Chapter 9
Critical Phenomena and Renormalization Theory

9.1   WHAT IS A PHASE TRANSITION?

This chapter will be devoted to the study of second-order phase transitions, but, before considering the particular case of second-order phase transitions, it is best to look in more detail at the question of how one defines a phase transition in general. The most familiar phase transitions, such as those between water, ice, and steam, are almost misleadingly clear, in that the properties of the phases involved are so strikingly different. However, even in this seemingly obvious case, the meaning of the word *phase* begins to become more subtle when we realize that we can convert a sample of pure liquid to pure gas with no phase transition, simply by moving the system along a trajectory around the critical point in the p-T plane (see Fig. 9.1). The phase transition lines do not necessarily separate the thermodynamic space into disjoint regions of different phases. Although it is possible to define precisely a phase transition point in the p-T plane, and we will do so presently, it is not possible to separate clearly the liquid phase points from the gas phase points.
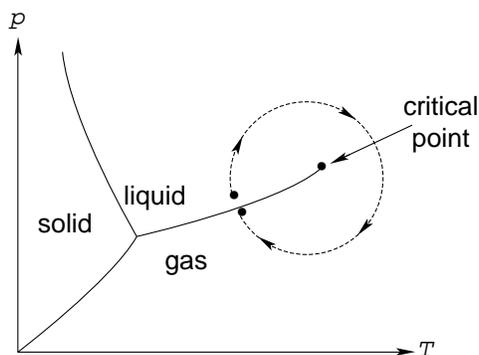

Fig. 9.1   By varying the values of p and T to move the system along the curve shown, it is possible to transform a liquid to a gas without encountering a phase transition line.

The phase transition encountered in the ideal Bose gas is typical of many, more subtle, phase transitions. Across the phase transition line, the density is continuous, the energy density is continuous, and even the specific heat is continuous. One must go to the derivative of C_V with respect to T in order to find a property that changes discontinuously. If phase transitions can be so delicate, what is the defining characteristic of a phase transition point?

"The ordinary gaseous and liquid states are, in short, only widely separated forms of the same condition of matter and can be made to pass into one another by a series of gradations so gentle that the passage shall nowhere present any interuption or break of continuity."
—— Thomas Andrews *Bakerian Lecture to the Royal Society.*(1869)
Andrews was the first person to demonstrate clearly the existence of a critical point in the liquid–gas transition.

The unambiguous definition of a phase transition involves the mathematical concept of analyticity. A mathematical function of many variables (we will consider the case of two variables) is called *analytic* at a point (x, y) if its Taylor expansion converges to the value of the function at every point within some finite circle about (x, y). That is, if

$$f(x + \Delta x, y + \Delta y) = f(x, y) + \sum_{m,n=0}^{\infty} f_{mn} \frac{(\Delta x)^m (\Delta y)^n}{m! n!} \tag{9.1}$$

whenever $\Delta x^2 + \Delta y^2 < a^2$ for some number $a > 0$, where $f_{mn} = \partial^{m+n} f / \partial x^m \partial y^n$. Single-phase regions in the p-T plane (or, for magnetic systems, in the H–T plane) are regions in which the appropriate thermodynamic potential [$G(T, p)$ for the p-T plane and $\phi(H, T)$ for the H–T plane] is an analytic function. They are bounded by curves along which the function is not analytic.

Equations (7.72) and (7.73) for $\alpha(n, \tau)$ the affinity of an ideal Bose gas, illustrate the point. This function must be calculated separately for the two different phases. Its value in one phase cannot be determined by smoothly extrapolating its values across the phase transition line. (See Fig. 9.2.)
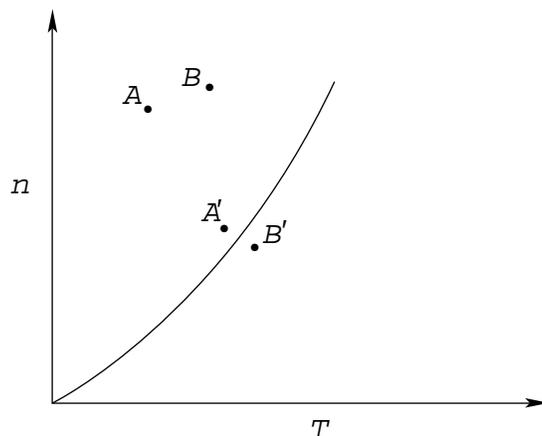

Fig. 9.2 One can calculate the value of $\alpha(n, T)$ at point B by expanding the function in a Taylor expansion centered at point A, but one cannot evaluate $\alpha(B')$ by using a Taylor expansion centered at A'.

This definition of a phase transition, in terms of the analyticity of the thermodynamic potential, presents a deep problem for the theory of statistical mechanics. To see what the problem is, let us consider a three-dimensional Ising model on a cubic lattice with $N = L^3$ points. The partition function is

$$Z(N, \beta, H) = \sum_C \exp\left(-\beta H \sum \sigma(\mathbf{r}) - \beta V \sum_{\mathrm{NN}} \sigma(\mathbf{r}) \sigma(\mathbf{r}') \right) \tag{9.2}$$

Each term in the sum over configurations is an analytic function of β and H. There are 2^N configurations. The sum of a finite number of analytic functions is analytic. Where are the phase transition points? The function defined in Eq. (9.2) is analytic for all values of β and H. This difficulty for many years caused knowledgeable people to have some doubts as to whether the formalism of statistical mechanics could properly treat phase transitions without some modification. Of course, models such as the Ising model, when treated

with mean-field theory, predict phase transitions. However, it was not clear whether or not those predictions were simply artifacts of the mean-field approximation that would vanish if an exact calculation could be made. The doubt was strengthened by the fact that the one-dimensional Ising model, which can be solved exactly, gives no phase transition in the exact solution but does give a phase transition in the mean-field approximation. It was only when Onsager was able to solve the two-dimensional Ising model exactly and show that it did predict a phase transition that these questions about the adequacy of statistical mechanics to treat phase transitions were finally put to rest. The resolution of the analyticity paradox can be given along the following lines. Recall that the laws of thermodynamics, and those of statistical mechanics, can only be used with complete confidence in the limit of large system size. Therefore, rather than looking at the total canonical potential for a finite system, we should be looking at something like the canonical potential per particle in the thermodynamic limit. That is,

$$\phi(\beta, H) = \lim_{N \to \infty} \big[\phi(N, \beta, H)/N\big] \tag{9.3}$$

By some fairly complicated mathematical analysis, it can be proved that the limit defined here exists for all reasonable Hamiltonian functions. But it is a fact of mathematics that the statement that a sequence of functions $f_N(x)$ converges, as $N \to \infty$, to a limit function $f(x)$ does *not* imply that df_N/dx converges to df/dx. Thus, even though $\phi(N, \beta, H)/N$ is analytic for every finite N, it is still possible for $\phi(\beta, H)$ to be nonanalytic. This may seem like mathematical quibbling, but Fig. 9.3 shows that it is this very effect (the fact that taking a derivative does not commute with taking a limit) that produces the nonanalytic behavior in the thermodynamic functions. This is just another example of the general rule that the proper subjects of thermodynamics and statistical mechanics are those characteristics of matter that appear in the thermodynamic limit.

9.2   SECOND-ORDER PHASE TRANSITIONS

A first-order phase transition involves a restructuring of the substance on a microscopic level. Looking at a small bit of the substance through a powerful microscope, one could easily detect the change that takes place in the material when T goes from just above a first order transition to just below it. In a gas-liquid transition, the density undergoes a finite jump. In a liquid-solid transition, a crystal lattice forms when none existed above the transition temperature and there is also a finite change in the density.

In contrast, a second-order phase transition could not be detected by observing a microscopic sample of the substance. Most second-order phase transitions separate a more symmetrical phase from a less symmetrical one. For example, the equilibrium state of the Ising model with no external field has up–down symmetry above T_c but does not have that symmetry below T_c. Of course, many (but not all) first-order transitions also separate more symmetrical from less symmetrical phases. The distinction between the two cases is that in first-order transitions there is a finite change in structure over an infinitesimal temperature interval—the substance is a translationally invariant liquid at any temperature above the transition and a noninvariant crystal at any temperature below it. In second-order transitions, the unsymmetrical state connects smoothly to the symmetrical state as T approaches T_c from below. (Usually, but not always, the unsymmetrical phase is the low-temperature phase.) Again, the Ising model is one of the simplest examples— the magnetization is nonzero below T_c and zero above T_c, but it is continuous, although not differentiable, through the transition. Because of this property, one could not detect a second-order transition by observing a microscopic sample. In a microscopic sample, the uncertainty in $\bar{\sigma}$ is always fairly large, because one is observing only a few fluctuating spins, and so one cannot distinguish between a zero value and a very small nonzero value.

On the other hand, if we move through the phase transition line on the trajectory shown in Fig. 9.4, by imposing a weak positive external field H and then slowly varying the value of H through zero to negative values, the average polarization of a single spin behaves in the following way. As $H \to 0$ from positive values, $\langle \sigma \rangle \to M(T)$, where $M(T)$ is the *finite* positive value of the spontaneous magnetization. A finite value of $\langle \sigma \rangle$ is not completely obscured by the random fluctuations in a finite microscopic sample, and can thus be observed. As we move from tiny positive values of H to tiny negative values, the average polarization $\langle \sigma \rangle$ changes *discontinuously* to $-M(T)$. Since this finite jump can be detected on a microscopic level, we say that all the points on the phase transition line, *except the endpoint of the line*, are points of first-order phase transitions. The endpoint of the line (the critical point in the Ising model) is a point of second-order phase transition.
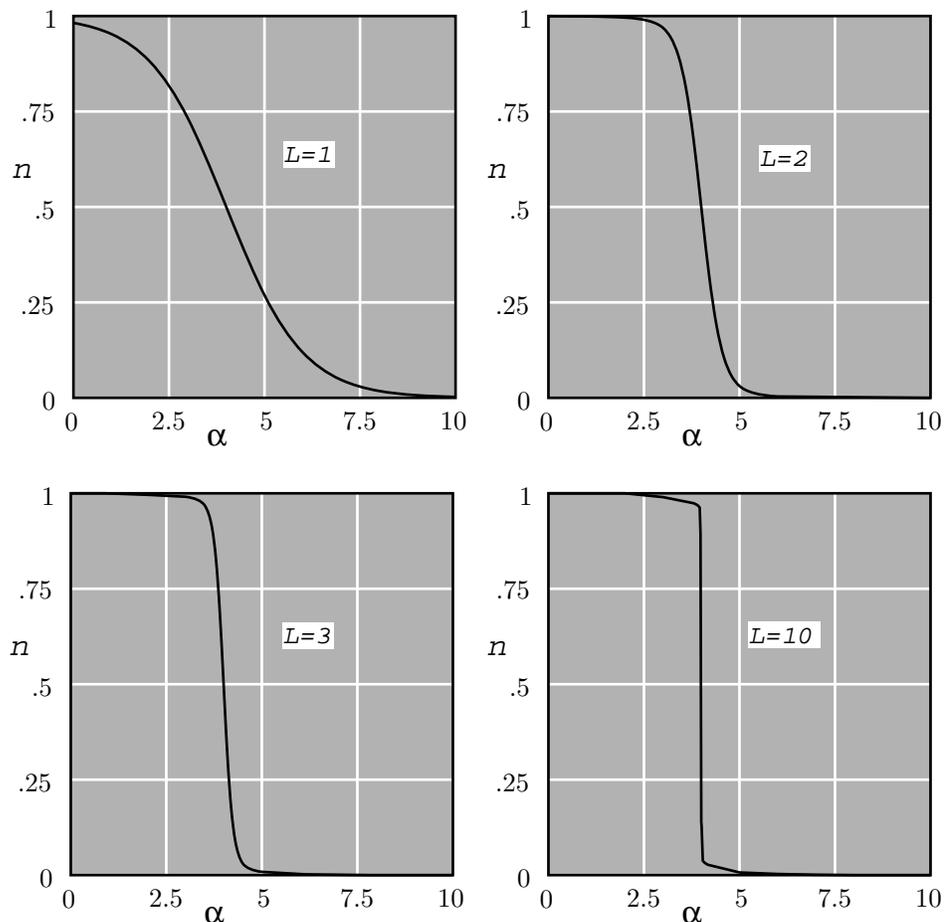
Fig. 9.3   The average number of particles per lattice site for the two-dimensional lattice gas with attractive nearest-neighbor interactions. This is the system that was analyzed in Section 8.9. All the graphs are for a value of $\beta v = -2$. Calculations have been made using the Monte Carlo method. Shown is the relationship between the affinity and the average occupation number for $L \times L$ lattices of various sizes, with periodic boundary conditions. It is clear that $n(\alpha)$ becomes a truly discontinuous function only in the limit of large lattice size. The curve for $L = 10$, although it looks discontinuous, is actually slightly rounded and not quite vertical.
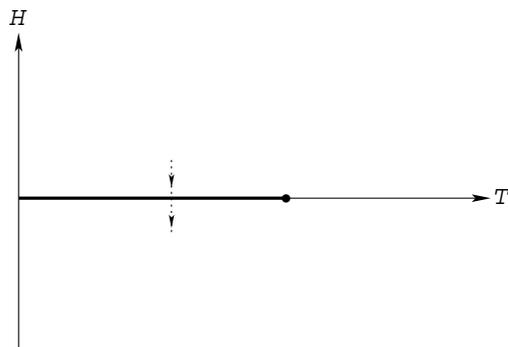

Fig. 9.4   If, at fixed T, the value of H is varied along the curve shown, there is a discontinuous finite change in the value of $\langle \sigma \rangle$ as the point $H = 0$ is passed. In a real system, this could be detected by observing a finite number of spins for a finite amount of time. Thus the transition is of first order, although it has no latent heat.

Most first-order phase transitions have a finite latent heat associated with them. However, it is easy to see that the first-order transition that has just been described has no latent heat. Therefore, the existence or nonexistence of a latent heat is not a reliable criterion for distinguising first-order from second-order transitions. The general criterion is that any phase transition that could be detected by observing a microscopically finite sample for a finite time is first order. All others are called second-order.

In a second-order transition from a more symmetrical to a less symmetrical phase, the quantity whose nonzero value distinguishes the unsymmetrical from the symmetrical state is called the *order parameter*. The order parameter for a uniaxial ferromagnet is the magnetization M, which is a real scalar, because the magnetization axis is fixed. For a ferromagnetic material in which the magnetization can point in any direction (called an isotropic ferromagnet), the order parameter is a vector magnetization $\mathbf{M}$. For the λ transition in liquid helium, the order parameter is usually taken to be the superfluid wave function $\psi(\mathbf{r})$ normalized so that $\psi^*\psi$ is equal to the superfluid density. The order parameter in that case is a complex scalar. In our analysis of second-order phase transitions, we will, for the most part, restrict ourselves to the three-dimensional Ising model, which has a real scalar order parameter, and only mention equivalent results for the the more complicated cases.

9.3   UNIVERSALITY AND CRITICAL EXPONENTS

The points in thermodynamic space at which second-order phase transitions occur are called *critical points*, and the behavior of systems at second-order phase transitions is generally referred to as *critical phenomena*. One of the striking characteristics of critical phenomena is the fact that certain detailed quantitative measures of a system's behavior near a critical point are quite independent of the details of the interactions between the particles making up the system. This characteristic of critical phenomena is called *universality*. The universal features are not only independent of the numerical details of the interparticle interactions, but are also independent of the most fundamental aspects of the structure of the system. For example, we mentioned that the order parameter $\bar{\sigma}$ for the 3D Ising model on a cubic lattice approached zero as the temperature approached the critical temperature from below as $(-t)^\beta$, where $\beta \approx 0.324$. What we mean by universality is illustrated by the fact that the value of β is independent of:

1. The numerical values of V_x, V_y, and V_z, in the case of an anisotropic Ising model (see the end of Section 8.21), so long as they are greater than zero. (If one of them is zero, then the system is not a three-dimensional system, but is a collection of completely noninteracting two-dimensional systems, and one thing that β *does* depend upon is the dimensionality of the system.)

