

## Statistical fields

### 2.1 Introduction

We noted in the previous chapter that the singular behavior of thermodynamic functions at a critical point (the termination of a coexistence line) can be characterized by a set of critical exponents  $\{\alpha, \beta, \gamma, \dots\}$ . Experimental observations indicate that these exponents are quite *universal*, i.e. independent of the material under investigation, and to some extent, of the nature of the phase transition. For example, the vanishing of the coexistence boundary in the condensation of  $\text{CO}_2$  has the same singular behavior as that of the phase separation of protein solutions into dilute and dense components. This universality of behavior needs to be explained. We also noted that the divergence of the response functions, as well as direct observations of fluctuations via scattering studies, indicate that fluctuations have long wavelengths in the vicinity of the critical point, and are correlated over distances  $\xi \gg a$ , where  $a$  is a typical interparticle spacing. Such correlated fluctuations involve many particles and a coarse-graining approach, in the spirit of the theory of elasticity, may be appropriate to their description. Here we shall construct such a *statistical field theory*.

We shall frame the discussion in the language of a magnetic system whose symmetries are more transparent, although the results are of more general applicability. Consider a material such as iron, which is experimentally observed to be ferromagnetic below a Curie temperature  $T_c$ , as in Fig. 1.4. The microscopic origin of magnetism is quantum mechanical, involving such elements as itinerant electrons, their spins, and their interactions, described by a microscopic Hamiltonian  $\mathcal{H}_{\text{mic}}$ . In principle, all thermodynamic properties of the system can be extracted from a partition function obtained by summing over all degrees of freedom, written symbolically as

$$Z(T) = \text{tr} \left[ e^{-\beta \mathcal{H}_{\text{mic}}} \right], \quad \text{with} \quad \beta = \frac{1}{k_B T}. \quad (2.1)$$

In practice, this formula is not of much use, as the microscopic Hamiltonian, and degrees of freedom, are too complicated to make a calculation possible.

A microscopic theory is certainly necessary to find out which elements are likely to produce ferromagnetism. However, given that there is magnetic behavior, such a theory is not necessarily useful to describe the disappearance of

magnetization as a result of thermal fluctuations. For addressing the latter, the (quantum) statistical mechanics of the collection of interacting electrons is an excessively complicated starting point. Instead, we make the observation that the important degrees of freedom close to the Curie point are long wavelength collective excitations of spins (much like the long wavelength phonons that dominate the heat capacity of solids at low temperatures). It thus makes more sense to focus on the statistical properties of these fluctuations which are ultimately responsible for the phase transition. Towards this end, we change focus from the microscopic scales to intermediate *mesoscopic* scales which are much larger than the lattice spacing, but much smaller than the system size. In a manner similar to the coarse graining process depicted in Fig. 1.1, we define a magnetization field  $\vec{m}(\mathbf{x})$ , which represents the average of the elemental spins in the vicinity of a point  $\mathbf{x}$ . It is important to emphasize that while  $\mathbf{x}$  is treated as a continuous variable, the function  $\vec{m}(\mathbf{x})$  does not exhibit any variations at distances of the order of the lattice spacing, i.e. its Fourier transform involves only wavevectors less than some *upper cutoff*  $\Lambda \sim 1/a$ .

The transformation from the original degrees of freedom to the field  $\vec{m}(\mathbf{x})$  is a change of variables. (This mapping is not invertible, as many microscopic details are washed out in the averaging process.) Again, it is in principle possible to obtain the corresponding probabilities for configurations of the field  $\vec{m}(\mathbf{x})$ , by transforming the original microscopic probabilities arising from the Boltzmann weight  $e^{-\beta\mathcal{H}_{\text{mic}}}$ . The partition function is preserved in the process, and can be written as

$$Z(T) = \text{tr} \left[ e^{-\beta\mathcal{H}_{\text{mic}}} \right] \equiv \int \mathcal{D}\vec{m}(\mathbf{x}) \mathcal{W}[\vec{m}(\mathbf{x})]. \quad (2.2)$$

The symbol  $\mathcal{D}\vec{m}(\mathbf{x})$  indicates integrating over all allowed configurations of the field, and will be discussed later. The different configurations of the field are weighted with a probability  $\mathcal{W}[\vec{m}(\mathbf{x})]$ , which is what we would like to find out.

While obtaining the precise form of  $\mathcal{W}[\vec{m}(\mathbf{x})]$  is not easier than solving the full problem, it is in fact possible to describe it in terms of a few phenomenological parameters. (This is similar to describing the energy cost of deforming a solid in terms of a few elastic moduli.) In the context of phase transitions, this approach was first applied by Landau to describe the onset of superfluidity in helium. In fact, the method can quite generally be applied to different types of systems undergoing phase transition, with  $\vec{m}(\mathbf{x})$  describing the corresponding order parameter field. We shall thus generalize the problem, and consider an  $n$ -component field, existing in  $d$ -dimensional space, i.e.

$$\mathbf{x} \equiv (x_1, x_2, \dots, x_d) \in \mathfrak{R}^d \quad (\text{space}), \quad \vec{m} \equiv (m_1, m_2, \dots, m_n) \in \mathfrak{R}^n \\ (\text{order parameter}).$$

Some specific cases covered in this general framework are:

$n = 1$  describes liquid–gas transitions, binary mixtures, as well as uniaxial magnets;

$n = 2$  applies to superfluidity, superconductivity, and planar magnets;

$n = 3$  corresponds to classical magnets.

While most physical situations occur in three-dimensional space ( $d = 3$ ), there are also important phenomena on surfaces ( $d = 2$ ), and in wires ( $d = 1$ ). Relativistic field theory is described by a similar structure, but in  $d = 4$ .

