

# Chapter 5

## Mean-Field Theory

### 5.1 Mean-Field Treatments of the Ising Model

In this Section, we are discussing various approaches to obtain a mean-field solution to the Ising model. In fact, several of the approaches will yield exactly identical results. The reason they are presented is that they highlight different ways of carrying out the approximation(s) that are commonly referred to as “mean-field approximations”. Essentially, they differ by whether one (i) neglects spin fluctuations around the mean or (ii) considers spins to behave statistically independently and by which part of the system one treats exactly (Bethe-Peierls mean-field theory).

#### 5.1.1 Weiss Molecular Field Theory

We start by identifying the *order parameter* of the magnet which distinguishes the ordered (magnetic) from the disordered (nonmagnetic) phase. For describing a paramagnetic to ferromagnetic transition, the obvious choice is the (*local*) *magnetization*

$$m = \langle s_i \rangle. \quad (5.1)$$

We now focus on a single spin,  $s_0$ , which on a hypercubic lattice in  $d$  dimensions has  $z = 2d$  nearest neighbours, which we label  $s_1, \dots, s_{2d}$ . The scenario considered is shown for the two-dimensional case in Fig. 5.1

The part of the Ising Hamiltonian containing spin  $s_0$  reads as follows, where we decompose the spins  $s_j$  into their mean value (the magnetization), and fluctu-

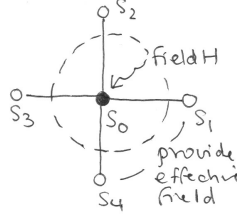


Figure 5.1: A spin  $s_0$  on a two-dimensional square lattice interacts with its nearest neighbours  $s_1, \dots, s_4$ .

ations around it,  $s_j = m + (s_j - m)$ :

$$\begin{aligned}\mathcal{H}_{s_0} &= -s_0 \left( J \sum_{j=1}^z s_j + H \right) \\ &= -s_0 (zJm + H) - Js_0 \sum_{j=1}^z (s_j - m)\end{aligned}$$

The fundamental assumption of mean-field theory is now *to set the fluctuations to 0*,  $(s_j - m) = (s_j - \langle s_j \rangle) \rightarrow 0$ , such that the resulting Hamiltonian reads:

$$\boxed{\mathcal{H}_{s_0}^0 = -s_0(zJm + H)} \quad (5.2)$$

This represents a non-interacting spin in an effective field  $H_{\text{eff}} = zJm + H$ . This Hamiltonian allows us to calculate  $\langle s_0 \rangle$ . The second step of mean-field theory is to argue that the chosen spin is not special at all, hence its mean must be identical to the magnetization. This gives us a *self-consistency condition*

$$\boxed{\langle s_0 \rangle \stackrel{!}{=} m} \quad (5.3)$$

As

$$\begin{aligned}\langle s_0 \rangle &= \frac{\text{tr } s_0 e^{\beta s_0 (zJm + H)}}{\text{tr } e^{\beta s_0 (zJm + H)}} \\ &= \frac{e^{+\beta(zJm + H)} - e^{-\beta(zJm + H)}}{e^{+\beta(zJm + H)} + e^{-\beta(zJm + H)}} \\ &= \tanh \beta(zJm + H)\end{aligned}$$

we obtain the following self-consistent equation for the magnetization:

$$\boxed{m = \tanh[\beta(zJm + H)]} \quad (5.4)$$

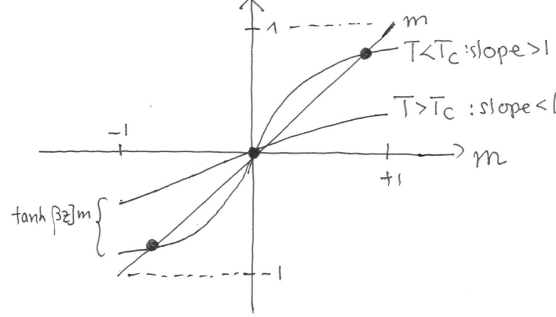


Figure 5.2: Graphical representation of the self-consistency equation for the magnetization in the Weiss mean field approximation.

While this equation cannot be solved analytically, the main features can be extracted anyways. For a finite field  $H \neq 0$ , we see for example that solutions change sign with the field:  $m(T, H) = -m(T, -H)$ .

The field-free case  $H = 0$  is more interesting. First of all,  $m = 0$  is always a solution, which corresponds to the paramagnetic regime. But if we draw both sides of the equation  $m = \tanh \beta z J m$  as a function of  $m$  (see Fig. 5.2), we see that there are two more solutions  $\pm m_0$  if the slope of the hyperbolic tangent at  $m = 0$  exceeds slope 1. Now the slope of the hyperbolic tangent is given by

$$\left. \frac{d}{dm} \tanh \beta z J m \right|_{m=0} = \frac{1}{\cosh^2 \beta z J m} (\beta z J) \Big|_{m=0} = \beta z J.$$

Hence, if  $\beta z J > 1$ , there are 3 solutions,  $m = 0$  and  $m = \pm m_0$ , which corresponds to the two  $Z_2$ -symmetry breaking solutions of an Ising magnet. The critical temperature is given by

$$\boxed{\beta_c z J = 1 \quad k_B T_c = z J} \quad (5.5)$$

For the hypercubic lattices, this means:

- There is a phase transition at  $k_B T_c = 2J$  in the one-dimensional case. In fact, we will see from an entropy argument due to Peierls and from an exact calculation in Chapter 7 that this is *wrong*; *there is no phase transition in 1D*. Of course, omitting all fluctuations is a serious approximation, but we will have to see why our theory fails even qualitatively.
- There is a phase transition at  $k_B T_c = 4J$  in the two-dimensional case. We will see from exact calculations in Chapter 7 that there is indeed a phase

transition, so our mean field theory is *qualitatively* right, but it is *quantitatively* wrong: the true transition temperature is at  $k_B T_c = 2.269J$ , hence overestimated. This is a typical feature of mean-field theories, because their neglect of fluctuations makes them *overestimate the tendency to order*.

- In three and more transitions, mean-field theory continues to predict (correctly) the existence of phase transitions, and the estimates for  $T_c$  get increasingly better ( $k_B T_c = 6J$  versus numerical  $k_B T_c = 4.511J$ ). This can be understood qualitatively: in higher dimensions, spin  $s_0$  is coupled to more and more neighbours, whose fluctuations around the mean (i.e. the magnetization) will increasingly tend to cancel each other (cf. the growth as  $1/\sqrt{N}$  of the relative fluctuations for  $N$  independent identically distributed random variables with the proviso that the neighbouring spins are not acting independently). This means that on average  $s_0$  indeed is coupled to an effective field  $zJm + H$ .

### 5.1.2 Mean-Field Theory and Bogolyubov Inequality

In this approach the essential approximation will consist in neglecting the statistical interdependence of the orientation of spins, and explore an inequality on free energies.