2. The structure of the lattice. If a ferromagnetic Ising model is defined on a face-centered cubic lattice, a hexagonal lattice, or, in fact, on any of the fourteen possible Bravais lattices in three dimensions, and the value of $\bar{\sigma}$ is determined very close to the ferromagnetic transition temperature for that lattice, then it is found that $\bar{\sigma}$ is proportional to $(-t)^\beta$ as $t \to 0$ with the same value of β as is shown by a cubic lattice.

3. The details of the interactions. The Ising model is defined as having only nearest-neighbor interactions. If longer-range interactions (next-nearest-neighbor, third-nearest-neighbor, etc.) are added, then, as long as they are chosen so that a ferromagnetic transition still occurs, $\bar{\sigma}$ will go to zero as $(-t)^\beta$ at the Curie point for the system, with the same value of β.

4. Whether the system is a lattice system or a three-dimensional gas with continuous coordinates and momenta. Consider any ordinary gas, even one with complex molecules, which have rotational and vibrational degrees of freedom, such as nitrogen, hexane, octane, etc. Measure the parameter, $\Delta n = n(\text{liquid}) - n(\text{gas})$, where n is the particle density, as a function of $t = (T - T_c)/T_c$ along the coexistence curve in the p-T plane. [The coexistence curve ends at the critical point. At that point $n(\text{liquid})$ becomes equal to $n(\text{gas})$.] As $T \to T_c$ from below, Δn approaches zero as $(-t)^\beta$ with the same value of β as the 3D Ising model. For the liquid–gas phase transition, the value of Δn is the order parameter. It is zero above the critical temperature and nonzero below it. That this system exhibits the same exponent as the 3D Ising model is really an astonishing fact since there seems to be nothing in common between a magnetic transition in a three-dimensional lattice model and the liquid–gas phase transition in a continuous system. (Also see Fig. 9.5.)

The order parameter exponent β is only one of a number of different exponents that can be defined at a critical phase transition. We will define some others shortly. They all share the characteristic of universality. Their values are independent of almost all detailed properties of the system. In fact, they generally depend
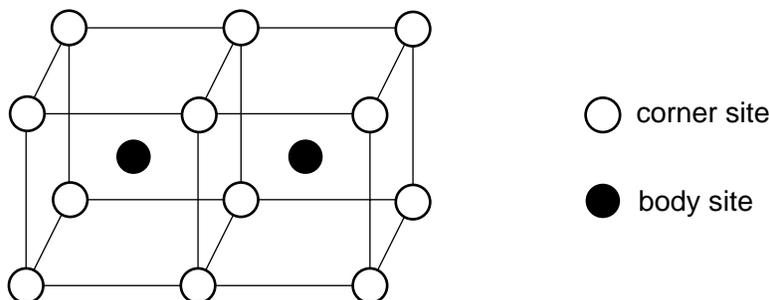
Fig. 9.5   Beta-brass is a binary alloy made up of equal numbers of zinc and copper atoms. It has a body-centered cubic (bcc) crystal structure. A bcc lattice can be defined by beginning with a cubic lattice, all of whose sites we will call *corner sites*, and adding an additional lattice site, called a *body site*, at the center of each cube. There are equal numbers of corner sites and body sites. In fact, there is no fundamental distinction between the set of corner sites and the set of body sites. The set of body sites forms a cubic lattice that could just as well have been called the corner sites. We define the order parameter $\Delta n = |Z_B - Z_C|/(Z_B + Z_C)$, where Z_B is the number of zinc atoms at the body sites and Z_C is the number of zinc atoms at the corner sites. In beta-brass, there is a phase transition at a temperature $T_c \approx 741$ K. Above T_c, $\Delta n = 0$, indicating that a zinc atom has an equal probability of being at a body or a corner site. Below T_c, $\Delta n > 0$ and, as $T \rightarrow T_c$, $\Delta n \sim (-t)^\beta$, with $\beta \approx 0.324$. The quantity Δn can be measured by X-ray diffraction studies.

on only two characteristics of the phase transition, namely, the number of components in the order parameter (one for a real number, two for a complex number or a two-dimensional vector, three for a vector, etc.) and the dimensionality of the system.

At zero external field, the specific heat of the three-dimensional Ising model, as a function of temperature, has an integrable singularity* of the form

$$C \sim \begin{cases} A_-(-t)^{-\alpha}, & \text{as } T \rightarrow T_c \text{ from below} \\ A_+ t^{-\alpha}, & \text{as } T \rightarrow T_c \text{ from above} \end{cases} \tag{9.4}$$

where, as usual, $t = (T - T_c)/T_c$ and the *specific heat exponent* α has the value

$$\alpha \approx 0.11 \pm 0.008 \tag{9.5}$$

A_- and A_+ are constants with the appropriate units. Since the right-hand side of Eq. (9.4) goes to infinity at $t = 0$, there is some question about what is actually meant, in a mathematical sense, by the equation. What the equation signifies is that, as $T \rightarrow T_c$ from below,

$$\lim_{T \rightarrow T_c} \left[C(T)(-t)^\alpha \right] = A_- \tag{9.6}$$

with a corresponding statement for the limit as $T \rightarrow T_c$ from above.

The magnetic susceptibility χ_m of the 3D Ising model at zero external field also shows a singularity at T_c. The form of the singularity defines a *susceptibility exponent* γ.

$$\chi_m(T, H = 0) \sim \begin{cases} B_-(-t)^{-\gamma}, & \text{as } T \rightarrow T_c \text{ from below} \\ B_+ t^{-\gamma}, & \text{as } T \rightarrow T_c \text{ from above} \end{cases} \tag{9.7}$$

where

$$\gamma = 1.24 \pm 0.004 \tag{9.8}$$

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* A function $f(x)$ has an integrable singularity at x_o if $f(x) \rightarrow \infty$ as $x \rightarrow x_o$ but the integral $\int_a^b f(x)\, dx$ for $a < x_o < b$ is finite. A good example is the function $\log(|x|)$, which has an integrable singularity at $x = 0$.
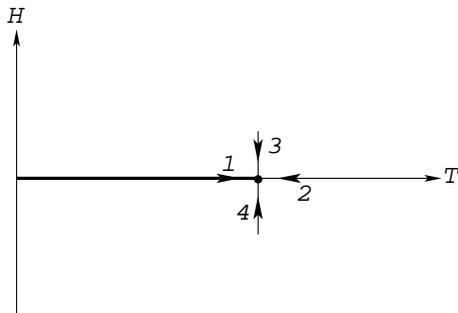
Fig. 9.6   The behavior of $\bar{\sigma}$ as one approaches the critical point in direction 1 defines the critical exponent β. The same thing along path 3 or 4 defines the exponent δ.

The critical exponent β describes how $\bar{\sigma}$ goes to zero as one approaches the critical point along the direction 1, shown in Fig. 9.6. It is defined by saying that, as $T \to T_c$ from below, $\bar{\sigma} \sim (-t)^{\beta}$

There is another critical exponent δ that indicates how $\bar{\sigma} \to 0$ along the directions 3 and 4. That is, at $T = T_c$ exactly, and for $H \to 0$,

$$|\bar{\sigma}| \sim C|H|^{1/\delta} \tag{9.9}$$

(That the exponent is written as $1/\delta$, rather than δ, is just an accident of history.) The same exponent is exhibited by a fluid system as one approaches the critical point by varying the pressure along the critical isotherm.

$$|n - n_c| \sim C|p - p_c|^{1/\delta} \tag{9.10}$$

where n_c and p_c are the particle density and pressure at the critical point. For that reason, δ is called the *critical isotherm exponent*. Its value is

$$\delta = 4.82 \pm 0.006 \tag{9.11}$$

When the same numbers appear in a variety of very different physical situations there must be some simple mechanism as work. But what can the magnetism of a uniaxial ferromagnet have in common with the condensation of carbon dioxide or the ordering transition in beta-brass? The Hamiltonian functions for the three systems are utterly different in structure. But ultimately it is the Hamiltonian function of each system that must determine the characteristics of all the phase transitions involving the system, including any critical exponents.

9.4   LANDAU THEORY

The physics of critical phenomena is subtle. Therefore, we will approach it in stages. We will begin with a simple thermodynamic analysis, due to L. D. Landau, that gives the same predictions for all the critical exponents as is given by the mean-field approximation. It has the advantage over mean-field theory of being based on a few general thermodynamic assumptions that do not involve the detailed microscopic model of the system. It can therefore be used, without significant modifications, to analyze the critical behavior of microscopically different systems. Since it predicts exactly the same behavior for each system, it explains the puzzling property of universality. Unfortunately, the universal behavior that the Landau theory predicts is wrong. For example, we have seen that mean-field theory predicts that, near T_c, $\bar{\sigma} \sim \sqrt{3}(-t)^{1/2}$, and therefore that the exponent $\beta = \frac{1}{2}$. But this disagrees with experiments and with more adequate theoretical analyses that do not use the mean-field approximation. They all show that $\beta \approx 0.324$. However, since a modification of the Landau theory plays a central role in the modern theory of critical phenomena, the time spent in presenting the theory will not be wasted. We will use the Landau theory to analyze a uniaxial ferromagnetic substance and then indicate how it can be applied to other systems.

In discussing the thermodynamics of a magnetic substance, one is free to use, as the "magnetic" variable, the magnetic field B, the magnetic displacement H, or the magnetic polarization of the substance M. The use of M, rather than B or H, has two advantages. First, it is completely determined by the microscopic state of the substance, without reference to external agents such as coils or pole pieces. The more important advantage is that the thermodynamic states of the substance are more adequately represented by the points
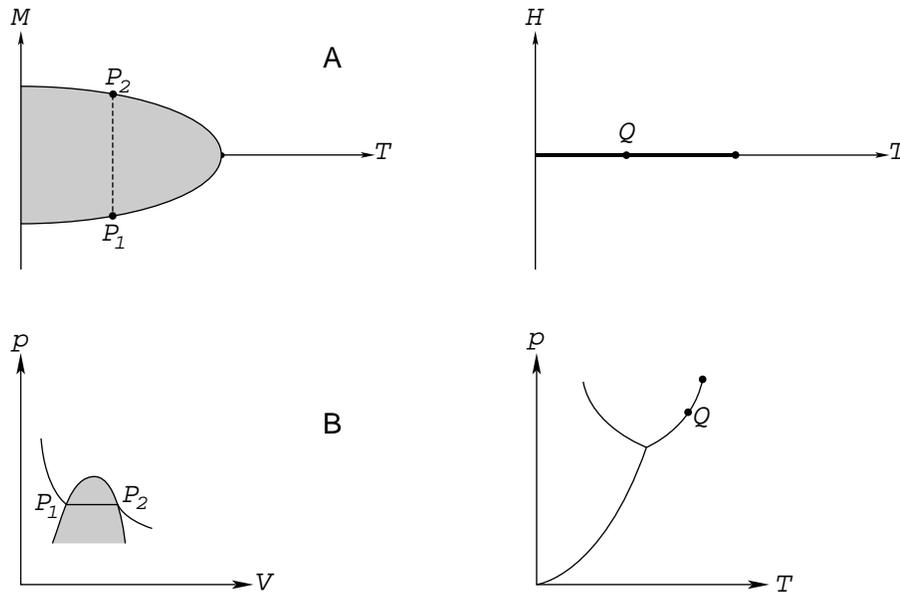
Fig. 9.7   (A) For a 3D Ising lattice, the set of thermodynamic states lying on the straight line between points P_1 and P_2 in the M–T plane are all mapped into the single point Q in the H–T plane. (B) A similar thing happens in liquid–gas transitions—the set of points between P_1 and P_2 in the p-V plane are mapped into the point Q in the p-T plane.

in the T–M plane, as opposed to the points in the T–H or T–B planes. The shaded region of the T–M plane, shown in Fig. 9.7(A), describes two-phase states, in which a portion of the substance is polarized in the up direction while the remainder is polarized in the down direction. This whole region is mapped into the single line, $H = 0$, $0 < T < T_c$, in the T–H plane. Thus single points in the T–H plane represent a multitude of possible macroscopic equilibrium states of the substance. A similar thing happens for fluids, where the region of two-phase (liquid and gas) states shown in the p-V plane collapses to the single-phase transition line in the p-T plane.

The Landau theory begins with some simple assumptions about the form of the canonical potential $\phi(T, M)$. The potential $\phi(T, M)$ is meant to be interpreted as the conditional canonical potential for a system of fixed magnetization *in the absence of an external magnetic field.* Recall that the conditional canonical potential is defined so that the probability of finding the system with magnetization M is proportional to $\exp \phi(M)$. From a microscopic point of view,

$$\phi(T, M) = \log\Big(\sum_C \delta\Big(\sum \mu_i - MV\Big) e^{-\beta E(C)}\Big) \tag{9.12}$$

where the sum on C is over all configurations of the system and μ_i is the magnetic moment of the ith particle in configuration C. The delta function limits the sum over configurations to those configurations that have a total magnetic moment equal to MV—that is, a magnetization equal to M. With no external field, this function is clearly symmetric in M. The Landau theory assumes that, for small values of M, it can be expanded as a power series in M.

$$\phi(T, M) = \phi_o(T) - VA(T)M^2 - VB(T)M^4 \tag{9.13}$$

The explicit factors of V in the second and third terms are included in order to make A and B independent of the system size. The minus signs, which suggest that the corresponding terms are negative, are included so that the stationary point at $M = 0$ is a maximum when A and B are positive.

Since we are interested in analyzing the thermodynamic properties of the system at the phase transition, where the thermodynamic functions are known to be nonanalytic, it may seem to be a fundamental error to assume that $\phi(T, M)$ is analytic in M. However, it is the equilibrium potential $\phi(T)$ that is nonanalytic.
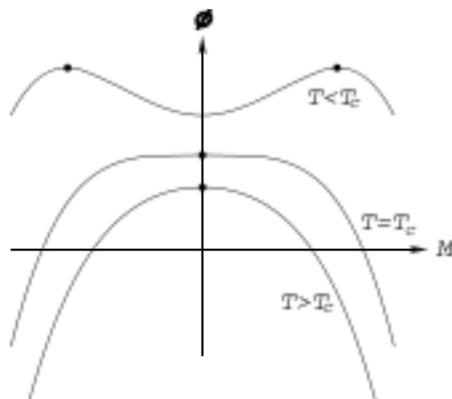
Fig. 9.8   If the function $\phi(T, M)$ is assumed to have the form given in Eq. (9.13), then, for T above T_c, $\phi(T, M)$ has single quadratic maximum at $M = 0$. One would therefore expect normal (that is, Gaussian) fluctuations about that most probable value of M. For $T = T_c$, the most probable value of M is still zero, but the probability distribution is much flatter, indicating a much larger probability of observing nonzero values. For $T < T_c$, we have spontaneous symmetry breakdown—the most probable values are the two nonzero values indicated. Notice that the fluctuations about those nonzero values would again be Gaussian, because the function is locally quadratic.

It will be shown that an analytic conditional potential $\phi(T, M)$ can still produce a nonanalytic equilibrium potential $\phi(T)$.

In the Landau theory, the critical temperature T_c is interpreted as the point at which $A(T)$ changes sign. That is, $A(T) > 0$ for $T > T_c$ and $A(T) < 0$ for $T < T_c$. $B(T)$ must remain positive or else the maximum of $\phi(T, M)$ would occur at $M = \pm\infty$. Since we are interested in the properties of the system in the vicinity of T_c, it is adequate to treat $A(T)$ as a linear function with a zero at T_c and to treat $B(T)$ as a constant. Thus we assume that

$$A(T) = at \;\; \text{and} \;\; B(T) = b \tag{9.14}$$

where a and b are constants and $t = (T - T_c)/T_c$, as usual.