## 2.2 The Landau–Ginzburg Hamiltonian

Using the coarse-grained weight in Eq. 2.2, we can define an effective Hamiltonian

$$\beta\mathcal{H}[\vec{m}(\mathbf{x})] \equiv -\ln \mathcal{W}[\vec{m}(\mathbf{x})], \quad (2.3)$$

which gives the probabilities of the field configurations by a Boltzmann factor. Guided by the steps outlined in the last chapter for generating the elastic theory of a deformed solid, we shall construct  $\beta\mathcal{H}[\vec{m}(\mathbf{x})]$  using the following principles:

**Locality and uniformity:** If a system consists of disconnected parts, the overall probability is obtained as a product of independent probabilities. A corresponding Hamiltonian as in Eq. (2.3) then decomposes into a sum of contributions from each location, going over to an integral in the continuum representation, i.e.

$$\beta\mathcal{H} = \int d^d\mathbf{x} \Phi[\vec{m}(\mathbf{x}), \mathbf{x}]. \quad (2.4)$$

Here,  $\Phi$  is an energy density, which can in principle have a different functional form at different locations. For a material that is *uniform* in space, different positions in  $\mathbf{x}$  are equivalent, and we can drop the explicit dependence of  $\Phi$  on  $\mathbf{x}$ . This will not be the case when the system is in an external potential, or has internal impurities. We are of course interested in more complicated systems in which, as a result of interactions, there is some coupling between different parts of the system. To this end, we generalize Eq. (2.4), by including gradients of the field, to

$$\beta\mathcal{H} = \int d^d\mathbf{x} \Phi[\vec{m}(\mathbf{x}), \nabla\vec{m}, \nabla^2\vec{m}, \dots]. \quad (2.5)$$

Once more, general non-local interactions can be described by including many derivatives. The “local” representation is useful when a good description can be obtained by including only a few derivatives. This is the case for short-range interactions (even including van der Waals interactions in liquid gas mixtures, but fails for long-range (such as Coulomb) interactions.<sup>1</sup>

<sup>1</sup> The precise borderline between long- and short-range interactions will be discussed later.

**Analyticity and polynomial expansions:** The functional form of  $\Phi$  is next written as an expansion in powers of  $\vec{m}$ , and its gradients. To justify such an expansion, let us again examine the simple example of a collection of independent degrees of freedom, say spins. The probability distribution at the microscopic level may be complicated; e.g. spins may be constrained to a fixed magnitude, or quantized to specific values. At the mesoscopic scale, the field  $\vec{m}$  is obtained by averaging many such spins. The averaging process typically simplifies the probability distribution; in most cases the central limit theorem implies that the probability distribution for the sum approaches a Gaussian form.<sup>2</sup> In constructing the statistical field theory, we are in fact searching for generalizations of the central limit theorem for describing interacting degrees of freedom. The key point is that in going from the microscopic to mesoscopic scales, non-analyticities associated with the microscopic degrees of freedom are washed out, and the probability distribution for the coarse-grained field is obtained by an analytic expansion in powers of  $\vec{m}$ . There are of course non-analyticities associated with the phase transition at the macroscopic scale. However, such singularities involve an infinity (macroscopic number) of degrees of freedom. By focusing on the mesoscopic scale we thus avoid possible singularities at both the short and long scales!

**Symmetries:** One element that survives the averaging process is any underlying microscopic symmetry. Such symmetries in turn constrain possible forms and expansions of the effective Hamiltonian. For example, in the absence of an external magnetic field, all directions for magnetization are equivalent, and hence  $\mathcal{H}[R_n \vec{m}(\mathbf{x})] = \mathcal{H}[\vec{m}(\mathbf{x})]$ , where  $R_n$  is a rotation in the  $n$ -dimensional order parameter space. A linear term in  $\vec{m}$  is not consistent with this symmetry, and the first term in an expansion is proportional to

$$m^2(\mathbf{x}) \equiv \vec{m}(\mathbf{x}) \cdot \vec{m}(\mathbf{x}) \equiv \sum_{i=1}^n m_i(\mathbf{x}) m_i(\mathbf{x}), \quad (2.6)$$

where  $\{m_i\}$  indicate the components of the vector field. Higher order terms in the series are constructed from

$$m^4(\mathbf{x}) \equiv (m^2(\mathbf{x}))^2, \quad m^6(\mathbf{x}) \equiv (m^2(\mathbf{x}))^3, \quad \dots$$

In constructing terms that involve gradients of the vector field, we should keep in mind the spatial symmetries of the system. In an *isotropic* system all directions in space are equivalent, and we should use combinations of derivatives that are invariant under spatial rotations. The simplest such term is

$$(\nabla \vec{m})^2 \equiv \sum_{i=1}^n \sum_{\alpha=1}^d \partial_{\alpha} m_i \partial_{\alpha} m_i, \quad (2.7)$$

<sup>2</sup> More precisely, upon averaging over  $n$  spins, the coefficient of  $m^2$  approaches a constant, while higher terms in the expansion decay as powers of  $n$ .

with  $\partial_\alpha$  indicating the partial derivative along the  $\alpha$ -th direction in space. If the different directions are not equivalent more terms are allowed. For example, in a two dimensional magnet on a rectangular lattice (unit cell aligned with the axes), the coefficients of  $\partial_1 m_i \partial_1 m_i$  and  $\partial_2 m_i \partial_2 m_i$  can be different. However, by appropriate rescaling of coordinates the leading gradient term can again be changed into the form of Eq. (2.7). A fourth order gradient term in an isotropic system is

$$(\nabla^2 \vec{m})^2 \equiv \sum_{i=1}^n \sum_{\alpha=1}^d \sum_{\beta=1}^d (\partial_\alpha \partial_\alpha m_i) (\partial_\beta \partial_\beta m_i),$$

and a possible quartic term in  $\vec{m}$  is

$$m^2 (\nabla \vec{m})^2 \equiv \sum_{i=1}^n \sum_{j=1}^n \sum_{\alpha=1}^d m_i m_j \partial_\alpha m_j \partial_\alpha m_i.$$

Anisotropies again lead to higher order terms which in general cannot be removed by simple rescalings.