#### Bogolyubov Inequality

Consider a classical Hamiltonian that can be decomposed into two parts,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1. \quad (5.6)$$

The decomposition is arbitrary but to make sense in the following it should be chosen such that the statistical physics of  $\mathcal{H}_0$  can be calculated more or less easily exactly, whereas  $\mathcal{H}_1$  contains all the difficult parts of the Hamiltonian. If we think of an Ising-like model, the partition functions are given as

$$Z = \sum_{\{s\}} e^{-\beta \mathcal{H}(s)} \quad Z_0 = \sum_{\{s\}} e^{-\beta \mathcal{H}_0(s)} \quad (5.7)$$

where we assume that we can calculate  $Z_0$ , but not  $Z$ . Then

$$\frac{Z}{Z_0} = \frac{\sum_{\{s\}} e^{-\beta(\mathcal{H}_0 + \mathcal{H}_1)}}{\sum_{\{s\}} e^{-\beta \mathcal{H}_0}} = \sum_{\{s\}} p_0(s) e^{-\beta \mathcal{H}_1(s)} = \langle e^{-\beta \mathcal{H}_1} \rangle_0, \quad (5.8)$$

where the expectation value is taken with respect to the probability distribution generated by  $\mathcal{H}_0$ . We now invoke the convexity inequality which says that for a function  $f(x)$  with  $f'(x) > 0$  and  $f''(x) > 0$  we have

$$f(\langle x \rangle_p) \leq \langle f(x) \rangle_p, \quad (5.9)$$

where the expectation value is taken with respect to some probability density  $p(x)$ . Then, setting  $x$  equal to  $\mathcal{H}_1$ , we have

$$\langle e^{-\beta \mathcal{H}_1} \rangle_0 \geq e^{-\beta \langle \mathcal{H}_1 \rangle_0}. \quad (5.10)$$

But the left-hand side is just  $Z/Z_0$ , hence

$$\frac{Z}{Z_0} \geq e^{-\beta \langle \mathcal{H}_1 \rangle_0}. \quad (5.11)$$

Taking the logarithm and using  $G = -k_B T \ln Z$  (both for  $Z$  and  $Z_0$ ), we obtain the *Bogolyubov inequality*:

$$\boxed{G \leq G_0 + \langle \mathcal{H}_1 \rangle_0} \quad (5.12)$$

The same expression also holds for  $F$ ; we anticipate that we work with  $G(T, H)$  rather than  $F(T, M)$ , i.e. subtract  $HM$  from the interaction energy of the Ising model. This expression can be reformulated a bit if we insert

$$G_0 = \langle \mathcal{H}_0 \rangle_0 - TS_0 \quad (5.13)$$

where the entropy  $S_0$  is given by

$$S_0 = -k_B \sum_{\{s\}} p_0(s) \ln p_0(s). \quad (5.14)$$

Then the Bogolyubov inequality takes the form

$$\boxed{G \leq \langle \mathcal{H} \rangle_0 - TS_0} \quad (5.15)$$

This shows that we can give a rigorous upper bound on the energy.

### Bogolyubov Inequality and Mean-Field Theory

We split the Hamiltonian  $\mathcal{H}$  of the Ising model in a way which depends on some control parameter  $\lambda$ , where the goal will be to choose it such as to minimize the free energy:

$$\mathcal{H}_0^{(\lambda)} = -\lambda \sum_i s_i \quad \mathcal{H}_1^{(\lambda)} = -J \sum_{\langle i,j \rangle} s_i s_j + (\lambda - H) \sum_i s_i \quad (5.16)$$

As  $\mathcal{H}_0^{(\lambda)}$  is a sum of single-spin terms,  $Z_0$  will be a product of single-spin partition functions  $e^{-\beta\lambda} + e^{+\beta\lambda} = 2 \cosh \beta\lambda$ :

$$Z_0 = (2 \cosh \beta\lambda)^N. \quad (5.17)$$

Then  $G_0 = -k_B T \ln Z$ . The expectation values of the spins are independent of each other and do not depend on the spin index:

$$\langle s_i \rangle_0 = \tanh \beta\lambda. \quad (5.18)$$

Due to independence, the expectation value of  $\mathcal{H}_1^{(\lambda)}$  reads

$$\mathcal{H}_1^{(\lambda)} = -\frac{1}{2} N J z \tanh^2 \beta\lambda + N(\lambda - H) \tanh \beta\lambda, \quad (5.19)$$

with  $z/2$  nearest-neighbour bonds. Then we have as variational ansatz from Eq. (5.12)

$$G(\lambda) = N[-\beta^{-1} \ln(2 \cosh \beta\lambda) - \frac{1}{2} J z \tanh^2 \beta\lambda + (\lambda - H) \tanh \beta\lambda] \quad (5.20)$$

which we seek to minimize to provide an upper bound on the free energy: differentiating with respect to  $\lambda$ , and setting  $dG/d\lambda = 0$ , we have

$$\lambda_{\min} - H = J z \tanh \beta\lambda_{\min}, \quad (5.21)$$

which upon insertion into  $G(\lambda)$  gives as variationally minimal free energy

$$G = -N k_B T \ln(2 \cosh \beta\lambda_{\min}) + \frac{N(\lambda_{\min} - H)^2}{2zJ}. \quad (5.22)$$

The magnetization per spin is then given by

$$m = -\frac{1}{N} \frac{dG}{dH} = -\frac{1}{N} \left( \frac{\partial G}{\partial H} + \frac{\partial G}{\partial \lambda} \frac{\partial \lambda}{\partial H} \right)_{\lambda_{\min}} = \frac{\lambda_{\min} - H}{Jz}. \quad (5.23)$$

Here we have used that  $\frac{\partial G}{\partial \lambda} = 0$  for  $\lambda = \lambda_{\min}$ . Inserting Eq. (5.21), we revert to the previously established relation

$$m = \tanh \beta(Jzm + H), \quad (5.24)$$

from which the analysis proceeds as before.

### 5.1.3 Bragg-Williams Mean-Field Theory

In this approach, the approximation made will again lead to an effective single-spin problem; instead of solving a self-consistency equation, we will minimize the resulting approximate free energy. The appeal of this approach is not any improved result, but a first insight into a very generic form of mean-field free energies.

We start by rewriting the Hamiltonian in terms of the number of nearest-neighbour bonds with both spins up ( $N_{++}$ ), both spins down ( $N_{--}$ ) and one up and one down ( $N_{+-}$ ); for a hypercubic lattice in  $d$  dimensions with  $z = 2d$  nearest neighbours, the total number of bonds for  $N$  sites is  $dN = Nz/2$  (assuming periodic boundary conditions). We also use  $N_{\pm}$ , the number of up and down spins;  $N = N_+ + N_-$ . Then the Hamiltonian can be expressed exactly as

$$\mathcal{H} = -J(N_{++} + N_{--} - N_{+-}) - H(N_+ - N_-). \quad (5.25)$$

As magnetization per site  $m = (N_+ - N_-)/N$ , therefore magnetization  $M = Nm = N_+ - N_-$ , we can express  $N_{\pm}$  in terms of  $m$ :

$$N_{\pm} = \frac{N(1 \pm m)}{2}. \quad (5.26)$$

The approximation now consists in a *decoupling* assumption: the spin states on different sites are statistically independent, and we have site-independent probabilities for  $s = \pm 1$  as

$$p_{\pm} = \frac{N_{\pm}}{N}. \quad (5.27)$$

We can now construct a free energy  $G = U - TS$ . Using the von Neumann expression  $S = -k_B \sum_k p_k \ln p_k$  and that entropy is simply additive for independent subsystems (i.e. individual spins), we have

$$S = -k_B N \left( \frac{N_+}{N} \ln \frac{N_+}{N} + \frac{N_-}{N} \ln \frac{N_-}{N} \right). \quad (5.28)$$

Under the decoupling assumption,  $N_{++}, N_{--}, N_{+-}$  can be traced back to  $N_{\pm}$ . There are  $Nz/2$  bonds. The probability that both spins are up is  $p_+^2$  due to statistical independence. Then

$$N_{++} = \frac{Nz}{2} p_+^2 = z \frac{N_+^2}{2N} \quad N_{--} = z \frac{N_-^2}{2N} \quad N_{+-} = z \frac{N_+ N_-}{N}. \quad (5.29)$$

We can now express the internal energy and hence the Gibbs free energy  $G(T, H) = \langle \mathcal{H} \rangle - TS$  as:

$$G(T, H) = -\frac{Jz}{2N} (N_+^2 + N_-^2 - 2N_+ N_-) - H(N_+ - N_-) + k_B T N \left( \frac{N_+}{N} \ln \frac{N_+}{N} + \frac{N_-}{N} \ln \frac{N_-}{N} \right), \quad (5.30)$$

which can be expressed in terms of magnetization per site  $m$  as

$$G(T, H) = -\frac{JzN}{2}m^2 - NHm + k_B T N \left( \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right). \quad (5.31)$$

The dependence on  $T$  is implicit in  $m$ . Passing to the intensive Gibbs free energy per site  $g = G/N$ , we now determine  $m$  by minimizing  $g$ , setting  $\partial g / \partial m = 0$ . The result is

$$0 = -Jzm - H + \frac{1}{2}k_B T \ln \frac{1+m}{1-m} \quad (5.32)$$

This looks new, but isn't, because  $\operatorname{arctanh} x = \frac{1}{2} \ln \frac{1+x}{1-x}$ . Hence, we recover  $m = \tanh \beta(Jzm + H)$ , and the same predictions for  $T_c$  and  $m(T)$ . The advantage of this approach is that we get an idea of the form of the free energy expressed in the order parameter  $m$ .