The quantity $\phi(T, M)$ is plotted as a function of M for temperatures less than, equal to, and greater than T_c in Fig. 9.8. For $T < T_c$, the maximum of $\phi(T < M)$, which should describe the equilibrium state, occurs at either of the two nonzero values shown in the figure. At those temperatures the system will exhibit a finite magnetization, even in the absence of any external magnetic field. Using Eqs. 9.13 and 9.14, the equilibrium value of M as a function of t is easy to calculate. Setting $\partial\phi(T, M)/\partial M = 0$ in the expression

$$\phi = \phi_o - VatM^2 - VbM^4 \tag{9.15}$$

gives the cubic equation

$$atM + 2bM^3 = 0 \tag{9.16}$$

This has the three solutions

$$M = 0 \;\; \text{and} \;\; \pm\sqrt{\frac{a}{2b}}(-t)^{1/2} \tag{9.17}$$

When t is positive, the $M = 0$ solution describes a maximum of $\phi(T, M)$ and the nonzero solutions are imaginary and therefore physically irrelevant. But for negative t the zero solution describes a local minimum of $\phi(T, M)$ and it is the now real nonzero solutions that describe the possible equilibrium values of the magnetization. It is obvious from Eq. (9.17) that the Landau prediction for the magnetization exponent is that $\beta = \frac{1}{2}$.

In order to calculate the specific heat below T_c, we must transform to the regular canonical potential $\phi(T)$. This is done by replacing the independent variable M in $\phi(T, M)$ by its equilibrium value as a function of T. For T less than but close to T_c, this gives

$$\phi(T) = \phi_o(T) - VatM^2(T) - VbM^4(T)$$
$$= \phi_o(T) + V\frac{a^2}{4b}\frac{(T - T_c)^2}{T_c^2} \tag{9.18}$$

The energy as a function of T is given by

$$
\begin{aligned}
E &= -\frac{\partial \phi}{\partial \beta} \\
&= kT^2 \frac{\partial \phi}{\partial T} \\
&= kT^2 \left(\phi'_o(T) + V \frac{a^2(T - T_c)}{2bT_c^2} \right)
\end{aligned}
\tag{9.19}
$$

The specific heat for $T < T_c$ is

$$
C = \frac{\partial E}{\partial T} = k \frac{\partial (T^2 \phi'_o)}{\partial T} + V \left(\frac{ka^2 T^2}{2bT_c^2} + \frac{ka^2 Tt}{bT_c} \right)
\tag{9.20}
$$

The limit of C as $T \to T_c$ from below is

$$
C = k \frac{\partial (T^2 \phi'_o)}{\partial T} \bigg|_{T_c} + V \frac{ka^2}{2b}
\tag{9.21}
$$

Above T_c, M is zero, and therefore the specific heat is given by the first term of Eq. (9.21). Thus in the Landau theory there is no singularity, but only a finite discontinuity in $C(T)$ at T_c of magnitude

$$
\Delta C = V \frac{ka^2}{2b}
\tag{9.22}
$$

In order to make this agree with Eq. (9.4), which defines the specific heat exponent α, we must choose $\alpha = 0$. This prediction disagrees with the experimental result given in Eq. (9.11).

   In order to calculate the magnetic susceptibility, it is necessary to have $\phi(T, M)$ in the presence of an external magnetic field. If a magnetic field B is present, then the energy of a configuration C is changed from $E(C)$ to $E(C) - B \sum \mu_i$. In that case

$$
\begin{aligned}
\phi(T, M) &= \log \left[\sum_C \delta \left(\sum \mu_i - MV \right) e^{-\beta E(C) + \beta B \sum \mu_i} \right] \\
&= \log \left[e^{\beta BMV} \sum_C \delta \left(\sum \mu_i - MV \right) e^{-\beta E(C)} \right] \\
&= \phi_{B=0}(T, M) + \beta BMV \\
&= \phi_o(T) + \beta BMV - V a t M^2 - V b M^4
\end{aligned}
\tag{9.23}
$$

Assuming that B is small and positive and that $T < T_c$, the plot of $\phi(T, M)$ as a function of M now has an asymmetrical double maximum. The unique equilibrium state is given by the higher maximum at positive M. The maximum occurs at the solution of $\partial \phi(T, M)/\partial M = 0$. This gives the equation

$$
\beta B - 2atM - 4bM^3 = 0
\tag{9.24}
$$

The point $B = 0$ and $t = 0$ is a singular point for the thermodynamic functions and therefore one must be very careful about the order in which limits and derivatives are taken. To calculate the susceptibility exponent γ, one must separately look at the limit of $(\partial M/\partial B)|_{B=0}$ as $t \to 0$ from below and above. We will first do the calculation for negative t. Equation (9.24) is an equation for $M(t, B)$. Taking the derivative of the equation with respect to B, setting B equal to zero, and defining χ_m as $\partial M/\partial B$ gives

$$
\beta - 2at\chi_m - 12bM^2(t, 0)\chi_m = 0
\tag{9.25}
$$

Replacing $M^2(t, 0)$ by its value $-at/2b$ obtained from Eq. (9.24) gives

$$
\chi_m = \frac{\beta_c}{4a}(-t)^{-1}
\tag{9.26}
$$

where $\beta_c = 1/kT_c$.

For positive values of t, M is proportional to B as $B \to 0$, and therefore the cubic term in Eq. (9.24) can be dropped. The magnetic susceptibility is then given by

$$\chi_m = \frac{M}{B} = \frac{\beta}{2a} t^{-1} \tag{9.27}$$

Comparing these results with Eq. (9.7) shows that the Landau theory prediction is that

$$\gamma = 1 \;\; \text{and} \;\; \frac{B_+}{B_-} = 2 \tag{9.28}$$

Notice that γ and the ratio B_+/B_- are both independent of the numerical values of the parameters a and b that appear in the thermodynamic function. (This is not true for the separate amplitudes, B_+ and B_-.) Thus, according to the Landau theory, these quantities should have the same value at the Curie point of all uniaxial ferromagnets. This prediction of universality for γ and the amplitude ratio B_+/B_- is supported by experimental observation, but the specific numbers predicted in Eq. (9.28) are not.

The isotherm exponent δ is calculated by setting $t = 0$ in Eq. (9.24). This gives

$$M = \left(\frac{\beta}{4b}\right)^{1/3} B^{1/3} \tag{9.29}$$

A comparison of this with the definition of δ given in Eq. (9.9) yields the estimate $\delta = 3$ for the isothermal exponent.

In Section 8.24 the mean-field approximation was used to calculate the order-parameter exponent β. The mean-field result was that $\beta = \frac{1}{2}$, in agreement with the Landau theory. Similar mean-field calculations of all the other exponents would show that all of the critical-point predictions of the mean field approximation are in agreement with those of Landau theory. Since mean field theory, which neglects correlation effects, is obviously a relatively crude approximation to reality, it is not surprising that it predicts critical exponents that do not agree with experiment or with more careful calculations. However, the Landau theory is a thermodynamic theory, and its basic assumption [that is, Eq. (9.13)] seems so reasonable that it is much more difficult to see why it fails so badly. In the next section we will see that the essential weakness of the Landau theory is that it neglects thermodynamic fluctuations.

9.5   CRITICAL-POINT FLUCTUATIONS

There are two ways of seeing that the careful treatment of large-scale fluctuations is important in any analysis of critical phenomena. The first is to consider an experimental effect, called *critical opalescence*. When a transparent fluid, such as water, is brought to its critical point, it becomes milky white, although it is quite clear at all neighboring pressures and temperatures. It is known that the effect is caused by the light being scattered, as it passes through the fluid, by small, disordered, spatially varying fluctuations in the fluid density. A spatially varying fluctuation in the density will create a similar fluctuation in the index of refraction, which will distort the wave fronts of a plane wave and cause a scattering of its energy flux.

The second way of seeing the importance of fluctuations at the critical point is to recall the relationship between energy fluctuations and specific heat that is expressed by the equation

$$\beta \, \Delta E = C^{1/2} \tag{9.30}$$

where $(\Delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2$ and C is the specific heat of the system. But, as $T \to T_c$, the specific heat of any system with a positive exponent, α, approaches infinity as $1/|t|^\alpha$. Equation (9.30), which is based on a Gaussian approximation to the function $\exp(\phi(T, M))$, is not really applicable right at the critical point, but it clearly indicates that fluctuations will be very large there. The fact that the magnetic susceptibility χ_m diverges at the critical point, combined with the relationship between χ_m and ΔM, shows that the magnetization will also exhibit large fluctuations at the critical point.

9.6   THE FLUCTUATION PROBABILITY

The equilibrium states of a macroscopic 3D Ising model show uniform magnetization. The magnetization M is zero above the transition temperature and finite below that temperature, but it is always uniform
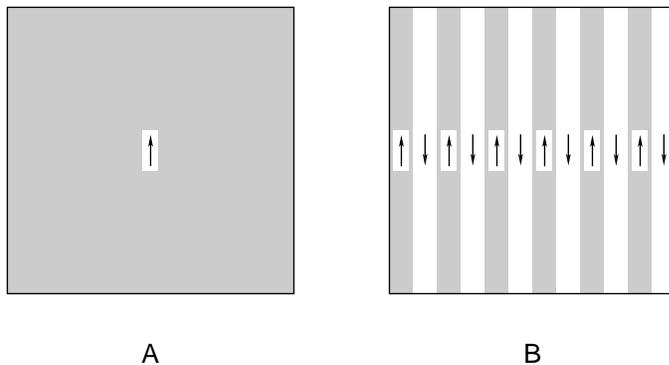
Fig. 9.9   (A) A magnetization pattern in which $M(\mathbf{r})$ is constant throughout the sample. In (B) the magnitude of $M(\mathbf{r})$ is constant, but its sign varies discontinuously from region to region. If the probability of any given pattern of magnetization is assumed to have the form given in Eq. (9.32), then the magnetization patterns shown in (A) and (B) would be equally probable, which seems obviously unreasonable.

throughout the sample. However, the fluctuations about the uniform average magnetization are, by their nature, nonuniform. In order to incorporate fluctuations into the thermodynamic analysis, it is necessary to construct some expression that describes the probability that the sample will be found with a particular spatially varying magnetization $M(\mathbf{r})$. It is easiest to begin at a temperature above T_c, so that the equilibrium value of M is zero. Above T_c the parameter at is positive, and the probable values of M are very small (of order $N^{-1/2}$). Therefore, the term proportional to M^4 can be neglected. That term becomes important only when t is very small or negative.

In the Landau theory, the magnetization is always assumed to be uniform and, with no external field and neglecting the M^4 term, the probability of obtaining a value M for the uniform magnetization is taken as

$$P(M) = C \exp(-atVM^2) \tag{9.31}$$

A natural way of extending the Landau theory to treat nonuniform patterns of magnetization would be to replace the term VM^2 by a term of the form $\int M^2(\mathbf{r})\, d^3\mathbf{r}$. That is, the probability of finding the sample with a magnetization pattern $M(\mathbf{r})$ would be taken as

$$P[M(\mathbf{r})] = C \exp\left(-at \int M^2(\mathbf{r})\, d^3\mathbf{r}\right) \tag{9.32}$$

This reduces to Eq. (9.31) when $M(\mathbf{r})$ is constant. Equation (9.32) would imply that the fluctuations in different macroscopic regions were statistically uncorrelated. That is, if we decompose the total volume V into two disjoint regions, V_1, and V_2, then, because

$$\int_V M^2 \, d^3\mathbf{r} = \int_{V_1} M^2 \, d^3\mathbf{r} + \int_{V_2} M^2 \, d^3\mathbf{r} \tag{9.33}$$

the probability of simultaneously getting a magnetization $M_1(\mathbf{r})$ within V_1 and a magnetization $M_2(\mathbf{r})$ within V_2 would be equal to the exponential of the sum of the integrals and therefore equal to the product of the separate probabilities.

9.7   THE GRADIENT EFFECT

The modification of Landau theory proposed neglects an important effect, namely the *gradient effect*. It would state that the probability of the two magnetization patterns shown in Fig. 9.9 were equal, which seems clearly unreasonable. The rapid back and forth changes in $M(\mathbf{r})$ shown in the pattern of Fig. 9.9(B) would require high-energy domain walls that would very much suppress the probability of occurrence of such a magnetization pattern. In the expression for the probability of a particular macrostate, some account must be taken of the rate of spatial variation (the gradient) of the magnetization. To determine the specific term that is necessary, one can refer to the results of the computer experiment carried out in Problem 8.26. It is

done on a two-dimensional Ising lattice, but the same result would be obtained in three dimensions. An Ising lattice in the form of a long tube, with a circumference of ten lattice units, is considered. The spins at one end of the tube are maintained at a fixed magnetization, $M = \langle \sigma \rangle = +1$. The average of the magnetization of a circular column of spins is then measured as a function of distance from the fixed end. $M(x) = \langle \sigma \rangle$, where the average is taken over all ten spins in the column at x and over a long Monte Carlo run at fixed temperature. It is found that the equilibrium value of $M(x)$ has an exponential form. That is, near the fixed column at $x = 0$,

$$M(x) = me^{-x/\ell} \tag{9.34}$$

where the *correlation length* ℓ increases as T approaches T_c. The exponential function is a solution of the equation

$$-\ell^2 \nabla^2 M + M = 0 \tag{9.35}$$

This is the equation that would be obtained by maximizing the following expression for the conditional canonical potential associated with a magnetization distribution $M(\mathbf{r})$. (See Problem 9.2.)

$$\phi(M) = \phi_o - \int_V \left[atM^2(\mathbf{r}) + c|\nabla M(\mathbf{r})|^2 \right] d^3\mathbf{r} \tag{9.36}$$

where $\ell^2 = c/at$. This expression for the value of the canonical potential to be assigned to any given pattern of magnetization seems to be adequate for $T > T_c$, where t is positive. In order to treat the case of zero or negative t, it will be necessary to again add a term of the form bM^4. The expression one then obtains is known as the *Landau–Ginsburg potential*.

$$\phi(T, M) = \phi_o - \int_V \left(atM^2 + bM^4 + c|\nabla M|^2 \right) d^3\mathbf{r} \tag{9.37}$$

The term proportional to $|\nabla M|^2$ will make the value of $\phi(M)$ large and negative for any function $M(\mathbf{r})$ that has very rapid variations in space. The probability of such a magnetization distribution, which is equal to $\exp \phi(M)$, will therefore be very small.

9.8   FUNCTIONAL INTEGRALS
The interpretation of the expression

$$P = C \exp\left[-\int \left(atM^2 + bM^4 + c|\nabla M|^2 \right) d^3\mathbf{r} \right] \tag{9.38}$$

as the probability of finding the system with the magnetization pattern $M(\mathbf{r})$ requires some careful mathematical analysis. In order for the expression to have any meaning as a probability, it must be normalized so that the sum of P over all possible distributions of magnetization $M(\mathbf{r})$ is one. But $M(\mathbf{r})$ is a function. How can one possibly take a sum over the vast set of conceivable functions, $M(\mathbf{r})$? Actually, there is a mathematical structure, called a *functional integral*, that was introduced by the mathematician Norbert Wiener to handle just such problems in probability theory. It was later rediscovered by Richard Feynman and used in a reformulation of fundamental quantum mechanics. Functional integration is a rather complex and difficult subject. Fortunately, the very fact that the Landau–Ginzburg theory must be interpreted as a macroscopic, thermodynamic theory of critical phenomena will allow us to avoid entirely the complexities of functional integration.