We shall demonstrate shortly that to describe magnetic systems, and in fact most transitions, it is sufficient to include only a few terms, leading to the so called *Landau–Ginzburg* Hamiltonian:

$$\beta \mathcal{H} = \beta F_0 + \int d^d \mathbf{x} \left[ \frac{t}{2} m^2(\mathbf{x}) + u m^4(\mathbf{x}) + \frac{K}{2} (\nabla m)^2 + \cdots - \vec{h} \cdot \vec{m}(\mathbf{x}) \right]. \quad (2.8)$$

The integration over the magnetic and non-magnetic degrees of freedom at short scales also generates an overall constant  $\beta F_0$ . This contribution to the overall free energy is analytic (as discussed earlier), and will be mostly ignored. Equation (2.8) also includes the contribution from the magnetic work  $\vec{B} \cdot \vec{m}$  to the Hamiltonian, where  $\vec{h} \equiv \beta \vec{B}$  and  $\vec{B}$  is the magnetic field.<sup>3</sup> The magnetic field may also generate higher order terms, such as  $m^2 \vec{m} \cdot \vec{h}$ , which are less important than the terms explicitly included above.

**Stability:** Since it originates from a well defined physical problem, the coarse-grained Boltzmann weight must not lead to any unphysical field configurations. In particular, the probability should not diverge for infinitely large values of  $\vec{m}$ . This condition implies that the coefficient of the highest order power of  $\vec{m}$ , e.g. the parameter  $u$  in Eq. (2.8), should be positive. There are related constraints on the signs of the terms involving gradients to avoid oscillatory instabilities.

The Landau–Ginzburg Hamiltonian depends on a set of *phenomenological parameters*  $\{t, u, K, \dots\}$ . These parameters are non-universal functions of

<sup>3</sup> Note that with the inclusion of work against the external field we are dealing with a Gibbs canonical ensemble, and  $-k_B T \ln Z$  is now the Gibbs free energy. This technical distinction is usually ignored, and we shall set  $-k_B T \ln Z = F$ , using the symbol usually reserved for the Helmholtz free energy.

microscopic interactions, *as well as external parameters such as temperature and pressure*. It is essential to fully appreciate the latter point which is a possible source of confusion. While the probability for a particular configuration of the field is given by the Boltzmann weight  $\exp\{-\beta\mathcal{H}[\vec{m}(\mathbf{x})]\}$ , this *does not imply* that all terms in the exponent are proportional to  $(k_B T)^{-1}$ . Such dependence holds only for the true microscopic Hamiltonian. The Landau–Ginzburg Hamiltonian is more correctly an effective free energy obtained by integrating over (coarse graining) the microscopic degrees of freedom, while constraining their average to  $\vec{m}(\mathbf{x})$ . It is precisely because of the difficulty of carrying out such a first principles program that we postulate the form of the resulting effective free energy on the basis of symmetries alone. The price paid is that the phenomenological parameters have unknown functional dependences on the original microscopic parameters, as well as on such external constraints as temperature (since we have to account for the entropy of the short distance fluctuations lost in the coarse-graining process). The constraints on these functional forms again arise from *symmetry, analyticity, and stability*, as discussed in the context of constructing the function form of  $\Phi[\vec{m}]$ . Notably, these mesoscopic coefficients will be analytic functions of the external parameters, e.g. expressible as power series in temperature  $T$ .

### 2.3 Saddle point approximation, and mean-field theory

By focusing only on the coarse-grained magnetization field, we have considerably simplified the original problem. Various thermodynamic functions (and their singular behavior) should now be obtained from the partition function

$$Z = \int \mathcal{D}\vec{m}(\mathbf{x}) \exp\{-\beta\mathcal{H}[\vec{m}(\mathbf{x})]\}, \quad (2.9)$$

corresponding to the Landau–Ginzburg Hamiltonian in Eq. (2.8). The degrees of freedom appearing in the Hamiltonian are functions of  $\mathbf{x}$ , the symbol  $\int \mathcal{D}\vec{m}(\mathbf{x})$  refers to a *functional integral*. In practice, the functional integral is obtained as a limit of discrete integrals: The continuous coordinate  $\mathbf{x} \equiv (x_1, x_2, \dots, x_d)$  is first discretized into a lattice of  $\mathcal{N}$  points  $\mathbf{i} \equiv (i_1, i_2, \dots, i_d)$ , at a lattice distance  $a$ ; the various derivatives are replaced with appropriate differences, and the functional integral is obtained as

$$\int \mathcal{D}\vec{m}(\mathbf{x}) \mathcal{F}\left[\vec{m}(\mathbf{x}), \frac{\partial \vec{m}}{\partial x_\alpha}, \dots\right] \equiv \lim_{\mathcal{N} \rightarrow \infty} \prod_{i=1}^{\mathcal{N}} d\vec{m}_i \mathcal{F}\left[\vec{m}_i, \frac{\vec{m}_{i_a+1} - \vec{m}_{i_a}}{a}, \dots\right].$$

There are in fact many mathematical concerns regarding the existence of functional integrals. These problems are mostly associated with having too many degrees of freedom at short distances, which allow for rather badly behaved functions. These issues need not concern us since we know that the underlying

problem has a well defined lattice spacing that restricts and controls the short distance behavior.