Let us focus on the field-free case  $H = 0$ . Then

$$g(T, 0) = -\frac{Jz}{2}m^2 + \frac{1}{2}k_B T [(1+m) \ln(1+m) + (1-m) \ln(1-m) - 2 \ln 2]. \quad (5.33)$$

Expanding the logarithm up to fourth order,

$$\ln(1 \pm x) \simeq \pm x - \frac{x^2}{2} \pm \frac{x^3}{3} - \frac{x^4}{4},$$

we find that

$$g(T, 0) = -k_B T \ln 2 + \frac{1}{2}(k_B T - Jz)m^2 + \frac{1}{12}k_B T m^4 + O(m^6). \quad (5.34)$$

Looking at the structure of the expansion of the logarithm, one sees that there are only even powers of  $m$  present. This is as it should be, as the Hamiltonian is invariant under reflection  $s_i \rightarrow -s_i$ , hence the sign of  $m$  may not appear. One can also see from the prefactors of the powers of  $m$  in the expansion that all higher orders  $m^6, m^8$ , etc. will have *positive* prefactors.

Using a more generic form and recognizing that  $(1/2)(k_B T - Jz) = (k_B/2)(T - T_c)$ , we have

$$g(T, 0) = a(T) + \frac{b(T)}{2}m^2 + \frac{c(T)}{4}m^4 + O(m^6) \quad (5.35)$$

where

- $a(T)$  is an irrelevant constant
- $b(T) > 0$  for  $T > T_c$ ,  $b(T) < 0$  for  $T < T_c$ : a sign change occurs at  $T = T_c$



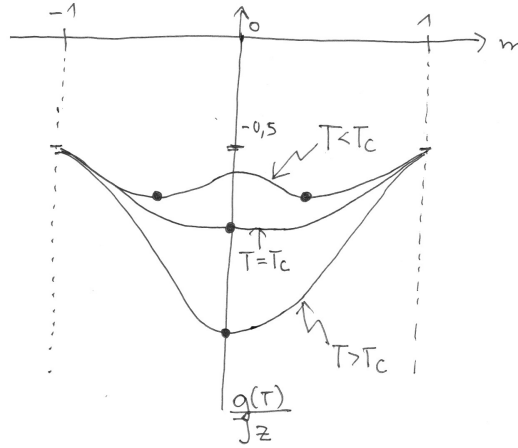


Figure 5.3: Gibbs free energy  $g$  from Eq. (5.33) as a function of  $m$  ( $|m| \leq 1$ ) for temperatures above, at and below the critical temperature. Dots indicate the magnetization that minimizes energy. At  $T = T_c$ , at the minimum the second (and third) derivative(s) vanish too, making the energy curve very flat.

- $b(T)$  is linear in  $(T - T_c)$
- $c(T) > 0$

We will encounter this form again in the framework of *Landau's theory of phase transitions*, where it will emerge as the minimum instance of the description of a continuous phase transition. The prefactors are for later convenience. Fig. 5.3 shows  $g$  above, at and below  $T_c$ . For symmetry reasons,  $g(m) = g(-m)$ . The shape depends on the sign of  $b(T)$ : above  $T_c$  it is positive, so there is a global minimum at  $m = 0$ . For  $T < T_c$  it is negative, such that a double-well structure emerges, where the minima sit at finite magnetization.

#### 5.1.4 Bethe Mean-Field Theory

Let us conclude by looking at one slightly more refined variety of mean-field theory due to Hans Bethe [H. Bethe, Proc. Roy. Soc. London **A150**, 552 (1935)]. It will show that there is room for qualitative and quantitative improvement, but also that certain features of mean-field theory are independent of the precise details of approximation. Last but not least, we will get a feeling how much more complicated calculations will become if one pushes the ideas of this section further.

In our original mean-field theory treatment due to Pierre Weiss (1865 – 1940), we considered uncorrelated *spins*. Obviously, the correlations will be strongest

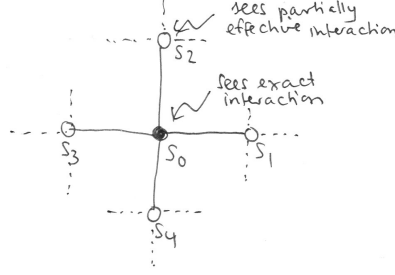


Figure 5.4: Smallest cluster on a square lattice: The interactions of a central spin  $s_0$  with its nearest neighbours  $s_1$  through  $s_4$  are treated exactly, whereas the surface spins of the cluster see only an effective field as far as their interactions with their other 3 neighbours are concerned.

between spins that are within each others immediate vicinity, and we can improve systematically by considering uncorrelated *clusters of spins* of increasing size.

The smallest cluster imaginable is a spin  $s_0$  together with its  $z$  nearest neighbours  $s_j$ , hence a cluster of  $z + 1$  spins, for example 5 spins on a square lattice (Fig. 5.4). Then  $s_0$  can interact exactly with its 4 neighbours. Those 4 neighbours interact exactly with  $s_0$ , of course, but see their own further three neighbours only through an effective field as in Weiss theory.

The Hamiltonian for the cluster can be written as

$$\mathcal{H}_c = -J s_0 \sum_{j=1}^z s_j - H s_0 - H' \sum_{j=1}^z s_j. \quad (5.36)$$

The last term contains the effective field interaction and the external field  $H$ , and will be related to the magnetization of the surrounding spins. As in simple Weiss theory, the field has to be determined self-consistently. Obviously, spin  $s_0$  in the center is treated on a different footing than the cluster surface spins  $s_j$ . But in a translationally invariant system there is no preferred spin site, and the magnetization of all spins must be identical. Hence the self-consistency condition reads

$$\langle s_0 \rangle = \langle s_j \rangle, \quad (5.37)$$

and this will be achieved by a proper choice of the effective field  $H'$ . To calculate

the magnetizations, we need

$$\begin{aligned}
 Z_c &= \sum_{\{s_j\}} \sum_{s_0=\pm 1} e^{\beta H s_0} e^{\beta J s_0 \sum_j s_j} e^{\beta H' \sum_j s_j} \\
 &= \sum_{\{s_j\}} \left( e^{+\beta H} \prod_j e^{\beta(J+H')s_j} + e^{-\beta H} \prod_j e^{\beta(-J+H')s_j} \right) \\
 &= e^{+\beta H} (2 \cosh \beta(J+H'))^z + e^{-\beta H} (2 \cosh \beta(J-H'))^z
 \end{aligned}$$

These steps can be rerun to calculate  $\langle s_0 \rangle$  and  $\langle s_j \rangle$ .