In attempting to give precise meaning to Eq. (9.38), we will consider a system that is in the form of a cube of side L, write the Cartesian components of $\mathbf{r}$ as x_1, x_2, and x_3, and assume that $M(x_1, x_2, x_3)$ satisfies periodic boundary conditions. It will simplify many of the later formulas if, for every integer K, we define the function

$$u_K(x) = \begin{cases} \sqrt{2}\cos kx, & \text{if } K > 0 \\ 1, & \text{if } K = 0 \\ \sqrt{2}\sin kx, & \text{if } K < 0 \end{cases} \tag{9.39}$$

where $k = 2\pi|K|/L$. Then the functions u_K satisfy the simple orthonormality relations

$$\int_o^L u_M(x)u_N(x)\, dx = L\delta_{MN} \tag{9.40}$$

Any real periodic function $f(x)$ with a period L can be expanded as the Fourier series

$$f(x) = \sum_K f_K \, u_K(x) \tag{9.41}$$

where

$$f_K = L^{-1} \int_o^L f(x) u_K(x) \, dx \tag{9.42}$$

Without this artifice, the special case $K = 0$ would require separate treatment in most of the following analysis. Introducing a single symbol $\mathbf{K}$ for the triplet of integers (K_1, K_2, K_3), we will expand M as a triple Fourier series, involving the *fluctuation amplitudes* $M_\mathbf{K}$.

$$M(x_1, x_2, x_3) = \sum_\mathbf{K} M_\mathbf{K} \, u_{K_1}(x_1) \, u_{K_2}(x_2) \, u_{K_3}(x_3) \tag{9.43}$$

The integers (K_1, K_2, K_3) are called the *mode numbers* corresponding to the wave vector $\mathbf{k} = 2\pi\mathbf{K}/L$. Clearly, the term with a wave vector $\mathbf{k}$ describes a fluctuation in the magnetization with a wavelength of size $2\pi/k$. But $M(\mathbf{r})$ is defined as the average magnetization within a volume, centered at $\mathbf{r}$, that contains very many individual spins. Variations in this function on any scale comparable to the lattice spacing have no meaning. They are microscopic details that have already been incorporated into the term $\phi_o(T)$. We must, in a somewhat arbitrary way, choose a minimum length scale Λ (and therefore a maximum wave vector $k_m = 2\pi/\Lambda$) for macroscopic fluctuations and declare that all details on a scale smaller than Λ are included in the ϕ_o term. That our arbitrary choice of Λ will not affect the outcome of any calculations very close to the critical point is shown by the results of Problem 9.7, where the reader is asked to plot the magnetic susceptibility per spin for systems of increasing size as a function of temperature. The sharp, high peak in χ_m, that is symptomatic of the critical phase transition, only becomes evident as L, the size of the system, becomes large. The fluctuations in M that are contributing to the divergence of χ_m are large-scale fluctuations. Such large-scale fluctuations are possible only in a large system. In a very large system, the small-scale fluctuations, whose calculation might be affected by our choice of Λ, make a contribution to χ_m that is negligible in comparison to the divergent contribution made by the large wavelength fluctuations, once we are sufficiently close to the critical point. Therefore, for the purpose of calculating the critical-point properties of the system, we can restrict the sum on $\mathbf{K}$ in Eq. (9.43) to the finite number of terms with $|\mathbf{K}| < L/\Lambda$.

The partition function Z is the sum of $\exp(-\beta E)$ over all possible configurations of the system. By assuming that the conditional canonical potential is given by Eq. (9.37), we have assumed that the sum of $\exp(-\beta E)$ over all those microscopic configurations that have a given set of fluctuation amplitudes $\{M_\mathbf{K}\}$ is equal to

$$Z(\{M_\mathbf{K}\}) = \exp\left(\phi_o - \int \left(atM^2 + bM^4 + c|\nabla M|^2\right) d^3\mathbf{r}\right) \tag{9.44}$$

where the function $M(\mathbf{r})$ is given in terms of the $M_\mathbf{K}$ by Eq. (9.43). The full partition function is the integral of $Z(\{M_\mathbf{K}\})$ over all values of the fluctuation amplitudes.

$$Z = e^{\phi_o} \int \exp\left[-\int \left(atM^2 + bM^4 + c|\nabla M|^2\right) d^3\mathbf{r}\right] \prod_\mathbf{K} dM_\mathbf{K} \tag{9.45}$$

Let us first evaluate this integral for $T > T_c$ by neglecting the term proportional to M^4. This is called the *Gaussian approximation*. Our first task is to evaluate the integral $\int \left(atM^2 + c|\nabla M|^2\right) d^3\mathbf{r}$ as an explicit function of the fluctuation amplitudes. This can easily be done by using the orthonormality relations [Eq. (9.40)] for the functions u_K and the identity

$$\int \nabla M \cdot \nabla M \, d^3\mathbf{r} = -\int M \, \nabla^2 M \, d^3\mathbf{r} \tag{9.46}$$

The result is that

$$\int \left(atM^2 + c|\nabla M|^2\right) d^3\mathbf{r} = L^3 \sum_\mathbf{K} (at + ck^2) M_\mathbf{K}^2 \tag{9.47}$$

where $k^2 = k_1^2 + k_2^2 + k_3^2 = (2\pi/L)^2(K_1^2 + K_2^2 + K_3^2)$. The integral for Z then factors into independent integrals over each of the variables $M_\mathbf{K}$.

$$Z = e^{\phi_o} \prod_\mathbf{K} \int_{-\infty}^{\infty} \exp\left[-L^3(at + ck^2)M_\mathbf{K}^2\right] dM_\mathbf{K}$$
$$= e^{\phi_o} \prod_\mathbf{K} \left(\frac{\pi/L^3}{at + ck^2}\right)^{1/2} \tag{9.48}$$

The canonical potential, including the contribution of the fluctuations, is

$$\phi = \phi_o + \frac{1}{2}\sum_\mathbf{K} \log\left(\frac{\pi/L^3}{at + ck^2}\right) \tag{9.49}$$

The energy is given by $-\partial\phi/\partial\beta$.

$$E = E_o - \frac{1}{2}\frac{\partial}{\partial\beta}\sum_\mathbf{K}\log\left(\frac{\pi/L^3}{at + ck^2}\right)$$
$$= E_o + \frac{1}{2}\frac{T^2}{T_c}\frac{\partial}{\partial t}\sum_\mathbf{K}\log\left(\frac{\pi/L^3}{at + ck^2}\right) \tag{9.50}$$
$$= E_o - \frac{1}{2}\frac{T^2}{T_c}\sum_\mathbf{K}\frac{a}{at + ck^2}$$

Since we are only interested in the singularity in the specific heat that occurs close to the critical point, we can set the smooth function T^2/T_c equal to T_c, its value at $T = T_c$. The specific heat, close to T_c, is equal to $\partial E/\partial T = (1/T_c)\partial E/\partial t$.

$$C = C_o + \frac{1}{2}\sum_\mathbf{K}\frac{a^2}{(at + ck^2)^2} \tag{9.51}$$

To evaluate the specific heat *at* the critical point, we must set $t = 0$, obtaining

$$C = C_o + \frac{1}{2}(a/c)^2\sum_\mathbf{K}k^{-4} \tag{9.52}$$

Clearly, the term with $\mathbf{k} = 0$ diverges. What is important to note, however, is that all of the long-wavelength modes give effectively divergent contributions to the specific heat. Consider the contribution to the sum of, let us say, the 1000 modes of smallest, but nonzero, k. They all have wave vectors of order L^{-1}. Thus each of them would contribute a term of order L^4. Since the specific heat is an extensive variable, and thus of order L^3, these contributions all diverge in the thermodynamic limit. Because of this *infrared divergence*, in the limit $t \to 0$, the term proportional to M^4 in the Landau–Ginsburg potential cannot be neglected.

9.9   THE CRITICAL DIMENSION

When the term BM^4 is included in Eq. (9.45), the integral no longer factors into independent integrals over each of the variables $M_\mathbf{K}$. It then becomes a very high-dimensional integral of a non-Gaussian exponential function, which cannot be evaluated. One can get some idea of the effect of the fourth-order term by calculating the partition function for an artificial situation in which all of the fluctuation modes except a single mode with mode numbers $\mathbf{K}$ are suppressed. In order to see an important effect of the dimensionality of the space, we will do this analysis for a space of unspecified dimension D. With only a single mode operating, the magnetization pattern is of the form

$$M(x_1, \ldots, x_D) = M_\mathbf{K}u_{K_1}(x_1)\cdots u_{K_D}(x_D) \tag{9.53}$$

This calculation will *not* allow us to determine the contributions to the canonical potential of the fluctuations in the macroscopic magnetization, because the integral for Z does not factor, and therefore the separate

fluctuations do not give independent contributions to ϕ. Near the critical point, the fluctuations of different wavelengths strongly interact with one another. The contribution to ϕ of the fluctuations at various wavelengths is not equal to the sum of the contributions of the wavelengths taken separately. However, this calculation will exhibit a certain characteristic of the problem that has been very important in finding a practical method of calculating critical exponents and other characteristics of critical phenomena.

With $M(\mathbf{r})$ given by Eq. (9.53), the spatial integral that appears in the exponent in Eq. (9.45) can be easily evaluated. At $T = T_c$, t is zero, and therefore, the terms we need to integrate are the $|\nabla M|^2$ term and the M^4 term. We are most interested in determining how these integrals depend upon the size of the system L and the spatial dimension D. In the following analysis, $k^2 = k_1^2 + \cdots + k_D^2 = 4\pi^2 K^2 L^{-2}$. First we note that

$$
\begin{aligned}
\int \nabla M \cdot \nabla M \, dx_1 \cdots dx_D &= - \int M \, \nabla^2 M \, dx_1 \cdots dx_D \\
&= k^2 L^D M_{\mathbf{K}}^2 \\
&= 4\pi^2 K^2 L^{D-2} M_{\mathbf{K}}^2
\end{aligned}
\tag{9.54}
$$

The M^4 integral is

$$
\begin{aligned}
\int M^4 dx_1 \cdots dx_D &= M_{\mathbf{K}}^4 \int_o^L u_{K_1}^4 dx_1 \int_o^L u_{K_2}^4 dx_2 \cdots \int_o^L u_{K_D}^4 dx_D \\
&\equiv I_{\mathbf{K}} L^D M_{\mathbf{K}}^4
\end{aligned}
\tag{9.55}
$$

The calculation of $I_{\mathbf{K}}$, which depends on the mode numbers, but is never far from one, is left as an exercise for the reader (see Problem 9.8). Using these formulas, one can evaluate the necessary integral

$$
\int (c|\nabla M|^2 + bM^4) \, d^D x = 4\pi^2 K^2 c L^{D-2} M_{\mathbf{K}}^2 + b I_{\mathbf{K}} L^D M_{\mathbf{K}}^4
\tag{9.56}
$$

With all other modes frozen at zero, the partition function is given by integrating $\exp[\phi_o - \int(c|\nabla M|^2 + bM^4)d^D x]$ over all possible values of the mode amplitude $M_{\mathbf{K}}$ [see Eq. (9.45)].

$$
Z = e^{\phi_o} \int_{-\infty}^{\infty} \exp\left(-4\pi^2 K^2 c L^{D-2} M_{\mathbf{K}}^2 - b I_{\mathbf{K}} L^D M_{\mathbf{K}}^4\right) dM_{\mathbf{K}}
\tag{9.57}
$$

In order to isolate the L dependence, we make a transformation of variables, $m = L^{(D-2)/2} M_{\mathbf{K}}$. Then

$$
Z = e^{\phi_o} L^{-(D-2)/2} \int \exp\left(-4\pi^2 K^2 c m^2 - b I_{\mathbf{K}} L^{4-D} m^4\right) dm
\tag{9.58}
$$

If $D > 4$ and $\mathbf{K} \neq 0$, then, because of the factor L^{4-D}, the second term in the exponent becomes negligible in comparison with the first in the thermodynamic limit, $L \to \infty$. But it is the M^4 term that produces the troublesome interactions between different modes. The same analysis is valid when any number of nonuniform modes exist simultaneously. In a space of more than four dimensions, the interaction terms are negligible in the thermodynamic limit, and therefore the partition function integral becomes a multiple Gaussian integral that can be evaluated.

Recall that, according to Eq. (9.52), the contribution to the specific heat, at $T = T_c$, of any nonuniform mode, calculated with the Gaussian approximation, was proportional to L^4, and therefore divergent in comparison with the ordinary specific heat, which is proportional to L^3. But, in dimension D, the ordinary specific heat is proportional to L^D. Thus, for $D > 4$, the separate terms in the Gaussian approximation each give a negligible contribution to the specific heat and, once the $\mathbf{K} = 0$ mode has been separated out, the discrete sum may be converted to an integral, using the usual rule that

$$
\sum_{\mathbf{K}} (\cdots) \to (L/2\pi)^D \int (\cdots) \, d^D k
\tag{9.59}
$$

The $\mathbf{K} = 0$ mode must, however, be treated separately. But the $\mathbf{K} = 0$ mode describes a uniform magnetization—just the sort of thing that is included in the simple Landau theory. Therefore, using the

simple Landau theory to calculate the contribution of the uniform mode and the Gaussian approximation for all the nonuniform fluctuations would allow one to calculate all of the critical exponents for systems in dimension D larger than four. This must seem to the reader like a completely empty result, since no real system is more than three dimensional. The point in looking at higher dimensional systems is that they are the closest solvable systems to the three-dimensional systems whose critical behavior we would like to calculate.

9.10   THE EPSILON EXPANSION

In contrast to textbook problems, most real problems that come up in physics cannot be solved exactly. One of the standard techniques for obtaining an approximate solution to an intractable mathematical problem is to find a solvable problem that is, in some sense, close to the given, unsolvable problem. The most common sense in which the solvable problem is close to the unsolvable one is that the two problems differ in the value of some numerical parameter λ. For example, it is impossible to calculate the orbits of the planets in the solar system, because of gravitational interactions between the planets. However, if the interplanetary interactions are turned off, then the problem of a planet moving in the gravitational field of the sun can be completely solved. We can relate the solvable problem to the unsolvable one as follows. We consider a sun of mass M and nine planets of masses $\lambda m_1, \lambda m_2, \ldots, \lambda m_9$, where λ is an adjustable parameter and m_i is the actual mass of the ith planet. For fixed λ and some given initial positions and velocities, let $\mathbf{R}_i(t, \lambda)$ be the trajectory of the ith planet. What we can calculate is $\mathbf{R}_i(t, 0)$. (When λ is very small, the planets move in the same way as "dust particles" in the field of the sun and their trajectories are simple ellipses, independent of their masses.) What we would like to know is $\mathbf{R}_i(t, 1)$. The *perturbation method* assumes that the function $\mathbf{R}_i(t, \lambda)$ can be expanded as a power series in λ.

$$\mathbf{R}_i(t, \lambda) = \mathbf{R}_i(t, 0) + \mathbf{R}_i'(t)\lambda + \mathbf{R}_i''(t)\lambda^2 + \cdots \tag{9.60}$$

It is possible to write the functions $\mathbf{R}_i'$, $\mathbf{R}_i''$, etc. as integrals involving the known functions $\mathbf{R}_i(t, 0)$. If t is not too large, the sizes of the terms in the series decrease rapidly, and it is a good approximation to cut off the infinite series after a few terms. In this way, one can construct useful, but not exact, analytic solutions to the problem of planetary motion.

In a similar way, it is possible to construct equations for critical-point parameters, such as exponents and amplitude ratios. The equations involve the parameter D, the space dimension, in such a way that they are meaningful for noninteger D. The parameter D is written in terms of an expansion parameter ϵ as

$$D = 4 - \epsilon \tag{9.61}$$

The equations can be solved exactly for $\epsilon = 0$, and the desired quantities (critical exponents, etc.) can be written as power-series expansions in ϵ. The next few sections will present the fundamental ideas needed to construct such equations.
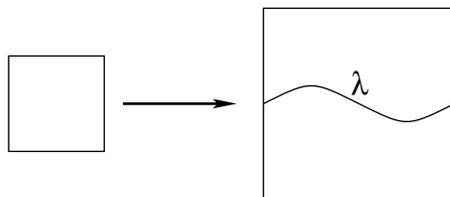

Fig. 9.10   When the size of a system at its critical temperature is increased, the important new degrees of freedom are fluctuations of a wavelength that could not have fit into the smaller system.