Even after all these simplifications, it is still not easy to calculate the Landau–Ginzburg partition function in Eq. (2.9). As a first step, we perform a *saddle point approximation* in which the integral in Eq. (2.9) is replaced by the maximum value of the integrand, corresponding to the *most probable* configuration of the field  $\vec{m}(\mathbf{x})$ . The natural tendency of interactions in a magnet is to keep the magnetizations vectors parallel, and hence we expect the parameter  $K$  in Eq. (2.8) to be positive.<sup>4</sup> Any variations in magnitude or direction of  $\vec{m}(\mathbf{x})$  incur an “energy penalty” from the term  $K(\nabla\vec{m})^2$  in Eq. (2.8). Thus the field is uniform in its most probable configuration, and restricting the integration to this subspace gives

$$Z \approx Z_{\text{sp}} = e^{-\beta F_0} \int d\vec{m} \exp \left[ -V \left( \frac{t}{2} m^2 + u m^4 + \cdots - \vec{h} \cdot \vec{m} \right) \right], \quad (2.10)$$

where  $V$  is the system volume. In the limit of  $V \rightarrow \infty$  the integral is governed by the saddle point  $\vec{m}$ , which maximizes the exponent of the integrand. The corresponding saddle point free energy is

$$\beta F_{\text{sp}} = -\ln Z_{\text{sp}} \approx \beta F_0 + V \min \{ \Psi(\vec{m}) \}_{\vec{m}}, \quad (2.11)$$

where

$$\Psi(\vec{m}) \equiv \frac{t}{2} \vec{m}^2 + u (\vec{m}^2)^2 + \cdots - \vec{h} \cdot \vec{m}. \quad (2.12)$$

The most likely magnetization will be aligned to the external field, i.e.  $\vec{m}(\mathbf{x}) = \vec{m}\hat{h}$ ; its magnitude is obtained from

$$\Psi'(\vec{m}) = t\vec{m} + 4u\vec{m}^3 + \cdots - h = 0. \quad (2.13)$$

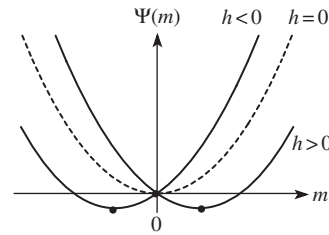
Surprisingly, this simple equation captures the qualitative behavior at a phase transition.

While the function  $\Psi(m)$  is analytic, and has no singularities, the saddle point free energy is Eq. (2.11) may well be non-analytic. This is because the minimization operation is not an analytic procedure, and introduces singularities as we shall shortly demonstrate. What justifies the saddle point evaluation of Eq. (2.10) is the thermodynamic limit of  $V \rightarrow \infty$ , and for finite  $V$ , the integral is perfectly analytic. In the vicinity of the critical point, the magnetization is small, and it is justified to keep only the lowest powers in the expansion of  $\Psi(\vec{m})$ . (We can later check self-consistently that the terms left out of the expansion are indeed small corrections.) The behavior of  $\Psi(m)$  depends strongly on the sign of the parameter  $t$ .

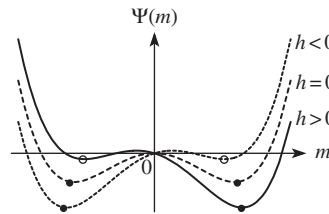
- (1) For  $t > 0$ , the quartic term is not necessary for stability and can be ignored. The solution to Eq. (2.13) is  $\vec{m} = h/t$ , and describes paramagnetic behavior. The most

<sup>4</sup> This is also required by the stability condition.

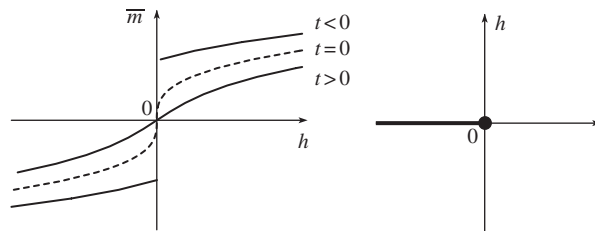
**Fig. 2.1** The function  $\Psi(m)$  for  $t > 0$ , and three values of  $h$ . The most probable magnetization occurs at the minimum of this function (indicated by solid dots), and goes to zero continuously as  $h \rightarrow 0$ .



**Fig. 2.2** The function  $\Psi(m)$  for  $t < 0$ , and three values of  $h$ . The most probable magnetization occurs at the *global* minimum of this function (indicated by solid dots), and goes to zero continuously as  $h \rightarrow 0$ . The metastable minimum is indicated by open dots.



**Fig. 2.3** The magnetization curves obtained from the solution of Eq. (2.13) (*left*), and the corresponding phase diagram (*right*).



probable magnetization is aligned to the magnetic field, and vanishes continuously as  $\vec{h} \rightarrow 0$ . The susceptibility  $\chi = 1/t$ , diverges as  $t \rightarrow 0$ .

- (2) For  $t < 0$ , a quartic term with a positive value of  $u$  is required to insure stability (i.e. a finite magnetization). The function  $\Psi(m)$  can now have two local minima, the global minimum being aligned with the field  $\vec{h}$ . As  $\vec{h} \rightarrow 0$ , the global minimum moves towards a non-zero value, indicating a spontaneous magnetization, even at  $\vec{h} = 0$ , as in a ferromagnet. The direction of  $\vec{m}$  at  $\vec{h} = 0$  is determined by the system's history, and can be realigned by an external field  $\vec{h}$ .

The resulting curves for the most probable magnetization  $\vec{m}(h)$  are quite similar to those of Fig. 1.4. The saddle point evaluation of the Landau–Ginzburg partition function thus results in paramagnetic behavior for  $t > 0$ , and ferromagnetic behavior for  $t < 0$ , with a line of phase transitions terminating at the point  $t = h = 0$ .