$$Z_c \langle s_0 \rangle = e^{+\beta H} (2 \cosh \beta(J+H'))^z - e^{-\beta H} (2 \cosh \beta(J-H'))^z \quad (5.38)$$

$$\begin{aligned}
 Z_c \langle s_j \rangle &= 2e^{+\beta H} \sinh \beta(J+H') (2 \cosh \beta(J+H'))^{z-1} \\
 &\quad - 2e^{-\beta H} \sinh \beta(J-H') (2 \cosh \beta(J-H'))^{z-1}
 \end{aligned} \quad (5.39)$$

Specializing to  $H = 0$ , the self-consistency condition (5.37) reduces to

$$\begin{aligned}
 &(\cosh \beta(J+H'))^z - (\cosh \beta(J-H'))^z \\
 &= \sinh \beta(J+H') (\cosh \beta(J+H'))^{z-1} - \sinh \beta(J-H') (\cosh \beta(J-H'))^{z-1},
 \end{aligned} \quad (5.40)$$

which can be rewritten as

$$\boxed{\left( \frac{\cosh \beta(J+H')}{\cosh \beta(J-H')} \right)^{z-1} = e^{2\beta H'}} \quad (5.41)$$

Obviously,  $H' = 0$  is always a solution. But again there are further solutions, because the right hand side diverges with  $H' \rightarrow \infty$ , whereas the left hand side converges to  $e^{2\beta(z-1)J}$ . So, if the slope of the left hand side exceeds that of the right hand side for  $H' = 0$ , there must be a further solution  $H'_0$  and by symmetry also  $-H'_0$ .

The derivative of the right hand side at  $H' = 0$  is  $2\beta e^{2\beta H'} = 2\beta$ . The derivative of the left hand side is a bit more involved, but in the end is just  $2\beta(z-1) \tanh \beta J$ . Hence, the transition temperature is reached when these expressions become identical,  $1 \stackrel{!}{=} (z-1) \tanh \beta_c J$  or

$$\coth \beta_c J = z - 1 \quad (5.42)$$

As  $\operatorname{arccoth} x = \frac{1}{2} \ln \frac{1-x}{1+x}$ , we obtain

$$\boxed{k_B T_c = \frac{2J}{\ln\left(\frac{z}{z-2}\right)}} \quad (5.43)$$

This leads to the following predictions:

- For a one-dimensional chain,  $z = 2$ , hence  $T_c = 0$ : there is no phase transition at finite temperature, which is a correct prediction *not* obtained in the simpler mean-field theory.
- For a two-dimensional square lattice  $z = 4$ , hence

$$k_B T_c = \frac{2J}{\ln 2} = 2.885J, \quad (5.44)$$

which is still far from the exact  $2.269J$ , but already much better than the original  $4J$  prediction.

One could now consider larger and larger clusters. Approximations will become better, but at the same time the calculational effort will explode. Ultimately, in vain: correlations will diverge at the transition temperature: some response function diverges at the transition, but this can be related to diverging two-point correlators due to a suitable fluctuation-dissipation theorem. No finite cluster will be able to account for this, so even these improved approaches will fail at the phase transition itself. Of course, this does not exclude reasonable results far away from the transition.

### 5.1.5 Construction of a Free Energy

Quite independent of these approximation schemes, we can construct a free energy as follows. We decompose a Hamiltonian into a non-interacting (hence easy) and interacting part,  $\mathcal{H}_\lambda = \mathcal{H}_0 + \lambda\mathcal{V}$ . In the case of the Ising model,

$$\mathcal{H}_0 = -H \sum_i s_i \quad \mathcal{V} = - \sum_{\langle i,j \rangle} s_i s_j \quad \lambda = J. \quad (5.45)$$

We now take  $\lambda \in [0, J]$  and introduce

$$G_\lambda = -k_B T \ln Z_\lambda = -k_B T \ln \text{tr} e^{-\beta \mathcal{H}_0 - \beta \lambda \mathcal{V}}. \quad (5.46)$$

Then  $G_0$  is the free energy of the simple non-interacting model, and  $G = G_J$  is the free energy of the Ising model. With the notation

$$\langle O \rangle_\lambda = \frac{1}{Z_\lambda} \text{tr} O e^{-\beta(\mathcal{H}_0 + \lambda \mathcal{V})} \quad (5.47)$$

we find that

$$\frac{dG}{d\lambda} = \langle \mathcal{V} \rangle_\lambda, \quad (5.48)$$

hence the exact result

$$G = G_J = G_0 + \int_0^J d\lambda \langle \mathcal{V} \rangle_\lambda. \quad (5.49)$$

The approximation comes in through  $\langle \mathcal{V} \rangle_\lambda$ , which one can evaluate at one of the several levels of approximation introduced here.

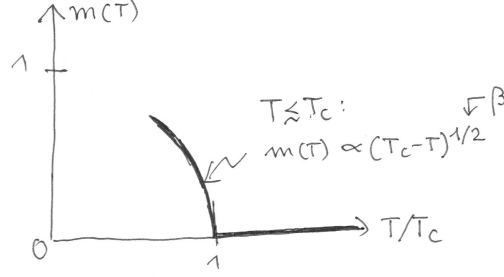


Figure 5.5: Power-law behaviour of the magnetization in mean-field prediction. Critical exponent  $\beta = 1/2$ .

### 5.1.6 Critical Exponents in Mean-Field Theory

Critical behaviour is characterized by singularities in various response functions.

#### Magnetization

For  $T < T_c$  close to  $T_c$ , magnetization  $m_0 \rightarrow 0$ . In this limit, we can expand  $\tanh x = x - x^3/3 + O(x^5)$  to obtain

$$m_0 = \beta z J m_0 - \frac{1}{3}(\beta z J)^3 m_0^3 + \dots \quad (5.50)$$

Dividing by  $m_0$ , we can solve as

$$m_0 = \pm \sqrt{3} \left( \frac{k_B T}{z J} \right)^{3/2} \left( \frac{z J}{k_B T} - 1 \right)^{1/2}. \quad (5.51)$$

Using  $T_c = z J / k_B$  we obtain

$$\boxed{m_0 = \pm \sqrt{3} \left( \frac{T}{T_c} \right)^{3/2} \left( \frac{T_c}{T} - 1 \right)^{1/2}} \quad (5.52)$$

The first factor depends only weakly on  $T$  around  $T_c$ ; the dominant contribution comes from the second factor which is singular at  $T = T_c$  (see Fig. 5.5):

$$m_0(T) \sim (T_c - T)^{1/2} \quad (T \rightarrow T_c^-) \quad (5.53)$$

Mean-field theory (correctly) predicts that the magnetization vanishes as a power law with temperature. The critical exponent, which is conventionally called

$\beta$ , is predicted to be  $\frac{1}{2}$  (which we will find to be incorrect; it is rather  $\approx 0.31$ ):

$$\boxed{m(T) \sim (T_c - T)^\beta \quad \beta = \frac{1}{2}} \quad (5.54)$$

### Susceptibility

In the magnetic case, we consider isothermal susceptibility per spin

$$\chi(T, H) = \left. \frac{\partial m}{\partial H} \right|_T, \quad (5.55)$$

which we obtain by taking the variation of the self-consistency equation  $m = \tanh \beta(zJm + H)$  in  $m$  and  $H$ . From

$$\delta m = \frac{1}{\cosh^2 \beta(zJm + H)} \beta z J \delta m + \frac{1}{\cosh^2 \beta(zJm + H)} \beta \delta h \quad (5.56)$$

susceptibility can be read off directly. In the case  $H = 0$  it reads

$$\chi(T, 0) = \frac{\beta}{\cosh^2 \beta(zJm + H) - \beta z J} \quad (5.57)$$

We now have to insert  $m$  as obtained in the mean-field approximation.