9.11   RENORMALIZATION THEORY

Although the Landau–Ginsburg theory is basically an adequate theory of critical phenomena, the complete intractability of the integral over fluctuation amplitudes for many years prevented any use of the theory to make calculations of critical parameters. The essential elements of a tractable calculational method were

supplied, in the early 1970s, by Kenneth Wilson of Cornell University. Wilson's analysis, which is called *renormalization theory*, begins with a study of what happens to the distribution of configurations of a system when one increases the size of the system. One can see why such a peculiar study might be relevant to critical phenomena by considering what new elements are introduced if we double the dimensions of a sample of ferromagnetic material at its critical temperature. (See Fig. 9.10.)

By doubling the size of the system, we have increased the number of microscopic degrees of freedom, but that is a trivial change, because the microscopic degrees of freedom in the larger system are basically identical to those in the smaller one. The new elements that have been added are fluctuations of a size that could not be accommodated in the smaller system. But it is exactly such large-scale fluctuations that are responsible for critical behavior. Thus, in looking only at the *changes* in going from a smaller to a larger system, all the details that are irrelevant to the critical point cancel out. The theoretical device used in the study is a two-step process, called a *renormalization transformation.*

1. In the first step, we scale up the size of the system by some factor larger than one. (This is all done theoretically—renormalization is not an experimental procedure.) What we aim to do is to compare the probability distribution for the configurations of the larger system with that of the smaller one. But this cannot be done immediately, because the larger system has more coordinates, and therefore many more possible configurations. The probability distributions would therefore be functions of very different numbers of variables and thus not directly comparable. To circumvent that difficulty, one carries out the second step.

2. We separate the coordinates in the larger system into a set of short-range coordinates and a set of long-range coordinates, in such a way that the number of long-range coordinates is equal to the total number of coordinates in the smaller system. We now compute the probability distribution for the long-range coordinates by integrating over the short-range coordinates. This leaves us with a probability function for the larger system that can be compared with that of the smaller system.

The procedure can be made clear by carrying it out in detail for the system shown in Fig. 9.11; a one-dimensional chain of coupled harmonic oscillators held fixed at its left end. The system is described by the $N+1$ coordinates, $x_o, x_1, \ldots, x_N$, where x_o is fixed at zero. The value of βE for a given configuration is assumed to be of the form

$$\beta E = K_1(x_1^2 + \cdots + x_{N-1}^2) + \tfrac{1}{2}K_1 x_N^2 + K_2 \sum_{n=1}^{N} (x_n - x_{n-1})^2 \qquad (9.62)$$

The spring constant K_1 has been reduced on the last particle to $K_1/2$ for a technical reason that will be made clear shortly. Such a modification would have no effect on the thermodynamic behavior of a very large system. The chain can be considered to be made up of N elementary *links*, such as shown in Fig. 9.11(B). To make up the chain, the mass points of the links are pasted together, thus increasing the interior spring constants from $K_1/2$ to K_1. In the canonical ensemble, the probability that the two ends of a single isolated link have coordinates x and y is proportional to the function

$$g_1(x,y) = \exp[-\tfrac{1}{2}K_1(x^2 + y^2) - K_2(x - y)^2] \qquad (9.63)$$

The partition function for the system is the integral of $\exp(-\beta E)$ over the N free coordinates, $x_1, \ldots, x_N$. It can be written as

$$Z_N = \int g_1(0, x_1) g_1(x_1, x_2) \cdots g_1(x_{N-1}, x_N)\, dx_1 \cdots dx_N \qquad (9.64)$$

We now increase the number of links to $2N$, writing the coordinates in the longer chain as $x_o, y_1, x_1, y_2, x_2, \ldots, y_N, x_N$. (Remember, x_o is defined as zero.) The partition function of the longer chain is

$$Z_{2N} = \int g_1(0, y_1) g_1(y_1, x_1) \cdots g_1(y_N, x_N)\, dy_1 \cdots dy_N\, dx_1 \cdots dx_N$$

$$= \int g_2(0, x_1) g_2(x_1, x_2) \cdots g_2(x_{N-1}, x_N)\, dx_1 \cdots dx_N \qquad (9.65)$$

where

$$g_2(x,y) = \int_{-\infty}^{\infty} g_1(x, z) g_1(z, y)\, dz \qquad (9.66)$$
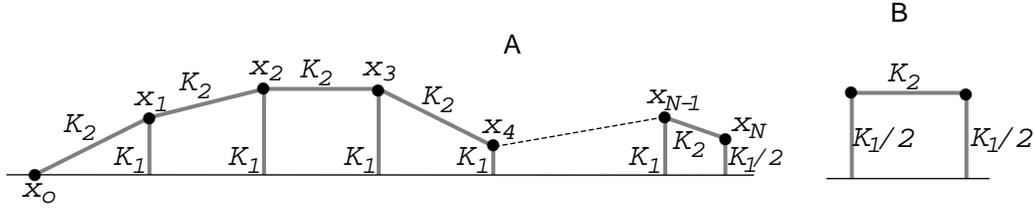
Fig. 9.11 (A) A system of $N+1$ particles that move only in the vertical direction. The potential energy has terms proportional to the square of the distance of a particle from its equilibrium position and terms proportional to the squares of the differences in the vertical coordinates of neighboring particles. (B) The system can be considered as being composed of N "links" of the form shown. What this really means is that the potential energy function is the sum of N terms of the form, $(K_1/2)(x_n^2 + x_{n-1}^2) + K_2(x_n - x_{n-1})^2$.

$g_2(x,y)$ is the unnormalized probability function for the end coordinates of a double link. With this transformation, the unnormalized configurational probability for the larger system, namely $g_2(x_o, x_1)g_2(x_1, x_2) \cdots g_2(x_{N-1}, x_N)$, is now in a form in which it can be compared with that of the smaller system. However, the coordinates in the larger system represent the endpoints of larger pieces (that is, double links) than those in the smaller system. The detailed integral for g_2 is not difficult to carry out.

$$g_2(x,y) = \int \exp[-\tfrac{1}{2}K_1(x^2 + y^2) - K_1 z^2 - K_2(x - z)^2 - K_2(z - y)^2] \, dz \tag{9.67}$$

The integral is done by expanding the quadratic polynomial, completing the square in z, and writing the rest in terms of x, y, and $x - y$.

$$
\begin{aligned}
\tfrac{1}{2}K_1&(x^2 + y^2) + K_1 z^2 + K_2(x - z)^2 + K_2(z - y)^2 \\
&= \tfrac{1}{2}(K_1 + 2K_2)(x^2 + y^2) + (K_1 + 2K_2)z^2 - 2K_2 z(x + y) \\
&= \tfrac{1}{2}(K_1 + 2K_2)(x^2 + y^2) + (K_1 + 2K_2)\Big(z - \frac{K_2(x + y)}{K_1 + 2K_2}\Big)^2 - \frac{K_2^2}{K_1 + 2K_2}(x + y)^2 \\
&= \tfrac{1}{2}K_1\Big(\frac{K_1 + 4K_2}{K_1 + 2K_2}\Big)(x^2 + y^2) + \frac{K_2^2}{K_1 + 2K_2}(x - y)^2 + (K_1 + 2K_2)\Big(z - \frac{K_2(x + y)}{K_1 + 2K_2}\Big)^2
\end{aligned}
\tag{9.68}
$$

With this we see that

$$g_2(x,y) = \Big(\frac{\pi}{K_1 + 2K_2}\Big)^{1/2} \exp[-\tfrac{1}{2}\tilde{K}_1(x^2 + y^2) - \tilde{K}_2(x - y)^2] \tag{9.69}$$

where $\tilde{K}_1 = K_1(K_1 + 4K_2)/(K_1 + 2K_2)$ and $\tilde{K}_2 = K_2^2/(K_1 + 2K_2)$. The factor $\sqrt{\pi/(K_1 + 2K_2)}$ is important in computing the partition function, but not in discussing the probability distribution, which would have to be normalized anyway. The configurational probability of the larger system has the same form as that of the smaller system, except for the fact that the parameters K_1 and K_2, have undergone the transformation

$$K_1 \to K_1\Big(\frac{K_1 + 4K_2}{K_1 + 2K_2}\Big) \quad \text{and} \quad K_2 \to \frac{K_2^2}{K_1 + 2K_2} \tag{9.70}$$

If we repeat this transformation, over and over again, we obtain the probability distribution for the endpoints of longer and longer links in a larger and larger system. The parameters K_1 and K_2 move as shown in the *renormalization flow diagram* in Fig. 9.12. If we begin with any nonzero value of K_1, then after repeated renormalizations the value of K_2 approaches zero and the value of K_1 approaches some point on the K_1 axis that depends on our starting values. If we begin with any point $K_1 > 0$ and $K_2 = 0$, then the point does not change under renormalization. Thus all the points on the K_1 axis are called *fixed points* of the renormalization flow. These are called trivial fixed points, because they describe systems in which $K_2 = 0$ and therefore the two ends of every link are statistically independent. That is, they
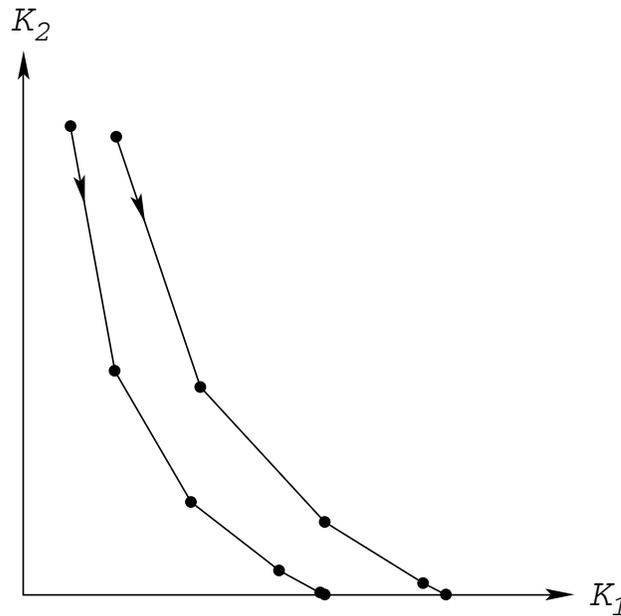
Fig. 9.12   Repeated renormalizations will bring any point with a nonzero value of K_1
to some fixed point on the K_1 axis. Different starting points within the K_1–K_2 plane
lead, in general, to different fixed points.

describe systems of noninteracting harmonic oscillators. Thus any system with a nonzero value of K_1, after
it is scaled a sufficient number of times, resembles a system with noninteracting coordinates. That after
many renormalization transformations neighboring particles become noninteracting is not surprising—the
coordinates of neighboring particles in the final system represent the positions of quite distant particles in
the original system.

9.12   THE NONTRIVIAL FIXED POINTS

If, in the initial system, $K_1 = 0$ exactly, then the renormalization flow equations say that K_1 remains zero and
that $K_2 \to K_2/2$. This does not look like a fixed point, but that impression is wrong. We have not yet used
up all of our freedom in mapping the larger system onto the smaller one. In comparing the configurations
of the larger system with those of the smaller one, we are free to scale the coordinates, defining coordinates
$\tilde{x}_1, \ldots, \tilde{x}_N$ in the larger system by the relations $x_n = \sqrt{2}\,\tilde{x}_n$. Then in terms of $\tilde{x}$ and $\tilde{y}$, with $K_1 = 0$,

$$g_2(\tilde{x}, \tilde{y}) = \left(\frac{\pi}{2K_2}\right)^{1/2} \exp[-K_2(\tilde{x} - \tilde{y})^2] \tag{9.71}$$

which means that the new probability distribution is the same as the original one. Since $g_2(\tilde{x}, \tilde{y})$ is not equal
to a function of $\tilde{x}$ times a function of $\tilde{y}$, the probability distribution for the configurations of the system will
not approach one for a system of noninteracting elements as the system size grows. The set of fixed points
along the K_2 axis are not trivial fixed points. Nontrivial fixed points describe states of the system that have
scale-invariant probability distributions. Let us confirm that this is so for the harmonically coupled chain
that we are considering.

9.13   SCALE INVARIANCE

If $K_1 = 0$, then the probability of a configuration $(x_1, x_2, \ldots, x_N)$ is equal to

$$P(x_1, x_2, \ldots, x_N) = C g_1(0, x_1) g_1(x_1, x_2) \cdots g_1(x_{N-1}, x_N) \tag{9.72}$$

where $g_1(x, y) = \exp[-K_2(x-y)^2]$. A small ensemble of configurations for such a system is shown in Fig. 9.13.
It is clear from the picture that the probability distribution for the system configurations resembles that of
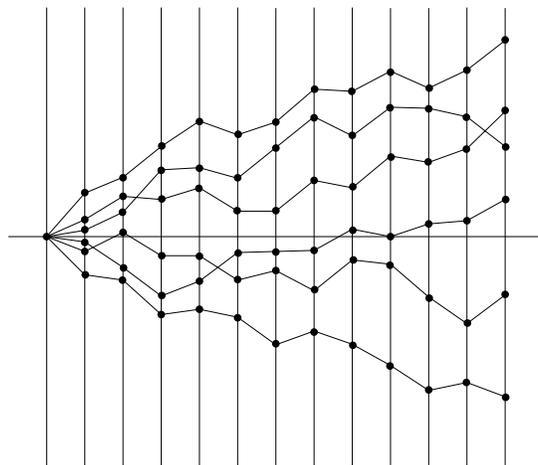
Fig. 9.13   A small ensemble of reasonably probable configurations of the system with $K_1 = 0$. The probability distribution for the system is the same as that for a random walk of N steps. As N increases, the fluctuations of the right end increase as $\sqrt{N}$. In contrast, when K_1 is not zero, the configurations remain close to the horizontal axis. Then the fluctuations about that axis provide a fixed scale of length and, as $N \to \infty$, a picture of the ensemble would show the configurations more and more concentrated on the axis.

a random walk of length N. (See Problems 1.24 to 1.26 for a definition of the random walk problem.) It is easy to confirm that it is precisely the probability distribution for a random walk of individual step size $a = 1/\sqrt{2K_2}$. Imagine that in the picture N is made so large that the individual steps are well beyond the limit of discernibility. Then the individual curves in the ensemble become examples of fractals. In that limit, an ensemble of random walks is known to have the characteristic that, if we take the piece of the picture between 0 and ℓ, blow it up by a factor L/ℓ in the horizontal direction, and by a factor of $\sqrt{L/\ell}$ in the vertical direction, then it will match exactly the original picture of the ensemble between 0 and L. Whenever the probability distribution for the configurations of a complex system has the property that, by scaling a few parameters, one can make the ensemble for a smaller system exactly match that of a larger system, then the probability distribution is said to be scale invariant. It can be shown that all nontrivial fixed points of renormalization transformations lead to scale-invariant probability distributions.

The two fundamental assumptions of Wilson's analysis of critical phenomena were that

1. At the critical point, the probability distribution for the fluctuations in the order parameter (the magnetization for ferromagnetic transitions) is scale invariant.
2. The scale-invariant distribution could be obtained as a nontrivial fixed point of a properly formulated renormalization transformation.