As noted earlier, the parameters  $(t, u, K, \dots)$  of the Landau–Ginzburg Hamiltonian are analytic functions of temperature, and can be expanded around



the critical point at  $T = T_c$  in a Taylor series as

$$\begin{cases} t(T, \dots) = a_0 + a_1(T - T_c) + \mathcal{O}(T - T_c)^2, \\ u(T, \dots) = u + u_1(T - T_c) + \mathcal{O}(T - T_c)^2, \\ K(T, \dots) = K + K_1(T - T_c) + \mathcal{O}(T - T_c)^2. \end{cases} \quad (2.14)$$

The expansion coefficients can be regarded as phenomenological parameters which can be determined by comparing to experiments. In particular, matching the phase diagrams in Figs. 1.4 and 2.3 requires that  $t$  should be a monotonic function of temperature which vanishes at  $T_c$ , necessitating  $a_0 = 0$  and  $a_1 = a > 0$ . Stability of the ferromagnetic phase in the vicinity of the critical point requires that  $u$  and  $K$  should be positive. The *minimal set of conditions* for matching the experimental phase diagram of a magnet to that obtained from the saddle point is

$$t = a(T - T_c) + \mathcal{O}(T - T_c)^2, \quad \text{with} \quad (a, u, K) > 0. \quad (2.15)$$

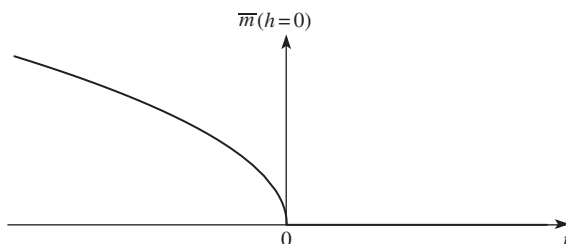
It is of course possible to set additional terms in the expansion, e.g.  $a$  or  $u$ , to zero, and maintain the phase diagram and stability by appropriate choice of the higher order terms. However, such choices are not *generic*, and there is no reason for imposing more constraints than absolutely required by the experiment.

Using Eq. (2.15), we can quantify the singular behaviors predicted by the saddle point evaluations of the free energy in Eqs. (2.11)–(2.13).

- **Magnetization:** In zero field, Eq. (2.13) reduces to  $\partial\Psi/\partial m = t\bar{m} + 4u\bar{m}^3 = \bar{m}(t + 4u\bar{m}^2) = 0$ , and we obtain

$$\bar{m}(h=0) = \begin{cases} 0 & \text{for } t > 0, \\ \sqrt{\frac{-t}{4u}} = \sqrt{\frac{a}{4u}} (T_c - T)^{1/2} & \text{for } t < 0. \end{cases} \quad (2.16)$$

For  $t < 0$ , the non-magnetized solution  $\bar{m} = 0$  is a maximum of  $\Psi(m)$ , and there is a spontaneous magnetization that vanishes with a universal exponent of  $\beta = 1/2$ . The overall amplitude is non-universal and material dependent.



**Fig. 2.4** The saddle point spontaneous magnetization vanishes with a square-root singularity.

Along the critical isotherm (the dashed line of Fig. 2.3), with  $t = 0$ , Eq. (2.13) gives

$$\bar{m}(t=0) = \left(\frac{h}{4u}\right)^{1/3}, \quad (2.17)$$

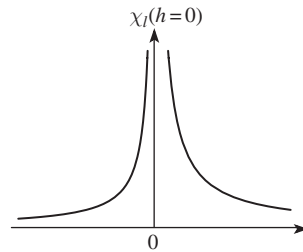
i.e.  $h \propto \bar{m}^\delta$ , with an exponent  $\delta = 3$ .

- **Susceptibility:** The magnetization is aligned to the external field,  $\vec{m} = \bar{m}(h)\hat{h}$ , its magnitude given by the solution to  $t\bar{m} + 4u\bar{m}^3 = h$ . The changes in the magnitude are governed by the *longitudinal susceptibility*  $\chi_\ell$ , whose inverse is easily obtained as

$$\chi_\ell^{-1} = \left.\frac{\partial h}{\partial \bar{m}}\right|_{h=0} = t + 12u\bar{m}^2 = \begin{cases} t & \text{for } t > 0, \text{ and } h = 0, \\ -2t & \text{for } t < 0, \text{ and } h = 0. \end{cases} \quad (2.18)$$

On approaching the critical point from either side, the zero field susceptibility diverges as  $\chi_\pm \sim A_\pm |t|^{-\gamma_\pm}$ , with  $\gamma_+ = \gamma_- = 1$ . Although the amplitudes  $A_\pm$  are material dependent, Eq. (2.18) predicts that their ratio is universal, given by  $A_+/A_- = 2$ . (We shall shortly encounter the *transverse susceptibility*  $\chi_t$ , which describes the change in magnetization in response to a field perpendicular to it. For  $h = 0$ ,  $\chi_t$  is always infinite in the magnetized phase.)

**Fig. 2.5** The zero field longitudinal susceptibility diverges at  $t = 0$ .



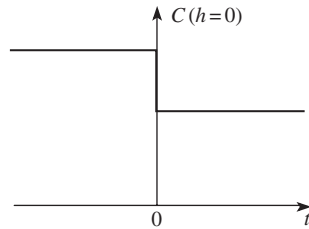
- **Heat capacity:** The free energy for  $h = 0$  is given by

$$\beta F = \beta F_0 + V\Psi(\bar{m}) = \beta F_0 + V \begin{cases} 0 & \text{for } t > 0, \\ -\frac{t^2}{16u} & \text{for } t < 0. \end{cases} \quad (2.19)$$

Since  $t = a(T - T_c) + \dots$ , to leading order in  $(T - T_c)$ , we have  $\partial/\partial T \sim a\partial/\partial t$ . Using similar approximations in the vicinity of the critical point, we find the behavior of the heat capacity at zero field as

$$C(h=0) = -T \frac{\partial^2 F}{\partial T^2} \approx -T_c a^2 \frac{\partial^2}{\partial t^2} (k_B T_c \beta F) = C_0 + V k_B a^2 T_c^2 \times \begin{cases} 0 & \text{for } t > 0, \\ \frac{1}{8u} & \text{for } t < 0. \end{cases} \quad (2.20)$$

The saddle point method thus predicts a discontinuity, rather than a divergence, in the heat capacity. If we insist on describing this singularity as a power law  $t^{-\alpha}$ , we have to choose the exponent  $\alpha = 0$ .