- $T > T_c$ : In this case,  $m = 0$  and

$$\chi(T, 0) = \frac{\beta}{1 - \beta z J} = \frac{\beta}{\beta_c z J - \beta z J} = \frac{1}{k_B(T - T_c)} \quad (5.58)$$

Susceptibility diverges as  $(T - T_c)^{-1}$  for  $T \rightarrow T_c^+$ .

- $T < T_c$ : Close to the transition,  $m$  will be small and we can expand  $\cosh^2 \epsilon \approx 1 + \epsilon^2$  to lowest non-trivial order. Then we obtain using Eq. (5.50)

$$\chi(T, 0) = \frac{\beta}{1 + (\beta z J)^2 m^2 - (\beta z J)} = \frac{\beta}{1 + 3(\beta z J - 1) - (\beta z J)} = \frac{1}{2k_B(T_c - T)}. \quad (5.59)$$

The susceptibility diverges with a power law both above and below the critical temperature  $T_c$ . By convention one uses the exponent(s)  $\gamma_{\pm}$ :

$$\boxed{\chi(T, 0) \sim A_{\pm} |T - T_c|^{-\gamma_{\pm}} \quad \gamma_{\pm} = 1 \quad A^+ = 2A^-} \quad (5.60)$$

### Heat Capacity

The heat capacity (which we consider at zero field  $H = 0$ ) is given by the derivative of the internal energy  $U$  with respect to temperature  $T$ . In the Weiss approximation  $U$  is given as

$$U = \langle \mathcal{H} \rangle = -J \sum_{\langle i,j \rangle} \langle s_i \rangle \langle s_j \rangle = -J \frac{Nz}{2} m^2. \quad (5.61)$$

At this level of approximation  $m^2$  is given by Eq. (5.52) as

$$m^2 = \begin{cases} 3 \left( \frac{T}{T_c} \right)^3 \left( \frac{T_c}{T} - 1 \right) = 3T_c^{-3} T^2 (T_c - T) & (T < T_c) \\ 0 & (T > T_c) \end{cases} \quad (5.62)$$

Upon insertion, we find that  $C = \partial U / \partial T = 0$  for  $T > T_c$ . For  $T < T_c$  we obtain

$$\frac{\partial U}{\partial T} = -J \frac{3Nz}{2} T_c^{-3} T (2T_c - 3T). \quad (5.63)$$

Approaching  $T_c$  from below, we obtain with  $T_c = Jz/k_B$

$$C = \frac{3}{2} N k_B. \quad (5.64)$$

Hence, in the Weiss mean-field theory the heat capacity does *not* exhibit a power-law divergence as  $C \sim B_{\pm} |T - T_c|^{-\alpha}$ , but it has a discontinuous jump at the phase transition. This is not confirmed by either exact calculation where available or experiment. More advanced mean-field schemes do not yield the correct qualitative behaviour, either.

### Critical Isotherm

The *critical isotherm*  $m(T_c, H)$  traces the dependence of  $m$  on  $H$  at the critical temperature  $T_c$ . To obtain it, we expand the Weiss consistency equation to third order in the hyperbolic tangent,

$$m = \beta(Jzm + H) - \frac{1}{3} [\beta(Jzm + H)]^3.$$

Using  $\beta_c z J = 1$  at criticality, this turns into

$$\beta_c H = \frac{1}{3} (m + \beta_c H)^3.$$

In the limit of very small field  $H \rightarrow 0$  we approximate the right hand side in lowest order to obtain

$$\boxed{\beta_c H = \frac{m^3}{3} \quad H \sim m^\delta \quad \delta = 3} \quad (5.65)$$

Here we have assumed  $H, m > 0$  for simplicity of the expression and called the exponent  $\delta$  by convention.

## 5.2 Landau Theory

In 1936, Lev Landau (1908 – 1968) developed a very simple theory of phase transitions that nevertheless manages to give a phenomenological description of both first order and second order phase transitions and their interplay.

The fundamental paradigm of Landau theory is that phase transitions are described by an *order parameter* which describes some local property of the system which is finite on the “ordered” side of the transition and zero on the “disordered” side. Its identification is the first crucial step: for Ising magnets it is obviously magnetization. In what follows we will first assume that the order parameter is a scalar, but in general it will be a  $n$ -dimensional vector.

The fundamental assumption of Landau theory is that the Gibbs free energy can be expanded in a power series of the order parameter  $m$ , where the only constraint are the underlying symmetries of the system, that should be respected. For example, an inversion symmetry of the system implies that only even powers of the order parameter may appear. We take  $m$  to be intensive, but nothing changes if we switch to the extensive  $M = Nm$  as order parameter.

The problem with this assumption is that the free energy cannot be truly expanded in a power series at the phase transition, because the phase transition is associated with some non-analyticity in some derivative of the free energy, which therefore should not exist. But we can describe phase transitions in Landau theory, and the reason for this is that the actual free energy is always some minimum of the free energy function. The minimum operation is *not* necessarily analytic, and we will see how it brings about non-analyticities.

Let us consider an Ising magnet at  $H = 0$ . The free energy should not depend on the sign of  $m$ :

$$G(T, m) = G(T, -m) \quad (5.66)$$

Therefore, only even powers of  $m$  should appear, and we expand as

$$G(m, T) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6 + \dots \quad (5.67)$$



The prefactors could of course be absorbed into the coefficients  $b(T), \dots$ , but are convenient once we take derivatives. But this varies from author to author, and in Chapter 6 on an extension of Landau theory, *Ginzburg-Landau theory*, we will find it convenient to choose another convention.

The important question is whether the functions  $b(T), c(T), \dots$  change sign, and if so, at which temperature? We will discuss various scenarios and see that they lead to continuous and first-order phase transitions as well as a new phenomenon, *tricritical points*.

### 5.2.1 Continuous Transitions

In the first scenario, we assume  $c, d, e > 0$  and

$$b(T) = b_0(T - T_c), \quad (5.68)$$

i.e. a Taylor expansion of  $b(T)$  up to linear order, where we assume  $b_0 > 0$ . Many physical systems can be represented like this; we have already seen one example in Section 5.1.3.

#### Magnetization

Under the provisions just made, we can identify the value of the order parameter via

$$0 \stackrel{!}{=} \left. \frac{\partial G}{\partial m} \right|_T = bm + cm^3 + dm^5 + \dots \quad (5.69)$$

Obviously,  $m = 0$  is a solution, corresponding to a disordered phase. Other solutions are given by  $0 = b(T) + c(T)m^2 + d(T)m^4 + \dots$ . Truncating after the second term for simplicity, we find  $m_0 = \pm \sqrt{-b(T)/c(T)}$  if  $b(T) < 0$ , hence  $T < T_c$ . Close to  $T_c$ , we can approximate  $c(T) \approx c(T_c) > 0$ , such that we obtain

$$\boxed{m_0 \approx \pm \sqrt{\frac{b_0}{c(T_c)}} \sqrt{T_c - T} \quad T \rightarrow T_c^-} \quad (5.70)$$

Graphically, we can represent three typical forms of the free energy for  $T > T_c$ ,  $T = T_c$  and  $T < T_c$  (Fig. 5.6). If temperature drops below  $T_c$ , instead of one extremum (more specifically, minimum) at  $m = 0$ , there are now three at  $m = 0, \pm m_0$ . As the free energy ultimately is monotonically growing for  $|m|$  large, the additional extrema must be minima, and the central extremum at  $m = 0$  must be a maximum. Hence, the order parameter is now given by  $m_0$ . This can be checked by evaluating the free energy for all three extrema explicitly. The order parameter  $m$  changes continuously at all times, hence there is no first order phase transition.