9.14   STABILITY OF FIXED POINTS

Looking at the renormalization flow diagram, one can see that a system point located close to, but not at, a nontrivial fixed point behaves, under repeated transformations, very differently from one located close to a trivial fixed point. The flow lines are all directed away from the nontrivial fixed points and toward the trivial ones. An initial point (K_1, K_2) that has K_2 very small but nonzero would be close to the trivial fixed point $(K_1, 0)$. Under repeated renormalizations, it would move toward that fixed point. However, an initial point with K_1 very small but nonzero, which would be close to the nontrivial fixed point $(0, K_2)$, would move steadily further from the K_2 axis, eventually coming to a trivial fixed point on the K_1 axis. For this reason, the trivial fixed points are called stable, in analogy with a stable equilibrium position of a mechanical system, while the nontrivial fixed points are called unstable fixed points. This is a general property of trivial and nontrivial fixed points. The nontrivial fixed points describe critical points of the associated thermodynamic system. At a critical point, the correlation functions for local macroscopic observables, such as the order parameter correlation function,

$$c(\mathbf{r}, \mathbf{r}') = \langle M(\mathbf{r})M(\mathbf{r}')\rangle \tag{9.73}$$

fall off as some power of $|\mathbf{r} - \mathbf{r}'|$. That is, *

$$\langle M(\mathbf{r})M(\mathbf{r}')\rangle \sim \frac{1}{|\mathbf{r} - \mathbf{r}'|^\lambda} \tag{9.74}$$

This can be seen to be a direct consequence of the assumption that the critical probability distribution is scale invariant. If a system of volume V is scaled to a volume s^3V, where s is some scaling parameter larger than one, then it should be possible, by comparing some scaled order parameter γM at the "corresponding points" in the new system (namely $s\mathbf{r}$ and $s\mathbf{r}'$) with the original order parameter at $\mathbf{r}$ and $\mathbf{r}'$, to obtain exactly the same correlation function. This implies that

$$\langle \gamma M(s\mathbf{r})\gamma M(s\mathbf{r}')\rangle = \langle M(\mathbf{r})M(\mathbf{r}')\rangle \tag{9.75}$$

With the correlation function given in Eq. (9.74), it is clear that this is satisfied for $\gamma = s^{\lambda/2}$.

$$\frac{\gamma^2}{|s\mathbf{r} - s\mathbf{r}'|^\lambda} = \frac{1}{|\mathbf{r} - \mathbf{r}'|^\lambda} \Rightarrow \gamma = s^{\lambda/2} \tag{9.76}$$

In any thermodynamic state that is not at the critical point, the correlation function at large distances has an exponential behavior.

$$c(\mathbf{r}, \mathbf{r}') \sim \frac{e^{-|\mathbf{r}-\mathbf{r}'|/\ell}}{r^\lambda} \tag{9.77}$$

where the parameter ℓ is the correlation length. There is no way of rescaling the order parameter by a factor γ that will make

$$\frac{\gamma^2}{s^\lambda}e^{-s|\mathbf{r}-\mathbf{r}'|/\ell} = e^{-|\mathbf{r}-\mathbf{r}'|/\ell} \tag{9.78}$$

for all values of $|\mathbf{r}-\mathbf{r}'|$. This shows that the probability distribution is not scale invariant. The correlation length ℓ acts as a standard of length that does not scale with the system size.

If the basic correlations in the system decay exponentially with a fixed correlation length, then after repeated renormalization transformations we will arrive at a set of long-range variables that are statistically independent. In the harmonically coupled chain those variables describe the endpoints of very long links. In a Landau–Ginsburg theory they will describe local magnetizations $M(\mathbf{r})$ that are averages over larger and larger domains. As the domains become much larger than the correlation length ℓ, the averages over different domains become statistically independent. When the renormalization process has produced statistically independent variables, then the set of parameters in the probability distribution (for the harmonically coupled chain, simply K_1 and K_2) will have reached a trivial fixed point. Thus the stability properties of the fixed points are closely associated with the decay of the correlation function in the states described by those fixed points. Unstable fixed points give power-law decay, while stable fixed points describe states with exponentially decaying correlation functions.

The renormalization flow diagram of the harmonically coupled chain has one feature that is not a general characteristic of such diagrams. That is that both the trivial and the nontrivial fixed points in the diagram form continuous lines (in this case, the K_1 and K_2 axes). It is very common for them to be, instead, discrete isolated points. However, there do exist other systems with continuous curves of fixed points.

9.15   THE CALCULATION OF EXPONENTS
In contrast to the Landau–Ginsburg theory, in which all calculations of critical properties were prevented by the impossibility of evaluating the partition function integral, the renormalization theory has allowed the accurate computation of the universal properties of critical phenomena, such as exponents and amplitude ratios. The reason for this practical success is that the desired quantities are entirely determined by the details of the renormalization flow diagram close to the nontrivial fixed point that represents the critical state of the system. As an example of how one relates critical exponents to flow diagrams, we will calculate

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* Usually the power λ in the following equation is written as $\lambda = D - 2 + \eta$, where D is the space dimension and η is yet another critical exponent.

two critical exponents that are associated with the correlation function of the harmonic chain. Before we do so, we will make a simple modification in our definition of the system. Instead of fixing the left end of the chain by demanding that $x_o = 0$, we will use periodic boundary conditions, defined by taking $x_o = x_N$, where N is the number of particles in the system. With periodic boundary conditions, the two-particle correlation function, to be defined, will be translationally invariant. This modification of the boundary conditions has no effect on the renormalization flow equations, $(K_1, K_2) \to (\tilde{K}_1, \tilde{K}_2)$, as can be easily confirmed by the reader.

In a uniaxial ferromagnet, the two-point correlation function is defined as the expectation value of the product of the magnetization at two different points, $\mathbf{r}_1$ and $\mathbf{r}_2$. Because of translational invariance, it is a function only of the relative variable $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. Another way of writing this is that

$$c(\mathbf{r}) = \langle M(\mathbf{R})M(\mathbf{R} + \mathbf{r})\rangle \tag{9.79}$$

where $\mathbf{R}$ is any point within the system. The equivalent function for the harmonic chain is

$$c(r|K_1, K_2) = \langle x_n x_{n+r}\rangle_K \tag{9.80}$$

where r is an integer, x_n is the coordinate of the nth mass point, and $\langle \ldots \rangle_K$ means the expectation value in a system with parameters K_1 and K_2. The dependence of the correlation function on the parameters of the system, K_1 and K_2, is shown explicitly because it will play an important part in the analysis.

We have seen that the probability distribution for the coordinates $\tilde{x}_n$ in the larger system with parameters K_1 and K_2 is identical to the probability distribution for the coordinates x_n in the smaller system with parameters $\tilde{K}_1$ and $\tilde{K}_2$, given in Eq. (9.70). This means that

$$\langle \tilde{x}_m \tilde{x}_n\rangle_K = \langle x_m x_n\rangle_{\tilde{K}} \tag{9.81}$$

But if in the larger system one uses an ordinary numbering of the coordinates, so that x_k is the coordinate of the kth particle (recall that in the previous analysis we called the particle coordinates $x_o, y_1, x_1, \ldots$), then

$$\tilde{x}_n = \frac{1}{\sqrt{2}}x_{2n} \tag{9.82}$$

In the renormalization transformation for the harmonic chain the factor s by which the size of the system is scaled up is 2. The factor γ by which the variables x_{2n} are scaled down to make the variables $\tilde{x}_n$ is $1/\sqrt{2}$. In order to facilitate the generalization of the following analysis to other possible scaling factors, we will rewrite Eq. (9.82) as

$$\tilde{x}_n = \gamma x_{sn} \tag{9.83}$$

Putting this into Eq. (9.81) immediately gives the important renormalization relation

$$\gamma^2 c(sr|K_1, K_2) = c(r|\tilde{K}_2, \tilde{K}_2) \tag{9.84}$$

If $K^* \equiv (K_1, K_2)$ is a fixed point, then $\tilde{K} = K^*$ and this relation can be written

$$\gamma^2 c(sr|K^*) = c(r|K^*) \tag{9.85}$$

This implies that, at the nontrivial fixed point, K^*, $c(r) = A/r^\lambda$ with λ and γ related by

$$\gamma = s^{\lambda/2} \tag{9.86}$$

Thus we see that γ, the scaling factor for the field, in combination with the scaling factor s, determines the power in the correlation function at the critical point. For the harmonic chain, $s = 2$ and $\gamma = 1/\sqrt{2}$, which shows that $\lambda = -1$.

The renormalization relation, Eq. (9.84), can be used to calculate another critical exponent that is associated with the correlation function. If K is not a fixed point, then the correlation function at large r takes an exponential form

$$c(r|K) \sim \frac{e^{-r/\ell}}{r^\lambda} \tag{9.87}$$

As $K_1 \to 0$, which means that K approaches a nontrivial fixed point, the correlation length ℓ, which depends on the values of K_1 and K_2, goes to infinity as some negative power of K_1.

$$\ell(K_1, K_2) \sim \ell_o K_1^{-\nu} \tag{9.88}$$

Using Eq. (9.87), the relation $\gamma^2 c(sr|K) = c(r|\tilde{K})$ can be written as

$$\frac{\gamma^2}{s^\lambda} e^{-sr/\ell(K)} = e^{-r/\ell(\tilde{K})} \tag{9.89}$$

Clearly λ must have the same value as it has at the critical point in order for γ^2/s^λ to be equal to one. The other relation we obtain is that

$$\frac{s}{\ell(K)} = \frac{1}{\ell(\tilde{K})} \tag{9.90}$$

or

$$\frac{\ell(K)}{\ell(\tilde{K})} = s \tag{9.91}$$

Using Eq. (9.88) and the fact that $s = 2$ gives

$$\lim_{K_1 \to 0} \frac{\tilde{K}_1^\nu}{K_1^\nu} = 2 \tag{9.92}$$

When the rescaling, $\tilde{x}_n = x_{2n}/\sqrt{2}$, is taken into account, the flow equations near a nontrivial fixed point take the form

$$K_1 \to 2K_1 \left(\frac{K_1 + 4K_2}{K_1 + 2K_2} \right) \quad \text{and} \quad K_2 \to \frac{2K_2^2}{K_1 + 2K_2} \tag{9.93}$$

Near $K_1 = 0$, the K_1 flow equation gives

$$\tilde{K}_1 \approx 4K_1 \tag{9.94}$$

Thus Eq. (9.92) says that $4^\nu = 2$ or

$$\nu = \tfrac{1}{2} \tag{9.95}$$

The harmonic chain is merely a toy model. It is of no intrinsic importance, but has been presented in order to illustrate the concepts and methods of renormalization theory in a situation where everything can be worked out exactly. For realistic systems, such as those described by the Landau–Ginsburg theory, the integrations necessary to determine the renormalization flow equations are quite complicated, and only the results of those integrations will be given here.

9.16   MOMENTUM-SPACE RENORMALIZATION

The renormalization transformation that has been used in analyzing the harmonic chain is an example of a *real-space renormalization* calculation, which means that the variables used in the calculation (that is, the x_ns) describe properties of the system at locations in real space. It is often more convenient to carry out the calculation in terms of variables that are Fourier components of the real-space variables. The fluctuation amplitudes $M_\mathbf{K}$ are a good example of such variables. One then says that the calculation is being done in momentum space, a terminology taken from quantum mechanics, where the momentum-space and real-space wave functions are just Fourier transforms of one another. To show how the renormalization transformation is done in momentum space, we will consider the renormalization theory analysis of the Landau–Ginsburg model in three dimensions.

The magnetization at point $\mathbf{r}$ is given in terms of the fluctuation amplitudes by the equation

$$M(\mathbf{r}) = \sum_\mathbf{K} M_\mathbf{K} \, u_{K_1}(x_1) \, u_{K_2}(x_2) \, u_{K_3}(x_3) \tag{9.96}$$

where the functions $u_K(x)$ are defined in Eq. (9.39) and the mode numbers, $\mathbf{K} = (K_1, K_2, K_3)$ are restricted to the range

$$|\mathbf{K}| < L/\Lambda \tag{9.97}$$

This restriction guarantees that the wavelengths of the fluctuations remain larger than Λ. We will only consider the case of zero external field. Then the probability distribution for the fluctuations in $M(\mathbf{r})$ is of the form

$$P[\{M_{\mathbf{K}}\}] = C \exp\left(-\int (AM^2 + bM^4 + c|\nabla M|^2)\, d^3\mathbf{r}\right) \tag{9.98}$$

In the simple Landau theory, the critical point occurs when $A = 0$. We will see that, when more accurate calculations are made using renormalization theory, the nontrivial fixed point, in fact, occurs at a slightly negative value of A, not at $A = 0$. That is why we have not written A as at.

The probability distribution is determined by the parameters A, b, and c. These are the equivalents, in the Landau–Ginsburg theory, of the parameters K_1 and K_2 for the harmonic chain. The momentum-space renormalization cycle has the following steps.

1. The size of the system in each direction is increased from L to $L' = sL$, where the scale factor s is any number larger than one. The number of fluctuation amplitudes will therefore increase. There will be one variable for each set of mode numbers (K_1, K_2, K_3) in the range

$$|\mathbf{K}| < L'/\Lambda \tag{9.99}$$

2. In order to reduce the number of variables to the previous value, the minimum allowable wavelength is increased from Λ to $\Lambda' = s\Lambda$. This restricts the allowable mode numbers to the range

$$|\mathbf{K}| < L'/\Lambda' = L/\Lambda \tag{9.100}$$

To obtain the new probability distribution, one must integrate over the eliminated fluctuation amplitudes. That is, one integrates over all those variables $M_{\mathbf{K}}$ with $\mathbf{K}$ in the range

$$L'/\Lambda' < |\mathbf{K}| < L'/\Lambda \tag{9.101}$$

3. The magnetization $M(\mathbf{r})$ is rescaled by multiplying it by some as yet undetermined scale factor γ.
4. The new probability distribution is for a magnetization field $M(\mathbf{r})$, defined within the volume $V' = (L')^3$. The old field was defined within the volume $V = L^3$. The new distribution can be mapped into the old volume by a scale transformation. Combining steps 3 and 4, the new magnetization variable is

$$\tilde{M}(\mathbf{r}) = \gamma M(\mathbf{r}/s) \tag{9.102}$$

The difficult step is Step 2, the integration. It cannot be done exactly, but it can be carried out using the ϵ expansion (or other approximation methods that we have not discussed). The details of the calculation are quite complicated and will not be given. We will only quote the results.

9.17   FIXED POINTS OF THE LANDAU–GINSBURG THEORY

What we are trying to determine are the fixed points, if any exist, in a fluctuation probability distribution of the Landau–Ginsburg form. A fixed point would mean a value of A, b, and c with the property that, if one started with a Landau–Ginsburg distribution having those values of the parameters and carried out the renormalization transformation defined, then the resulting probability distribution would still be of the Landau–Ginsburg form with the same parameter values.

One case in which the integration is not difficult is the case $b = 0$. In that case the integral in the exponent of Eq. (9.98) is

$$\int (AM^2 + c|\nabla M|^2)\, d^3\mathbf{r} = \sum_{\mathbf{K}} (A + ck^2) M_{\mathbf{K}}^2 \tag{9.103}$$

Integrating over the variables $M_{\mathbf{K}}$ with $\mathbf{K}$ in the shell $L'/\Lambda' < |\mathbf{K}| < L'/\Lambda$ simply produces a factor in front of the exponential that can be absorbed into the normalization constant. The probability distribution, after the integration of step 2, is of the same form as the starting one with the same value of the parameters. However, one must still complete steps 3 and 4. When that is done the completed transformation has the form

$$\int_{V'} (AM^2 + c|\nabla M|^2)\, d^3\mathbf{r} \to \frac{s^3}{\gamma^2} \int_V [A\tilde{M}^2(\mathbf{x}) + s^{-2}c|\nabla \tilde{M}(\mathbf{x})|^2]\, d^3\mathbf{x} \tag{9.104}$$

where $\mathbf{x} = \mathbf{r}/s$. The parameter A will remain unchanged if we choose $\gamma = s^{3/2}$, but then the parameter c will remain constant only if its value is zero. Thus there is a line of fixed points defined by the equations

$$b = 0, \quad c = 0, \quad \text{and} \quad 0 < A < \infty \tag{9.105}$$

The fact that $c = 0$ means that the values of the magnetization at different points $\mathbf{r}_1$ and $\mathbf{r}_2$ are statistically independent in the thermodynamic limit. The states described by these fixed points are noncritical states in which the correlation function decays exponentially with some correlation length ℓ. After many renormalizations [recall that, in each renormalization, we keep only the long-wavelength components of $M(\mathbf{r})$] the function $M(\mathbf{r})$ varies very slowly with $\mathbf{r}$. It is an average of the magnetization over a subvolume of size Λ. When $\Lambda \gg \ell$, these subvolumes become statistically independent. Another way of saying the same thing is that two points with a separation $r = |\mathbf{r}_1 - \mathbf{r}_2|$ in the starting volume are mapped into points with a separation sr after the renormalization. If r is not zero, then sr eventually becomes much larger than the correlation length ℓ and the magnetizations at the two points become statistically independent. As expected, the renormalization flow equations show that these fixed points are stable. Any initial state close to this line of fixed points flows into it.

