be a good approximation* near $T_c$. The power law behavior of thermodynamic quantities near $T_c$ survives (and occurs both above and below $T_c$ in the more accurate description) but the powers or exponents are different than the values calculated in mean field theory, and are no longer simple rationals.

5. Because of the power law singularities of the thermodynamic potentials near $T_c$, it is not possible to classify phase transitions into higher orders (second, third etc.) according to which derivative of the free energy is discontinuous (the Ehrenfest classification): we simply have first order transitions, where the entropy, or volume etc. is discontinuous, and second order transitions where such variables are continuous.

## Analogies between liquid-gas and Ising ferromagnet transitions

Although we have approached these two transitions from different perspectives, there are in fact close similarities. In particular the critical point in the liquid-gas system is directly analogous to the transition temperature in the Ising ferromagnet. The relationship is displayed in Fig. 3. The analogies are in fact *quantitative*—the transitions at the critical points are said to be in *the same universality class*. For example the density discontinuity below the liquid-gas critical point grows as $(T_c - T)^\beta$ where $\beta$ has the same value as

in the growth of the magnetization below $T_c$ in the Ising ferromagnet $M \sim (T_c - T)^\beta$, and the compressibility in the gas diverges near $T_c$ in the same way that the susceptibility does at the magnet transition!

The main difference between the two transitions is that the magnetic field is an externally applied, symmetry breaking field that can be set to zero. In the liquid-gas there is no symmetry between the two states below $T_c$ (the dense liquid and rarefied gas), and the value of $P$ yielding the transition (corresponding to $B = 0$ in the magnetic case) is not *a priori* obvious.

### When is mean field theory exact?

Mean field theory is often a useful first approach giving a qualitative prediction of the behavior at phase transitions. It becomes exact when a large number of neighbors participate in the interaction with each spin, since then the fluctuations in the effective field indeed become small compared with the mean. This happens in high enough spatial dimension $d$, or for long range interactions. A handout describes the infinite range Ising model, and also introduces a useful formal approach known as the Hubbard-Stratonovich transformation, demonstrating this. This is an advanced topic you can consult if you are interested.

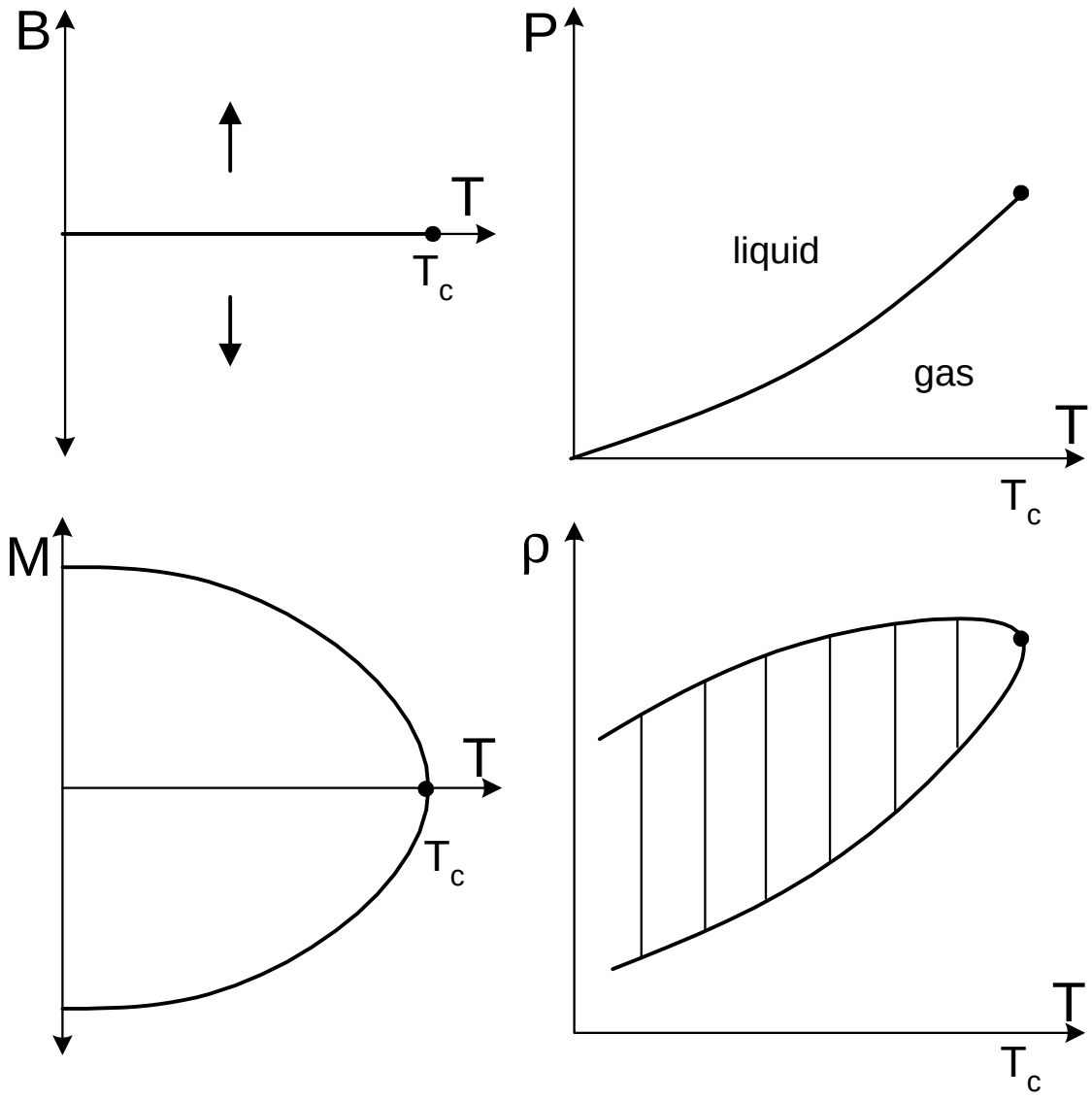


Figure 3: Analogy between Ising ferromagnet transition (left panels) and liquid-gas transition (right panels).