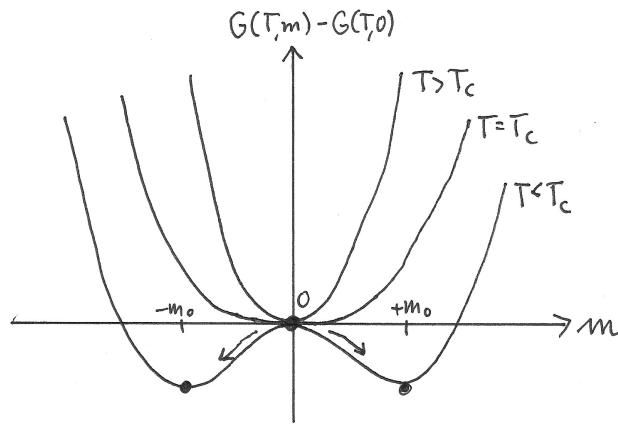


Figure 5.6: Shapes of the free energy versus order parameter  $m$  in Landau theory (scenario for a continuous phase transition,  $c, d, e > 0$ ): above  $T_c$ , there is one global minimum at  $m = 0$ . Positive prefactors of the higher powers of  $m$  ensure stability, i.e. prevent a minimum of the free energy at some unphysical diverging value of  $m$ . At  $T_c$ , the free energy becomes flat at  $m = 0$ , i.e. the derivative develops three zeros. Two of the extrema separate away at  $T < T_c$  and are minima due to symmetry and the stability requirement. Their positions give the new values of the order parameter  $\pm m_0$ .

### Heat Capacity

In order to see how a non-analyticity is generated at  $T_c$ , we consider the heat capacity  $C = T(\partial S/\partial T)$ . Entropy  $S$  itself is a first derivative,

$$S = -\frac{\partial G}{\partial T} = -a' - \frac{b'}{2}m^2 - \frac{c'}{4}m^4 - \dots - \frac{b}{2}(m^2)' - \frac{c}{4}(m^4)', \quad (5.71)$$

where the primes indicate derivatives with respect to temperature. Taking another derivative, we obtain

$$C = -Ta'' - Tb'(m^2)' - \frac{Tb}{2}(m^2)'' - \frac{Tc''}{4}m^4 - \frac{Tc'}{2}(m^4)' - \frac{Tc}{4}(m^4)'' - \dots \quad (5.72)$$

in orders up to  $m^4$ .  $b'' = 0$  as  $b$  is linear in  $T$ .

For  $T > T_c$ ,  $m = 0$ ; so are all derivatives of  $m$ . Hence

$$C = -Ta'' \quad (T > T_c) \quad (5.73)$$

For  $T < T_c$ , we consider  $m^2 = (b_0/c)(T_c - T)$ . Then  $(m^2)' = -b_0/c$  and  $(m^2)'' = 0$ . At the same time  $m^4 = (b_0^2/c^2)(T_c - T)^2$ , hence  $(m^4)' = -(2b_0^2/c^2)(T_c - T)$  and  $(m^4)'' = 2b_0^2/c^2$ .

Close to the transition,  $m$  is very small but changes rapidly. Therefore we can assume

$$m^4 < (m^4)' \ll (m^4)'' \quad (5.74)$$

and the dominant contributions to  $C$  read for  $T \rightarrow T_c^-$ :

$$C = -Ta'' - Tb'(m^2)' - (Tc/4)(m^4)'' = -Ta'' + \frac{Tb_0^2}{2c} \quad (5.75)$$

Hence, we have a drop (discontinuity) in  $C$  right at  $T_c$ , going towards higher temperatures:

$$\Delta C = \frac{T_c b_0^2}{2c} \quad (5.76)$$

This scenario of Landau theory therefore describes a *continuous phase transition*. The critical exponent of the order parameter is  $\beta = 1/2$ , the critical exponent of the heat capacity is by convention set to  $\alpha = 0$ .

### 5.2.2 First-Order Transitions

The situation changes if we assume that  $c(T)$  has a sign change, too, which we assume to happen at  $T^*$ :  $c(T) < 0$  for  $T < T^*$  and  $c(T) > 0$  for  $T > T^*$ . If  $c(T) < 0$ , the stability of the system has to be ensured by  $d(T), e(T) > 0$ . The consequences of the sign change of  $c(T)$  depend on which scenario prevails:

- (1)  $T^* < T_c$  will give again a continuous phase transition
- (2)  $T^* > T_c$  will give a first-order phase transition
- (3)  $T^* = T_c$  will give a tricritical point

### Continuous Phase Transition

Let us briefly discuss the first case (1). For  $T > T^*$  we have exactly the same scenario as before,  $c(T) > 0$ , and the sign change of  $b(T)$  at  $T_c$  generates a continuous phase transition. The sign change in  $c(T)$  at the lower temperature  $T^*$  does not generate any additional minima. To see this, consider

$$0 = \left. \frac{\partial G}{\partial m} \right|_T = bm + cm^3 + dm^5 = m(b + cm^2 + dm^4). \quad (5.77)$$

$m = 0$  is always a solution. For the alternative solutions, we focus on the positive solutions of the quadratic equation  $0 = b + cx + dx^2$ , because  $x = m^2 \geq 0$ . The two solutions read

$$x_{\pm} = -\frac{c}{2d} \pm \frac{1}{2d} \sqrt{c^2 - 4db}. \quad (5.78)$$

If we are below  $T_c$ ,  $b < 0$ . Hence, the square root is greater than  $|c|$ , and there is only one positive solution

$$m^2 = x_+ = -\frac{c}{2d} + \frac{1}{2d} \sqrt{c^2 - 4db} > 0, \quad (5.79)$$

independent of the sign of  $c$ .

### First-Order Phase Transition

Let us now turn to the more exciting case (2). We reconsider the analysis of the solutions of  $0 = m(b + cm^2 + dm^4)$ .  $m = 0$  is always a solution. The solutions of  $0 = b + cx + dx^2$  with  $x = m^2$  read again

$$x_{\pm} = -\frac{c}{2d} \pm \frac{1}{2d} \sqrt{c^2 - 4db}, \quad (5.80)$$

but the different pattern of sign changes leads to a substantially different outcome.

- For  $T > T^* > T_c$ ,  $b, c, d > 0$ . Then the square root is either imaginary (no real solution for  $x$ ) or less than  $c$  (no positive solution for  $x$ ).  $m = 0$  remains the only solution, as would also be clear from a graphical inspection.

- For  $T^* > T > T_c$ ,  $b, d > 0$  but  $c < 0$ . Then  $-c/(2d) > 0$ , and there might be 2 positive solutions for  $x$ , hence 4 additional solutions for  $m_0$  (symmetric about  $m = 0$ ). If  $c^2 - 4db < 0$ , there are again no positive solutions, hence only  $m = 0$ . If  $c^2 - 4db > 0$ , there are now two positive solutions for  $x$ , hence  $m^2$ . There must be a temperature  $\tilde{T}$  with  $T_c < \tilde{T} < T^*$  where this happens, as  $b \rightarrow 0$  as  $T \rightarrow T_c^+$ . This corresponds to 4 new solutions for the order parameter,  $\pm\sqrt{x_+}$  and  $\pm\sqrt{x_-}$ . Due to stability and symmetry, the 5 extrema must be ordered min – max – min – max – min. What the physical system now does is a competition between the minimum at  $m = 0$  and the two minima at  $m_0 = \pm\sqrt{-\frac{c}{2d} + \frac{1}{2d}\sqrt{c^2 - 4db}}$ : which one is a global minimum of the free energy? The phase transition will happen if they all have the same free energy at some temperature  $T_1$ .