**Fig. 2.6** The saddle point approximation predicts a discontinuous heat capacity.

## 2.4 Continuous symmetry breaking and Goldstone modes

For zero field, although the microscopic Hamiltonian has full rotational symmetry, the low-temperature phase does not. As a specific direction in  $n$ -space is selected for the net magnetization  $\vec{M}$ , there is *spontaneous symmetry breaking*, and a corresponding *long-range order* is established in which the majority of the spins in the system are oriented along  $\vec{M}$ . The original symmetry is still present globally, in the sense that if all local spins are rotated together (i.e. the field transforms as  $\vec{m}(\mathbf{x}) \mapsto \mathfrak{R}\vec{m}(\mathbf{x})$ ), there is no change in energy. Such a rotation transforms one ordered state into an equivalent one. Since a uniform rotation costs no energy, by continuity we expect a rotation that is slowly varying in space (e.g.  $\vec{m}(\mathbf{x}) \mapsto \mathfrak{R}(\mathbf{x})\vec{m}(\mathbf{x})$ , where  $\mathfrak{R}(\mathbf{x})$  only has long wavelength variations) to cost very little energy. Such low energy excitations are called *Goldstone modes*. These collective modes appear in any system with a *broken continuous symmetry*.<sup>5</sup> Phonons in a solid provide a familiar example of Goldstone modes, corresponding to the breaking of translation and rotation symmetries by a crystal structure.

The Goldstone modes appearing in diverse systems share certain common characteristics. Let us explore the origin and behavior of Goldstone modes in the context of *superfluidity*. In analogy to Bose condensation, the superfluid phase has a macroscopic occupation of a single quantum ground state. The order parameter,

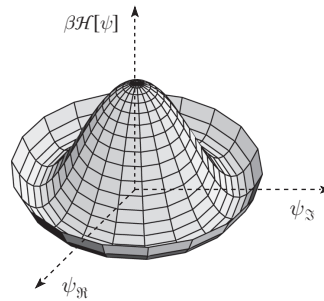
$$\psi(\mathbf{x}) \equiv \psi_{\mathfrak{R}}(\mathbf{x}) + i\psi_{\Im}(\mathbf{x}) \equiv |\psi(\mathbf{x})|e^{i\theta(\mathbf{x})}, \quad (2.21)$$

can be roughly regarded as the ground state component (overlap) of the actual wavefunction in the vicinity of  $\mathbf{x}$ .<sup>6</sup> The phase of the wavefunction is not an observable quantity and should not appear in any physically measurable

<sup>5</sup> There are no Goldstone modes when a discrete symmetry is broken, since it is impossible to produce slowly varying rotations from one state to an equivalent one.

<sup>6</sup> A more rigorous derivation proceeds by second quantization of the Hamiltonian for interacting bosons, and is beyond our current scope.

**Fig. 2.7** The Landau–Ginzburg Hamiltonian of a superfluid for  $t < 0$ .



probability. This observation constrains the form of the effective coarse grained Hamiltonian, leading to an expansion

$$\beta\mathcal{H} = \beta F_0 + \int d^d\mathbf{x} \left[ \frac{K}{2} |\nabla\psi|^2 + \frac{t}{2} |\psi|^2 + u |\psi|^4 + \dots \right]. \quad (2.22)$$

Equation (2.22) is in fact equivalent to the Landau–Ginzburg Hamiltonian with  $n = 2$ , as can be seen by changing variables to the two component field  $\vec{m}(\mathbf{x}) \equiv (\psi_{\Re}(\mathbf{x}), \psi_{\Im}(\mathbf{x}))$ . The superfluid transition is signaled by the onset of a finite value of  $\psi$  for  $t < 0$ . The Landau–Ginzburg Hamiltonian (for a uniform  $\psi$ ) has the shape of a wine bottle (or Mexican hat) for  $t < 0$ .

Minimizing this function sets the magnitude of  $\psi$ , but does not fix its phase  $\theta$ . Now consider a state with a slowly varying phase, i.e. with  $\psi(\mathbf{x}) = \bar{\psi} e^{i\theta(\mathbf{x})}$ . Inserting this form into the Hamiltonian yields an energy

$$\beta\mathcal{H} = \beta\mathcal{H}_0 + \frac{\bar{K}}{2} \int d^d\mathbf{x} (\nabla\theta)^2, \quad (2.23)$$

where  $\bar{K} = K\bar{\psi}^2$ . As in the case of phonons we could have guessed the above form by appealing to the invariance of the energy function under a uniform rotation: Since a transformation  $\theta(\mathbf{x}) \mapsto \theta(\mathbf{x}) + \theta_0$  should not change the energy, the energy density can only depend on gradients  $\theta(\mathbf{x})$ , and the first term in the expansion leads to Eq. (2.23). The reasoning based on symmetry does not give the value of the *stiffness parameter*. By starting from the Landau–Ginzburg form which incorporates both the normal and superfluid phases we find that  $\bar{K}$  is proportional to the square of the order parameter, and vanishes (softens) at the critical point as  $\bar{K} \propto \bar{\psi}^2 \propto t$ .

We can decompose the variations in phase of the order parameter into independent normal modes by setting (in a region of volume  $V$ )

$$\theta(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \theta_{\mathbf{q}}. \quad (2.24)$$

Taking advantage of translational symmetry, Eq. (2.23) then gives

$$\beta\mathcal{H} = \beta\mathcal{H}_0 + \frac{\bar{K}}{2} \sum_{\mathbf{q}} q^2 |\theta(\mathbf{q})|^2. \quad (2.25)$$

We can see that, as in the case of phonons, the energy of a Goldstone mode of wavenumber  $\mathbf{q}$  is proportional to  $q^2$ , and becomes very small at long wavelengths.