According to Eq. (9.104), one can obtain another fixed point by letting $A = 0$ and $\gamma = s^{1/2}$. However, with $b = 0$, that set of parameter values does not describe a normalizable probability distribution. It is actually outside the physically allowable parameter space.

9.18   THE WILSON FIXED POINT

If b is not zero, then the integration over the fluctuation variables $M_{\mathbf{K}}$ that is required in the renormalization transformation becomes very difficult. In fact, it is impossible to carry out exactly. We have seen that if the space dimension D is larger than 4, then the bM^4 term becomes negligibly small. It is therefore possible to expand the required integral as a power series in $\epsilon = 4 - D$. In order to determine the fixed points, it is enough to calculate the renormalization flow equations for an expansion factor s only marginally larger than one. Assuming that $s = 1 + \delta$, we will simply quote the results of the renormalization transformation, given to first order in ϵ and δ. The renormalization equation for the parameter c is unchanged from Eq. (9.104). That is

$$c \to \frac{s}{\gamma^2} c \tag{9.106}$$

In order to find a fixed point with a nonzero value of c, we must choose the order parameter scaling factor, $\gamma = s^{1/2}$. The renormalization flow equations for the other two parameters, A and b, take a simpler form if they are written in terms of the equivalent variables

$$x = \frac{\Lambda^2}{2\pi^2} A \quad \text{and} \quad y = \frac{3}{2\pi^2} b \tag{9.107}$$

They are

$$x \to \tilde{x} = x + (2x + y - xy)\delta \tag{9.108}$$

and

$$y \to \tilde{y} = y + (\epsilon y - 3y^2)\delta \tag{9.109}$$

Of course, γ has been chosen so that $\tilde{c} = c$, and, therefore, that parameter will no longer be explicitly considered.

To determine the fixed point, we set $\tilde{x} = x$, $\tilde{y} = y$, and recall that, for a three-dimensional system, $\epsilon = 1$. The resulting equations have two solutions. The first, $(x^*, y^*) = (0, 0)$, is the unphysical solution that was rejected previously. The other, called the Wilson fixed point, is at

$$(x^*, y^*) = (-\tfrac{1}{5}, \tfrac{1}{3}) \tag{9.110}$$

To first order in ϵ, this gives the correct distribution of fluctuations at the critical point for any system with a scalar order parameter in three dimensions, such as the 3D Ising model.

9.19   DIFFERENTIAL FLOW EQUATIONS

Using the fact that $\log s = \log(1 + \delta) \approx \delta$, one can write the renormalization equations given in differential form.

$$\frac{dx}{d(\log s)} = \lim_{\delta \to 0} \frac{\tilde{x} - x}{\delta} = 2x + y - xy \tag{9.111}$$

and

$$\frac{dy}{d(\log s)} = \lim_{\delta \to 0} \frac{\tilde{y} - y}{\delta} = \epsilon y - 3y^2 \tag{9.112}$$

The flow lines produced by these differential equations are shown in Fig. 9.14.
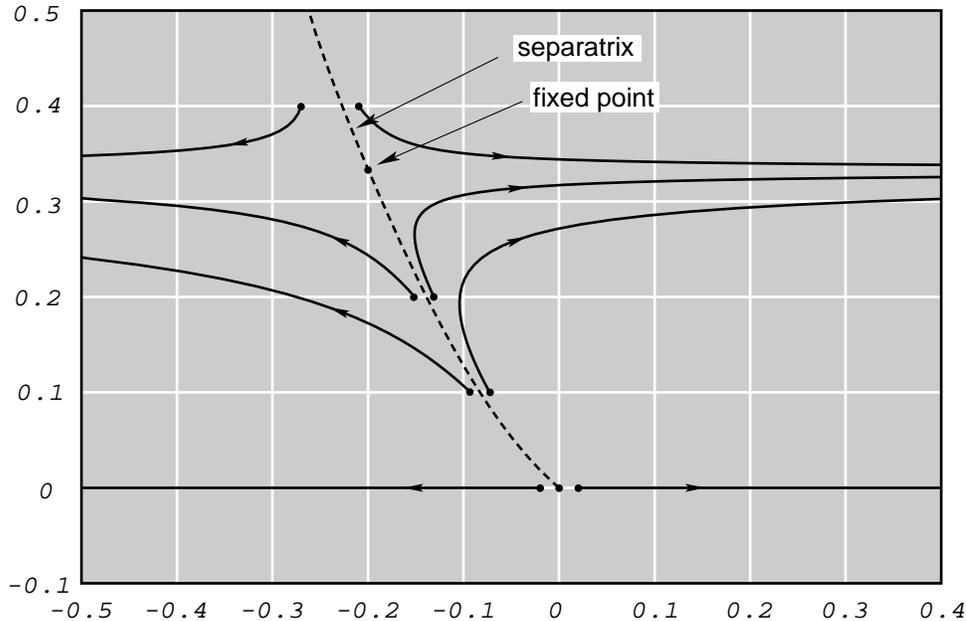

Fig. 9.14   The renormalization flow pattern described by Eqs. (9.111) and (9.112). All points to the right of the dotted line, called the separatrix, flow, as $s \to \infty$, to $x = +\infty$. The points to the left of the separatrix flow to $x = -\infty$. The points on the separatrix flow to the Wilson fixed point. Those points describe fluctuation probability distributions for a system at a critical point. One thing that must be kept in mind is that this renormalization flow diagram depends on the fact that we have chosen the scaling parameter γ equal to $s^{1/2}$. For those points that flow to $x = \pm\infty$ this is clearly wrong. Had we chosen $\gamma = s^{3/2}$, those points would flow to noncritical fixed points with $c = 0$ and A either negative or positive, indicating that the system was either below or above the critical temperature.

In the vicinity of the Wilson fixed point (x^*, y^*), the differential equations can be linearized by writing x as $x^* + \Delta x$ and y as $y^* + \Delta y$ and then ignoring second-order terms in Δx and Δy. One then obtains the following linearized flow equations for the variables Δx and Δy. They are valid only close to the fixed point, but that is exactly where we are most interested in the details of the renormalization flow.

$$\frac{d(\Delta x)}{d(\log s)} = \tfrac{5}{3}\Delta x + \tfrac{6}{5}\Delta y \tag{9.113}$$

and

$$\frac{d(\Delta y)}{d(\log s)} = -\Delta y \tag{9.114}$$

Let us first look at the equation for Δy. It can be written in the form $d\log(\Delta y) = d\log(s^{-1})$, which has the solution $\Delta y(s) = \Delta y(1)/s$. Thus, if the parameter y is initially displaced from its fixed point value y^*, it will monotonically move to that value under renormalization. A parameter with that characteristic is called

an *irrelevant parameter*. The logic behind calling a parameter irrelevant if it flows to its fixed point value under renormalization is that, insofar as the study of critical phenomena is concerned, such a parameter can simply be set equal to its fixed point value. One is only interested in very large systems, and, therefore, it is reasonable to assume that a number of renormalizations have already been done, which would be enough to bring all irrelevant parameters to their fixed point values.

The Landau–Ginsburg distribution is actually only an approximation to the true critical point probability distribution. Once the renormalization integrals are calculated to more than first order in ϵ, it is found that the strict Landau–Ginsburg form has no nontrivial fixed point. After one renormalization, a distribution function of the Landau–Ginsburg form is converted to one of a more general form, with terms such as M^6, M^8, $M^2|\nabla M|^2$, $|\nabla M|^4$, etc.. Therefore, in order to find a fixed point, one must start with a completely general probability distribution for the fluctuations in the order parameter. The coefficients of all the terms (actually infinite in number, although their size at the fixed point drops rapidly as the power of M increases) are completely determined by the fixed point condition that the distribution function must reproduce itself under a renormalization transformation. Also, these extra parameters are all irrelevant parameters, so that they automatically flow to their fixed point values. For that reason, one can discuss all the essential physics of the critical point in terms of the simple Landau–Ginsburg distribution. However, these terms do affect the values of critical properties when things are calculated to higher than first order in ϵ.

If $y = y^*$ but x is displaced slightly from its fixed point value, then the flow equation for Δx is

$$\frac{d(\Delta x)}{d \log s} = \tfrac{5}{3}\,\Delta x \qquad\qquad (9.115)$$

It is clear that the point will move farther and farther from the fixed point. Eventually, it will come to the line of trivial fixed points. For this reason, x is called a *relevant parameter*. We will see that the only other relevant parameter in the theory is the magnetic field B, which we have set equal to its fixed point value of zero in this discussion.

Renormalization theory is such an abstract construction that it is necessary, even at the hazard of appearing repetitious, to review periodically the physical meaning of the mathematical operations. The flow equations clearly do not describe the physical movement of anything. They describe a purely intellectual procedure in which one looks at more and more macroscopic variables in larger and larger systems. What is involved is obviously a form of thermodynamic limit, as outlined in Chapter 3. The rescaling of the order parameter M at each renormalization step is analogous to something that is done in the proof of the Central Limit Theorem. In that proof, one must look at the variable $T = (x_1 + \cdots + x_N)/\sqrt{N}$. If one looks at the average, $x = (x_1 + \cdots + x_N)/N$, then the fluctuations disappear as $N{\to}\infty$. If one looks at the sum, $S = x_1 + \cdots + x_N$, then they blow up in that limit. The scaling factor $1/\sqrt{N}$ is just enough to give a nontrivial probability distribution in the thermodynamic limit. In the same way, one must rescale M with just the right factor in order to keep the fluctuations in view as one takes the thermodynamic limit. In fact, renormalization theory can be considered as a major extension of the Central Limit Theorem from systems of independent variables to systems with significant interactions. The trivial fixed points, where the observables become statistically independent in the thermodynamic limit, give Gaussian probability distributions that correspond exactly to the usual Central Limit Theorem. However, because of the interactions and the statistical correlations that they produce, completely different limiting probability distributions are also possible. They are described by the nontrivial fixed points, which have much more complex fluctuation probability distributions. Renormalization theory shares with the Central Limit Theorem the marvelous characteristic that the detailed mathematical form of the probability distributions in the thermodynamic limit depend very little on the microscopic details of the system. It is certainly remarkable that the complicated distribution at the fixed point, which cannot even be written down in any finite formula, is not determined by the physical details of the real system, but by a purely mathematical fixed point condition. In the macroscopic limit, where thermodynamics becomes valid, statistical effects dominate everything else and limit the fluctuation distribution function to those few forms (including the Gaussian distribution) that satisfy the fixed point condition.

The essential characteristic of the flow equations, for determining critical exponents, is the rate at which all relevant parameters diverge from the fixed point as s is increased. Equation (9.115) for Δx can be written as

$$d(\log \Delta x) = \tfrac{5}{3} d(\log s) \qquad\qquad (9.116)$$

This has the solution

$$\Delta x(s) = \Delta x(1)s^{5/3} \qquad (9.117)$$

The parameter x is proportional to the parameter A. In the Landau theory, the critical point occurred at $A = 0$, and, therefore, near the critical point, A could be assumed to be proportional to $t = (T - T_c)/T_c$. Now that we have determined the correct value for A at the critical point (at least to order ϵ), we can again express A in terms of t. We do this by writing x in the form $\Delta x = x - x^* = Ct$, where the constant C cannot be determined by renormalization theory. Putting this into Eq. (9.117) gives

$$t = s^{5/3}t_o \qquad (9.118)$$

where $t_o = \Delta x(1)/C$. Again we must ask ourselves what this equation means. It does not mean that, as we look at larger and larger systems, we change the temperature as a function of the system size. All the systems in the thermodynamic limit sequence are at the same temperature. What is meant is that the probability distribution for the scaled-up variables in the scaled-up system, at temperature t_o, is the same as the probability distribution for the starting variables in the starting system at temperature $t_o s^{5/3}$. This is reasonable. As one looks at larger and larger scale variables at fixed temperature, they become less correlated. As one looks at a fixed set of variables at larger and larger values of t, they also become less correlated. Equation (9.118) gives an equivalence between the two effects.

9.20   THE MAGNETIC FIELD

If we ignore the irrelevant parameter y, then, close to the critical point, for sufficiently large systems, the fluctuation distribution is determined by the single parameter t, the deviation of the temperature from its critical value. However, this is true only because we have been assuming that there is no external magnetic field. It is known that the critical point occurs only at $B = 0$. Therefore B must be a relevant parameter. The calculation of the renormalization flow equations in the presence of an external magnetic field is even more complicated than in the zero-field case, and thus we will again only quote the results. To first order in ϵ, near the critical point, a nonzero magnetic field scales as

$$B = s^{5/2}B_o \qquad (9.119)$$

The specific numbers $\frac{5}{3}$ and $\frac{5}{2}$, in Eqs. (9.118) and (9.119) are obtained when the ϵ expansion is cut off after the linear term. If the expansion is carried further, then the form of the equations remains the same but the numerical values of the exponents are modified. Therefore, we will write the equations in the more general form

$$t = s^{y_t}t_o \quad \text{and} \quad B = s^{y_B}B_o \qquad (9.120)$$

and use the first-order values, $y_t = \frac{5}{3}$ and $y_B = \frac{5}{2}$, only when we want specific numbers for a calculation.

9.21   THE SCALING FORMULAS

Very close to the critical point, those properties that show nonanalytic behavior, such as the susceptibility and the specific heat, are dominated by the large-scale fluctuations in the order parameter. For that reason, the part of the canonical potential that is contributed by the microscopic degrees of freedom [for example, the ϕ_o term in Eq. (9.37)] may be ignored in the calculation of specifically critical properties. That fact, when combined with the scaling properties of t and B, will be seen to yield simple algebraic formulas for the various critical exponents in terms of the two parameters y_t and y_B.

Consider a large ferromagnetic system of, let us say, 10^{25} microscopic coordinates. Choose some number K, such as 10^{20}, that is very large but still much smaller than the total number of coordinates. Let $\hat{\phi}(t, B, V)$ be that part of the canonical potential that is due to the K fluctuation modes of largest wavelength. Very close to the critical point we can treat $\hat{\phi}$ as the total canonical potential. The distribution of the K largest modes for a system of volume s^3V at temperature t and field B is the same as it is for a system of volume V at temperature $s^{y_t}t$ with a field $s^{y_B}B$. Integrating over that distribution to obtain $\hat{\phi}$ gives the relationship

$$\hat{\phi}(t, B, s^3V) = \hat{\phi}(s^{y_t}t, s^{y_B}B, V) \qquad (9.121)$$

Taking a derivative of Eq. (9.121) with respect to V and defining the canonical potential density $f(t, B) = \phi(t, B, V)/V = \partial\phi(t, B, V)/\partial V$ gives the basic scaling relation that we will use to derive the exponent formulas.

$$s^3 f(t, B) = f(s^{y_t} t, s^{y_B} B) \tag{9.122}$$

We are actually making an assumption in this analysis, namely that the singular part of the canonical potential is itself an extensive quantity (i.e. proportional to V). This is called the *hyperscaling* property. There are some statistical mechanical models in which this hyperscaling assumption is not valid.