We therefore solve for

$$G(m_0) - G(0) = \frac{1}{2}b(T_1)m_0^2 + \frac{1}{4}c(T_1)m_0^4 + \frac{1}{6}d(T_1)m_0^6 \stackrel{!}{=} 0 \quad (5.81)$$

One solution would obviously be provided by  $m_0 = 0$ . Of interest to us is the alternative solution

$$\frac{1}{2}b(T_1) + \frac{1}{4}c(T_1)m_0^2 + \frac{1}{6}d(T_1)m_0^4 = 0, \quad (5.82)$$

where we insert our previous result for  $m_0$ , namely  $b(T_1) = -c(T_1)m_0^2 - d(T_1)m_0^4$ . Then

$$0 = -\frac{1}{3}d(T_1)m_0^2 - \frac{1}{4}c(T_1) \quad (5.83)$$

which we can solve trivially for

$$m_0^2 = -\frac{3c(T_1)}{4d(T_1)} \quad (5.84)$$

as the value where the phase transition happens. As there is a sudden jump in the value of the order parameter, the phase transition at  $T = T_1$  is a *first-order phase transition*.

To check that this transition happens above  $T_c$ , hence preempts the continuous phase transition, we determine

$$b(T_1) = -d(T_1)m_0^4 - c(T_1)m_0^2 = \frac{3c(T_1)^2}{16d(T_1)} > 0. \quad (5.85)$$

If  $b(T_1) > 0$ , then  $T_1 > T_c$ .

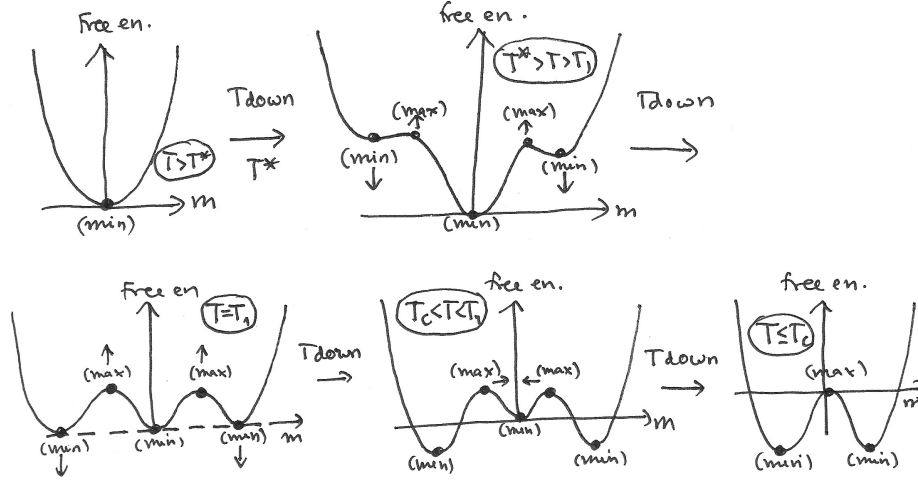


Figure 5.7: Shapes of the free energy versus order parameter  $m$  in Landau theory (scenario for a first-order phase transition:  $c$  changes sign at a higher temperature  $T^*$  than  $b$  (at  $T_c$ )): we descend with temperature. Above  $T^*$ , there is one global minimum at  $m = 0$ . Positive prefactors of the higher powers of  $m$  ensure stability, i.e. prevent a minimum of the free energy at some unphysical diverging value of  $m$ . At some  $\tilde{T}$ , the free energy develops five extrema, with minima for the largest values of  $m$  and  $m = 0$ . At  $T_1 > T_c$ , the two outlying minima turn from local into global minima, a first-order phase transition happens. At  $T = T_c$  the two maxima merge into the central minimum, which becomes a maximum. At  $T < T_c$ , there is a maximum separating two minima.

- For  $T < T_c < T^*$ , nothing special happens. If  $b$  turns negative, the second (smaller) solution of the quadratic equation turns negative, and we are back to three solutions for  $m$ , namely  $m = 0$  and  $m = \pm m_0$ . The latter two must then be minima, which they already were. The two vanishing maxima merge at  $T = T_c$  into the central minimum, which then turns into a maximum.

The shapes of the free energy are shown for illustrative purposes in Fig. 5.7.

### 5.2.3 Tricritical Points

The situation that  $T^* = T_c$ , that both  $b(T)$  and  $c(T)$  change sign at exactly the same temperature, might seem such a rare coincidence that it is of no practical relevance. This is maybe true if temperature is the only control parameter in the system. As soon as there is at least a second such “tuning” parameter, it may be

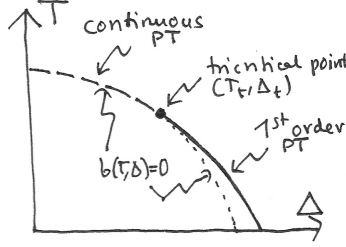


Figure 5.8: Tricritical phase transition: The dashed-dotted line is the line of *potential* locations of continuous phase transitions, as  $b = 0$ . They however only happen in the dashed part, because they are preempted by a first-order transition line. The matching point of the first-order and continuous PT (phase transition) lines is the *tricritical point*  $(T_t, \Delta_t)$ . The slopes of both curves are identical at  $(T_t, \Delta_t)$ .

possible to engineer exactly this situation. A good example is provided by the Blume-Emery-Griffiths model for mixtures of  $^3\text{He}$  and  $^4\text{He}$ . Here, we will not be very specific about this tuning parameter  $\Delta$ ; except that we take it to be intensive. Still assuming symmetry with respect to the sign of the order parameter, the free energy is given in Landau theory as

$$G(T, m, \Delta) = a(T, \Delta) + \frac{1}{2}b(T, \Delta)m^2 + \frac{1}{4}c(T, \Delta)m^4 + \frac{1}{6}d(T, \Delta)m^6. \quad (5.86)$$

Consider Fig. 5.8.  $b(T, \Delta) = 0$  defines a line on which a continuous phase transition will happen, unless it is preempted (as just discussed) by a first-order phase transition, which will happen if  $c$  changes sign for a higher temperature than  $b$ . Assume that we can control  $c(T, \Delta)$  in the following way. Calling the temperatures of sign changes again  $T_c$  for  $b$  and  $T^*$  for  $c$ ,

- $\Delta > \Delta_t$ :  $T^* > T_c$
- $\Delta < \Delta_t$ :  $T^* < T_c$

This gives the scenario shown in the Fig. 5.8. The matching point of the first-order and continuous PT lines is the *tricritical point*  $(T_t, \Delta_t)$ . Let us now discuss the behaviour of the transition lines at the tricritical point. To simplify notation, we introduce  $b_T$  and  $b_\Delta$  (and similarly for  $c$ ) for the partial derivatives  $\partial b / \partial T|_\Delta$  and  $\partial b / \partial \Delta|_T$ .

The location of the first-order transitions is given by [Eq. (5.85)]

$$b(T, \Delta) = \frac{3c^2(T, \Delta)}{16d(T, \Delta)}, \quad (5.87)$$

and the location of the (possible) continuous phase transitions by

$$b(T, \Delta) = 0. \quad (5.88)$$

The slope of this critical line is given by

$$\left. \frac{d\Delta}{dT} \right|_{\text{crit}} = -\frac{b_T}{b_\Delta}. \quad (5.89)$$

At the same time, we can take the variation of the first-order line to turn Eq. (5.87) into

$$b_\Delta \delta\Delta + b_T \delta T - \frac{6c(c_T \delta T + c_\Delta \delta\Delta)}{16d} + \frac{3c^2}{16d^2} (d_T \Delta T + d_\Delta \delta\Delta) = 0. \quad (5.90)$$

This gives a slope of the first-order line as

$$\left. \frac{d\Delta}{dT} \right|_{\text{first order}} = -\frac{b_T - (3/8)(cc_T/d) + (3c^2/16d^2)d_T}{b_\Delta - (3/8)(cc_\Delta/d) + (3c^2/16d^2)d_\Delta} = -\frac{b_T - (3/8)cc_T + bd_T}{b_\Delta - (3/8)cc_\Delta + bd_\Delta}. \quad (5.91)$$

At the tricritical point,  $b \rightarrow 0$ ,  $c \rightarrow 0$ , hence

$$\left. \frac{d\Delta}{dT} \right|_{\text{first order, tricritical}} = -\frac{b_T}{b_\Delta}. \quad (5.92)$$

The slopes of (5.89) and (5.92) are therefore identical, there is no kink where the transition lines join.