## 2.5 Discrete symmetry breaking and domain walls

For a one component (scalar) field, there are two possible values for the magnetization in the ordered phase. While the two possible states have the same energy, it is not possible to continuously deform one into the other. In this case, as well as in other systems with discrete symmetry breaking, different states in the same sample are separated by sharp domain walls. To demonstrate this, consider a scalar field with the Landau–Ginzburg Hamiltonian for  $t < 0$  and  $h = 0$ . A domain wall can be introduced by forcing the two sides of the system to be in different states, e.g. by requiring  $m(x \rightarrow -\infty) = -\bar{m}$  and  $m(x \rightarrow +\infty) = +\bar{m}$ . In between, the most probable field configuration is obtained by minimizing the energy, and satisfies

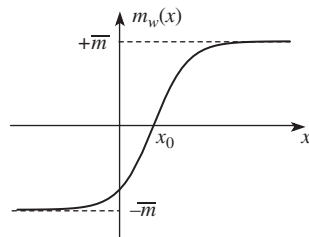
$$\frac{d^2 m_w(x)}{dx^2} = t m_w(x) + 4u m_w(x)^3. \quad (2.26)$$

By using the identity  $d^2 \tanh(ax)/dx^2 = a^2 \tanh(ax) [1 - \tanh^2(ax)]$ , it can be easily checked that the profile

$$m_w(x) = \bar{m} \tanh \left[ \frac{x - x_0}{w} \right], \quad (2.27)$$

is a solution to the above nonlinear differential equation, provided

$$w = \sqrt{\frac{2K}{-t}}, \quad \text{and} \quad \bar{m} = \sqrt{\frac{-t}{4u}}. \quad (2.28)$$



**Fig. 2.8** Profile of the domain wall in a system with discrete symmetry breaking.

The above solution separates regions where the magnetization approaches its two possible bulk values of  $\pm \bar{m}$ . The domain wall between the two regions is centered at an arbitrary position  $x_0$ , and has a width  $w$ . On approaching the phase transition at  $t = 0$  this width diverges as  $(T_c - T)^{-1/2}$ . The width  $w$  is in fact proportional to the correlation length of the system, which will be calculated in the next chapter.

The free energy cost of creating a domain wall in the system can be obtained by examining the energy difference to a uniformly magnetized solution, as

$$\begin{aligned}\beta F_w &\equiv \beta F[m_w(x)] - \beta F[\bar{m}] \\ &= \int d^d \mathbf{x} \left[ \frac{K}{2} \left( \frac{dm_w}{dx} \right)^2 + \frac{t}{2} (m_w^2 - \bar{m}^2) + u (m_w^4 - \bar{m}^4) \right].\end{aligned}\quad (2.29)$$

Simple algebraic manipulations then give

$$\beta F_w = -\frac{t}{2} \bar{m}^2 \int d^d \mathbf{x} \cosh^{-4} \left( \frac{x-x_0}{w} \right) = -\frac{t}{2} \bar{m}^2 w \mathcal{A} \int_{-\infty}^{\infty} \frac{dy}{\cosh^4 y} = -\frac{2}{3} t \bar{m}^2 w \mathcal{A}, \quad (2.30)$$

where  $\mathcal{A}$  is the cross-sectional area of the system normal to the  $x$  direction. The free energy per unit area is proportional to the bulk energy density, multiplied by the width of the domain wall. On approaching the phase transition, the above calculation predicts that the interfacial free energy vanishes as  $(T_c - T)^{3/2}$ .

## Problems for chapter 2

1. *Cubic invariants:* When the order parameter  $m$ , goes to zero discontinuously, the phase transition is said to be first order (discontinuous). A common example occurs in systems where symmetry considerations do not exclude a cubic term in the Landau free energy, as in

$$\beta \mathcal{H} = \int d^d \mathbf{x} \left[ \frac{K}{2} (\nabla m)^2 + \frac{t}{2} m^2 + c m^3 + u m^4 \right] \quad (K, c, u > 0).$$

- (a) By plotting the energy density  $\Psi(m)$ , for uniform  $m$  at various values of  $t$ , show that as  $t$  is reduced there is a discontinuous jump to  $\bar{m} \neq 0$  for a positive  $\bar{t}$  in the saddle point approximation.
  - (b) By writing down the two conditions that  $\bar{m}$  and  $\bar{t}$  must satisfy at the transition, solve for  $\bar{m}$  and  $\bar{t}$ .
  - (c) Note that the correlation length  $\xi$  is related to the curvature of  $\Psi(m)$  at its minimum by  $K\xi^{-2} = \partial^2 \Psi / \partial m^2|_{\text{eq}}$ . Plot  $\xi$  as a function of  $t$ .
2. *Tricritical point:* By tuning an additional parameter, a second order transition can be made first order. The special point separating the two types of transitions is known as a tricritical point, and can be studied by examining the Landau–Ginzburg Hamiltonian

$$\beta \mathcal{H} = \int d^d \mathbf{x} \left[ \frac{K}{2} (\nabla m)^2 + \frac{t}{2} m^2 + u m^4 + v m^6 - h m \right],$$

where  $u$  can be positive or negative. For  $u < 0$ , a positive  $v$  is necessary to insure stability.