To analyze the behaviour right at the tricritical point, we remember that in thermodynamics external control parameters come with conjugate quantities such that in energy expressions terms like  $-pdV$  or  $\mu dN$  appear. Let us call  $\zeta$  the intensive conjugate quantity to  $\Delta$ . Then, if  $g = G/N$ , we have

$$\zeta = -\left. \frac{\partial g}{\partial \Delta} \right|_T, \quad (5.93)$$

where the sign is an arbitrary convention. Along the first-order transition line, we have, using the values for  $m$  at both sides of the transition, to lowest order

$$\zeta_+ \approx -a_\Delta \quad \zeta_- \approx -a_\Delta + \frac{3}{8d}(b_\Delta c + c_\Delta b). \quad (5.94)$$

Then

$$\delta\zeta = \zeta_+ - \zeta_- \approx -\frac{3}{8d}(b_\Delta c + c_\Delta b). \quad (5.95)$$

(The difference was written such as to make  $\delta\zeta > 0$ .) In the  $T$ - $\zeta$  plane, the phase diagram therefore looks somewhat like in Fig. 5.9: there is a coexistence region opening up below  $T_t$ .



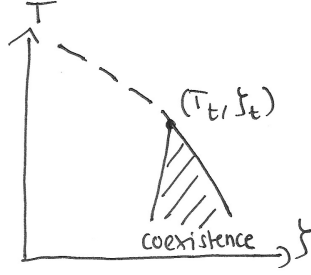


Figure 5.9: Coexistence region below  $T_t$  in a  $T$ - $\zeta$  plane, where  $\zeta$  is conjugate to the control parameter  $\Delta$ .

As previously discussed, the order parameter at the tricritical point must obey

$$m^2 = -\frac{c}{2d} + \sqrt{c^2/4d^2 - b/d}. \quad (5.96)$$

Now we approach the tricritical point, hence  $b \rightarrow 0$  and  $c \rightarrow 0$ . If both are small, then it is reasonable to assume (at first) that  $|b| \gg |c^2|$  and  $|b/d| \gg c^2/4d^2$ . If this holds, we can neglect the contributions from  $c/2d$  and obtain

$$m(T) = (b/d)^{1/4} \sim (b_0/d)^{1/4} (T_t - T)^{1/4} \quad \beta = \frac{1}{4} \quad (\text{tricritical}) \quad (5.97)$$

for temperatures below  $T_t$ . But if we approach the tricritical point along the critical line  $b = 0$ ,  $|b/d| < c^2/4d^2$  in a narrow region around it. In this narrow region, we find that  $m^2 \propto c$ . Linearizing  $c$  around its zero at  $T = T_t$ , we obtain the “normal” critical behaviour

$$m(T) = (T_t - T)^{1/2} \quad \beta = \frac{1}{2} \quad (\text{critical}) \quad (5.98)$$

for temperatures below  $T_t$ .

The crossover line between the two types of criticality is defined by  $b/d \approx c^2/4d^2$ . With additional calculations, one can determine all critical and tricritical exponents as

$$\begin{array}{lll} \beta_c = \frac{1}{2} & \gamma_c = 2 & \alpha_c = -1 \\ \beta_c = \frac{1}{4} & \gamma_c = 1 & \alpha_c = \frac{1}{2} \end{array} \quad (5.99)$$

A sketch of the regions is given in Fig. 5.10.

### 5.2.4 Symmetry and First-Order Transitions

So far, we have assumed a fundamental invariance of  $G(T, m)$  with respect to a sign change in  $m$ . Let us now consider the case

$$G(T, m) \neq G(T, -m). \quad (5.100)$$

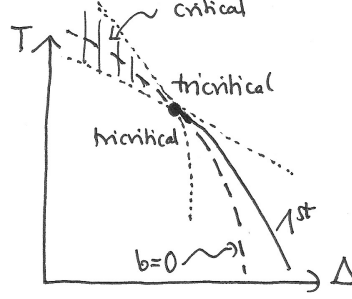


Figure 5.10: Critical and tricritical regions in the vicinity of the tricritical point  $(T_t, \Delta_t)$  in a  $T$ - $\Delta$  diagram.

This opens up the possibility of *odd* powers of  $m$  appearing in the free energy expansion. It is easy to show that by a suitable transformation  $m \rightarrow m + \tilde{m}$  one can make the linear term always disappear. The most general form of the free energy therefore reads

$$G(T, m) = a(T) + \frac{1}{2}b(T)m^2 - \frac{1}{3}c(T)m^3 + \frac{1}{4}d(T)m^4. \quad (5.101)$$

The sign in front of the  $m^3$  term is of course arbitrary; it is chosen such that the interesting physics happens for  $c(T) > 0$  (for all  $T$ ). As before,  $b(T) \simeq b_0(T - T_c)$ . Then the finite order parameter  $m_0$  is given by

$$0 \stackrel{!}{=} \left. \frac{\partial G}{\partial m} \right|_{m_0} = bm_0 - cm_0^2 + dm_0^3, \quad (5.102)$$

hence  $0 = b - cm_0 + dm_0^2$ . The transition happens if  $G(T_1, m_0) = G(T_1, 0)$ , this determines

$$m_0 = \frac{2c}{3d}. \quad (5.103)$$

A simple calculation gives that at the transition

$$b = \frac{2c^2}{9d} > 0, \quad (5.104)$$

hence there is a first-order transition at  $T_1 > T_c$ . A sketch of the free energies at various temperatures is shown in Fig. 5.11.

In this case, the first-order transition is not due to a sign change in  $c$ , but to the appearance of a cubic term due to the breaking of the inversion symmetry! Had we reversed the sign of the  $m^3$  term,  $m_0 < 0$  instead of  $m_0 > 0$ , which

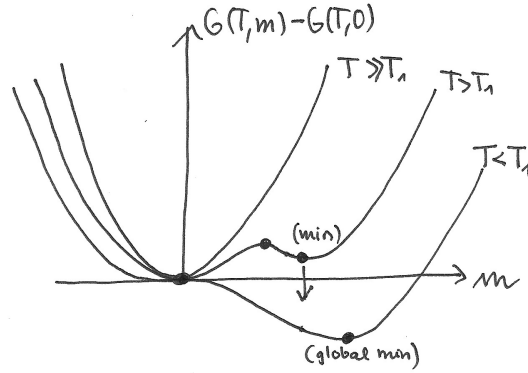


Figure 5.11: Free energies in the presence of a cubic term: At some temperature, a local minimum at finite order parameter  $m_0$  turns into a global minimum, replacing  $m = 0$  and generating a first-order phase transition.

now is different physics. Indeed, if we associate a continuous phase transition with symmetry breaking, there can't be a continuous phase transition for lack of a breakable symmetry.

A classical example for such a symmetry-driven first-order transition is provided by the  $q$ -state *Potts model*

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} \delta_{s_i, s_j} \quad s_i = 0, 1, \dots, q-1 \quad (5.105)$$

for  $q = 3$  (for  $q = 2$  we revert to the Ising model).