- (a) By sketching the energy density  $\Psi(m)$ , for various  $t$ , show that in the saddle point approximation there is a first order transition for  $u < 0$  and  $h = 0$ .
- (b) Calculate  $\bar{t}$  and the discontinuity  $\bar{m}$  at this transition.
- (c) For  $h = 0$  and  $v > 0$ , plot the phase boundary in the  $(u, t)$  plane, identifying the phases, and order of the phase transitions.
- (d) The special point  $u = t = 0$ , separating first and second order phase boundaries, is a *tricritical* point. For  $u = 0$ , calculate the tricritical exponents  $\beta$ ,  $\delta$ ,  $\gamma$ , and  $\alpha$ , governing the singularities in magnetization, susceptibility, and heat capacity. (Recall:  $C \propto t^{-\alpha}$ ;  $\bar{m}(h = 0) \propto t^\beta$ ;  $\chi \propto t^{-\gamma}$ ; and  $\bar{m}(t = 0) \propto h^{1/\delta}$ .)
3. *Transverse susceptibility*: An  $n$ -component magnetization field  $\vec{m}(\mathbf{x})$  is coupled to an external field  $\vec{h}$  through a term  $-\int d^d \mathbf{x} \vec{h} \cdot \vec{m}(\mathbf{x})$  in the Hamiltonian  $\beta \mathcal{H}$ . If  $\beta \mathcal{H}$  for  $\vec{h} = 0$  is invariant under rotations of  $\vec{m}(\mathbf{x})$ ; then the free energy density ( $f = -\ln Z/V$ ) only depends on the absolute value of  $\vec{h}$ ; i.e.  $f(\vec{h}) = f(h)$ , where  $h = |\vec{h}|$ .
- (a) Show that  $m_\alpha = \langle \int d^d \mathbf{x} m_\alpha(\mathbf{x}) \rangle / V = -h_\alpha f'(h)/h$ .
- (b) Relate the susceptibility tensor  $\chi_{\alpha\beta} = \partial m_\alpha / \partial h_\beta$ , to  $f''(h)$ ,  $\vec{m}$ , and  $\vec{h}$ .
- (c) Show that the transverse and longitudinal susceptibilities are given by  $\chi_t = m/h$  and  $\chi_\ell = -f''(h)$ ; where  $m$  is the magnitude of  $\vec{m}$ .
- (d) Conclude that  $\chi_t$  diverges as  $\vec{h} \rightarrow 0$ , whenever there is a spontaneous magnetization. Is there any similar a priori reason for  $\chi_\ell$  to diverge?

4. *Superfluid  $\text{He}^4$ - $\text{He}^3$  mixtures*: The superfluid  $\text{He}^4$  order parameter is a complex number  $\psi(\mathbf{x})$ . In the presence of a concentration  $c(\mathbf{x})$  of  $\text{He}^3$  impurities, the system has the following Landau–Ginzburg energy

$$\beta \mathcal{H}[\psi, c] = \int d^d \mathbf{x} \left[ \frac{K}{2} |\nabla \psi|^2 + \frac{t}{2} |\psi|^2 + u |\psi|^4 + v |\psi|^6 + \frac{c(\mathbf{x})^2}{2\sigma^2} - \gamma c(\mathbf{x}) |\psi|^2 \right],$$

with positive  $K$ ,  $u$  and  $v$ .

- (a) Integrate out the  $\text{He}^3$  concentrations to find the effective Hamiltonian,  $\beta \mathcal{H}_{\text{eff}}[\psi]$ , for the superfluid order parameter, given by

$$Z = \int \mathcal{D}\psi \exp(-\beta \mathcal{H}_{\text{eff}}[\psi]) \equiv \int \mathcal{D}\psi \mathcal{D}c \exp(-\beta \mathcal{H}[\psi, c]).$$

- (b) Obtain the phase diagram for  $\beta \mathcal{H}_{\text{eff}}[\psi]$  using a saddle point approximation. Find the limiting value of  $\sigma^*$  above which the phase transition becomes discontinuous.
- (c) The discontinuous transition is accompanied by a jump in the magnitude of  $\psi$ . How does this jump vanish as  $\sigma \rightarrow \sigma^*$ ?
- (d) Show that the discontinuous transition is accompanied by a jump in  $\text{He}^3$  concentration.
- (e) Sketch the phase boundary in the  $(t, \sigma)$  coordinates, and indicate how its two segments join at  $\sigma^*$ .

- (f) Going back to the original joint probability for the fields  $c(\mathbf{x})$  and  $\Psi(\mathbf{x})$ , show that  $\langle c(\mathbf{x}) - \gamma\sigma^2 |\Psi(\mathbf{x})|^2 \rangle = 0$ .
- (g) Show that  $\langle c(\mathbf{x})c(\mathbf{y}) \rangle = \gamma^2\sigma^4 \langle |\Psi(\mathbf{x})|^2 |\Psi(\mathbf{y})|^2 \rangle$ , for  $\mathbf{x} \neq \mathbf{y}$ .
- (h) Qualitatively discuss how  $\langle c(\mathbf{x})c(0) \rangle$  decays with  $x = |\mathbf{x}|$  in the disordered phase.
- (i) Qualitatively discuss how  $\langle c(\mathbf{x})c(0) \rangle$  decays to its asymptotic value in the ordered phase.

5. *Crumpled surfaces:* The configurations of a crumpled sheet of paper can be described by a vector field  $\vec{r}(\mathbf{x})$ , denoting the position in three-dimensional space,  $\vec{r} = (r_1, r_2, r_3)$ , of the point at location  $\mathbf{x} = (x_1, x_2)$  on the flat sheet. The energy of each configuration is assumed to be invariant under translations and rotations of the sheet of paper.

- (a) Show that the two lowest order (in derivatives) terms in the quadratic part of a Landau–Ginzburg Hamiltonian for this system are:

$$\beta\mathcal{H}_0[\vec{r}] = \sum_{\alpha=1,2} \int d^2\mathbf{x} \left[ \frac{t}{2} \partial_\alpha \vec{r} \cdot \partial_\alpha \vec{r} + \frac{K}{2} \partial_\alpha^2 \vec{r} \cdot \partial_\alpha^2 \vec{r} \right].$$

- (b) Write down the lowest order terms (there are two) that appear at the quartic level.
- (c) Discuss what happens when  $t$  changes sign, assuming that quartic terms provide the required stability (and  $K > 0$ ).