In order to obtain the magnetization exponent β in terms of the two basic fixed point parameters y_t and y_B, we differentiate this equation with respect to B and use the thermodynamic relation $M(t, B) = kT\partial f(t, B)/\partial B$ with T set equal to T_c (since t is assumed to be very small).

$$s^3 M(t, B) = s^{y_B} M(s^{y_t} t, s^{y_B} B) \tag{9.123}$$

The exponent β is defined by saying that, for very small negative t, $M(t, 0) \approx A(-t)^\beta$. Setting B to zero in Eq. (9.123) and assuming that t is a small negative number, gives the relation

$$s^3 (-t)^\beta = s^{y_B + \beta y_t} (-t)^\beta \tag{9.124}$$

which implies that

$$y_B + \beta y_t = 3 \tag{9.125}$$

or

$$\beta = \frac{3 - y_B}{y_t} \tag{9.126}$$

Using the values to first order in ϵ, $y_t = \frac{5}{3}$ and $y_B = \frac{5}{2}$, gives the exponent value

$$\beta = 0.3 \tag{9.127}$$

which is much closer to the experimentally observed value of 0.324 than is the mean-field prediction, $\beta = 0.5$. Taking higher powers in the ϵ expansion of y_B and y_t eliminates the remaining discrepancy.

9.22   THE SUSCEPTIBILITY EXPONENT

To evaluate the susceptibility exponent in terms of y_t and y_B, we take a derivative of Eq. (9.123) with respect to B and then set B equal to zero.

$$s^3 \chi_m(t, 0) = s^{2y_B} \chi_m(s^{y_t} t, 0) \tag{9.128}$$

The exponent γ was defined by Eq. (9.7), which says that the magnetic susceptibility in zero field, close to the critical temperature, has the form $\chi_m \sim B_\pm |t|^{-\gamma}$. Using this in Eq. (9.128) gives

$$s^3 |t|^{-\gamma} = s^{2y_B - \gamma y_t} |t|^{-\gamma} \tag{9.129}$$

which shows that

$$2y_B - \gamma y_t = 3 \tag{9.130}$$

or

$$\gamma = \frac{2y_B - 3}{y_t} \tag{9.131}$$

Using the values to first order in ϵ for y_B and y_t gives $\gamma = 1.2$—quite close to the experimental value of 1.24. Again, higher-order terms bring the predictions completely in line with the experimental results. Other cases will be left to the problems and exercises.

9.23   REAL-SPACE RENORMALIZATION

The Landau–Ginsburg potential is a thermodynamic object, and therefore the renormalization theory that is based on it has all the advantages and disadvantages of any thermodynamic calculation. It is not based on

any detailed microscopic model of the system, and it is therefore applicable to a wide class of systems that have only some broad features in common. The disadvantage in this is that the theory provides no method of relating the detailed features of the microscopic Hamiltonian, such as the spin–spin interaction strength, to the thermodynamic properties of the system, like the phase transition temperature. It is obvious that any theory that does not distinguish between a ferromagnetic solid and a nonmagnetic fluid must leave out many physically important details.

There is another version of renormalization theory, illustrated by the calculation that was made involving the harmonic chain, that does begin from a detailed microscopic model of the system. This real-space renormalization method, being based on a microscopic picture of the system, is properly a part of statistical mechanics, rather than thermodynamics. It has become a particularly powerful technique for analyzing systems with discrete variables, such as the Ising model.
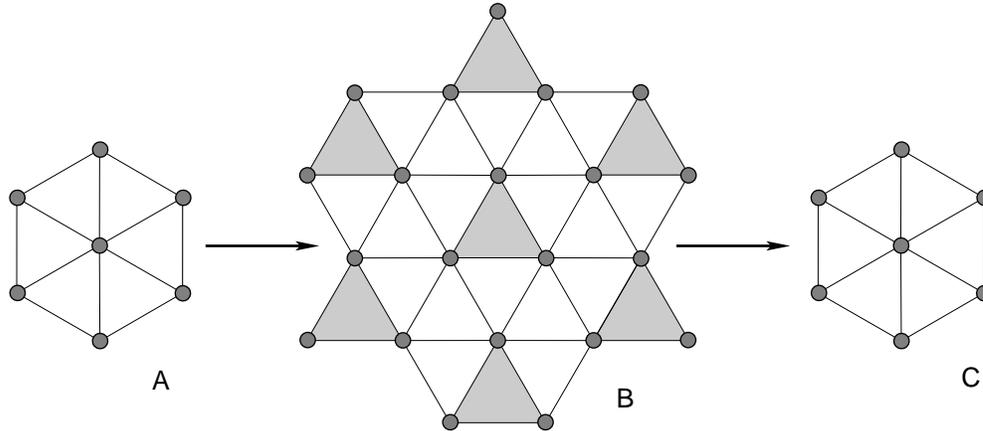

Fig. 9.15   System A is expanded by a factor of three to make System B. The site spins in System B are grouped into sets of three, called blocks. Associated with each block, is a block spin variable, whose value is ±1, depending upon whether the sum of the vertex spins is positive or negative. The set of block spins is equivalent to another seven-spin system (System C), which differs from System A only in having an altered Hamiltonian function.

As an example of a real-space renormalization calculation for a discrete system, we consider the arrays of two-valued spins shown in Fig. 9.15. The leftmost array, which we will call System A, has seven spins in a hexagonal pattern on a triangular lattice. The renormalization procedure consists of the following two steps.
 1. The dimensions of System A are increased by a factor of $\sqrt{3}$, and each spin is replaced by three spins to produce a larger, related system of 21 spins (System B) on a similar triangular lattice. The spin–spin interactions in the second system are assumed to be the same as those in the first, so that System B is simply a larger version of System A.
 2. The 21 spins in System B, shown by filled dots, will be called it site spins. They can each take the values of ±1. The probability of any configuration is given by

$$P(\sigma_1, \ldots, \sigma_{21}) = Z^{-1} \exp H(\sigma_1, \ldots, \sigma_{21}) \tag{9.132}$$

where $H = -\beta E$ and E is the energy of the spin system. Although it is dimensionless and is proportional to minus energy, the function H is usually called the Hamiltonian of the system. (It is really a conditional canonical potential, but we will follow the more standard nomenclature.) We will not assume that E necessarily has the simple Ising model form that involves only nearest neighbor interactions. Each of the shaded triangles is called a block, and associated with each block is a two-valued *block spin* variable $\tilde{\sigma}$, defined as follows.

$$\tilde{\sigma} = S(\sigma + \sigma' + \sigma'') \tag{9.133}$$

where σ, σ', and σ'' are the site spins at the three vertices of the block and $S(n)$ is the *sign function*,

$$S(n) = \begin{cases} -1, & \text{for } n < 0 \\ 0, & \text{for } n = 0 \\ +1, & \text{for } n > 0 \end{cases} \tag{9.134}$$

The procedure of assigning the values ± 1 to the block spin variables, according to whether most of the site spins are up or down, is called *majority rule*. As can be seen, there are seven block spins, arranged in a hexagonal array, similar to System A. We define a new block spin Hamiltonian, $\tilde{H}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7)$, by the relation

$$\exp \tilde{H}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7) = {\sum}' \exp H(\sigma_1, \ldots, \sigma_{21}) \tag{9.135}$$

where the prime on the summation sign indicates that the sum is taken only over those configurations that give the set of block spin values that are indicated on the left hand side. Another way of writing this is

$$\exp \tilde{H}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7) = \sum \delta(\tilde{\sigma}_1 - S_1) \cdots \delta(\tilde{\sigma}_7 - S_7) \exp H(\sigma_1 \ldots, \sigma_{21}) \tag{9.136}$$

where $S_i \equiv S(\sigma_i + \sigma_i' + \sigma_i'')$ and σ_i, σ_i', and σ_i'' are the site spins at the vertices of the ith block. With this definition of the block spin Hamiltonian, it is easy to see that the probability for the block spin variables is

$$\tilde{P}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7) = \tilde{Z}^{-1} \exp \tilde{H}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7) \tag{9.137}$$

This renormalization transformation maps the 21-spin system with the Hamiltonian $H(\sigma_1, \ldots, \sigma_{21})$ into a 7-spin system, System C, similar to the starting system, but with a Hamiltonian $\tilde{H}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_7)$. If the Hamiltonian in the starting system had some particularly simple form, such as

$$H = K \sum_{\text{NN}} \sigma_i \sigma_j \tag{9.138}$$

there is no reason to expect that form to be retained in the mapping. In fact, the renormalized Hamiltonian will usually be of a more complicated form. It will generally have next-nearest-neighbor terms, three-spin terms, etc.

$$\tilde{H} = \tilde{K}_1 \sum_{\text{NN}} \tilde{\sigma}_i \tilde{\sigma}_j + \tilde{K}_2 \sum_{\text{NNN.}} \tilde{\sigma}_i \tilde{\sigma}_j + \tilde{K}_3 \sum_{\text{triangles}} \tilde{\sigma}_i \tilde{\sigma}_j \tilde{\sigma}_k + \cdots \tag{9.139}$$

This effect is known as a *proliferation of interactions*. The same effect occurs in the momentum-space renormalization of the Landau–Ginsburg potential when the calculation is done beyond first order in epsilon.

The aim of the calculation is to find a starting Hamiltonian

$$H = K_1 \sum_{\text{NN}} \sigma_i \sigma_j + K_2 \sum_{\text{NNN.}} \sigma_i \sigma_j + K_3 \sum_{\text{tri.}} \sigma_i \sigma_j \sigma_k + \cdots \tag{9.140}$$

with the property that its form and the specific values of its parameters are preserved under the transformation. In practical calculations one starts with a Hamiltonian with a finite (and fairly small) number of parameters, such as K_1, K_2, and K_3. One then makes some approximation to the exact renormalization transformation that prevents the proliferation of interactions and thus gives a renormalized Hamiltonian of the same form but with new parameters. That is,

$$(K_1, K_2, K_3) \rightarrow (\tilde{K}_1, \tilde{K}_2, \tilde{K}_3) \tag{9.141}$$

The solutions of the equation

$$(K_1, K_2, K_3) = (\tilde{K}_1, \tilde{K}_2, \tilde{K}_3) \tag{9.142}$$

define the fixed points of the transformation. For Ising systems, there are usually two trivial fixed points and a nontrivial one that describes the critical properties of the system. One trivial fixed point has the values $K_1 = K_2 = K_3 = 0$. Since the Hamiltonian is related to the energy by $H = -\beta E$, having $H = 0$ is equivalent to having infinite temperature. At this trivial fixed point the site spins are totally uncorrelated. But if the site spins are uncorrelated, then the block spins will also be. That is why $H = 0$ is always a fixed point. The other trivial fixed point occurs at zero temperature, or infinite interaction strength. In that case, the site spins are perfectly correlated—if one of them is up, then they are all up; if one of them is down, then they are all down. But again, if that is true of the site spins, then it will also be true of the block spins, which explains why that case is a fixed point. Both trivial fixed points are stable. The interesting
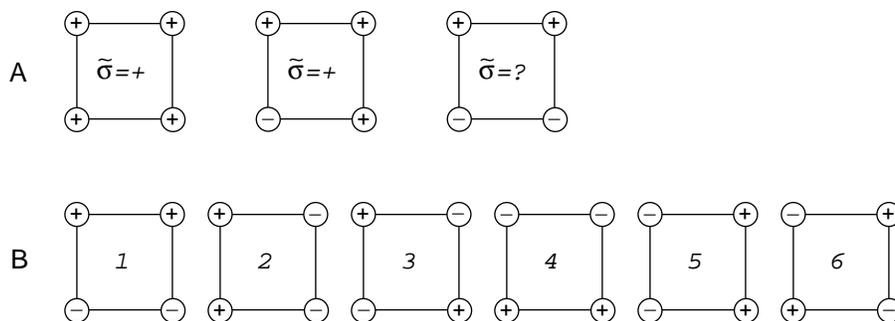
Fig. 9.16   It is obvious that a block spin value of $+1$ should be assigned to the first two configurations in (A), but it is not clear what block spin value should be assigned to the third. The six site-spin configurations that give an ambiguous block spin value are shown in (B).

fixed point, which one hopes will at least approximately describe the critical properties of the system, is the third, unstable one.

There is a wide variety of different approximation schemes, designed to prevent the proliferation of interactions. We will illustrate some of them in the exercises that are associated with this chapter. The properties of the renormalization flow equations near the nontrivial fixed point give the critical exponents of the system.

Although the calculational details of the method will be left to the exercises, there are a number of important general points that should be discussed here.

1. What is really needed is a renormalization transformation for an infinite (or at least very large) system, rather than one for a system like a seven-spin hexagon. However, no one has been able to compute the renormalization transformation for even a mildly complex Hamiltonian on an infinite lattice. Fortunately, although most properties of small systems are very different than the corresponding properties of very large systems, the renormalization transformation itself, which can be used to calculate the critical behavior of an infinite system, is affected very little by the size of the system. Thus the scheme has the marvelous characteristic of allowing one to make reasonably accurate calculations on very large systems by doing a calculation on a very small one.

2. It was no accident that our introduction to the real-space renormalization method was based on a triangular Ising lattice. In a square lattice a new problem appears that would have significantly complicated the analysis. The problem, called *block spin ambiguity*, is illustrated in Fig. 9.16. In a square lattice, one would usually form blocks from sets of four site spins. If the block spin variables are to take the values ± 1, so that they have the same form as the site spin variables, then it becomes very unclear what block spin value should be assigned to the six block configurations that have zero total spin. This problem can be resolved in a number of different ways. Some people have simply assigned a block spin value of $+1$ to three of the configurations, such as (1), (2), and (3) and a value of -1 to the others. This can be done in four different ways if one adds the natural restriction that reversing all of the spins in a configuration should reverse the value of the block spin. Another way of treating the problem is to allow the block spin variables to have the three possible values, ± 1 and 0. This procedure has the drawback that it maps the original system of two-valued spins onto a system of three-valued spins, but all subsequent renormalizations will take the system of three-valued spins into itself. In the exercises, we will illustrate still other methods of resolving the problem of block spin ambiguity.

3. In contrast to the momentum-space renormalization method, the real-space renormalization method allows one to make a prediction of the critical temperature T_c. To illustrate how this is done, let us imagine making a calculation in which only two Hamiltonian parameters, K_1 and K_2, are used, where K_1 is the nearest-neighbor interaction strength and K_2 is the next-nearest-neighbor strength, as in Eq. (9.140). Using some particular finite system, one can compute a renormalization flow diagram, as shown in Fig. 9.17. We will assume that the physical system that we are interested in is an Ising lattice with only nearest-neighbor interactions. For such a system,

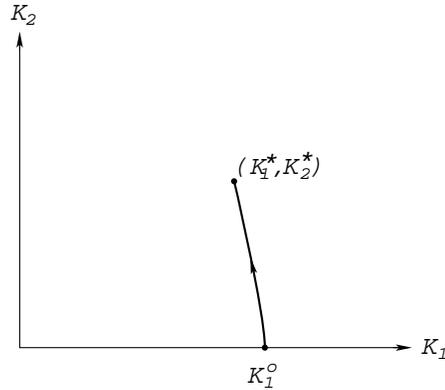$$E = -V \sum_{\text{NN}} \sigma_i \sigma_j \tag{9.143}$$

Fig. 9.17   The point $(K_1^o, 0)$ flows, under renormalization, to the fixed point (K_1^*, K_2^*). This means that the physical system, with interaction strength K_1^o will be at its critical point. Since $K_1 = V/\tau$, the critical temperature is given by $\tau_c = V/K_1^o$.

with some particular fixed value of V. Therefore, in the physical system, $K_1 = V/kT$ and $K_2 = 0$. From the renormalization flow diagram, one can find the point on the K_1 axis, call it K_1^o, that flows to the nontrivial fixed point under repeated renormalizations. The equation

$$K_1^o = V/kT_c \tag{9.144}$$

then allows one to calculate T_c.

  4. The real-space renormalization method is particularly valuable in analyzing two-dimensional systems because the alternative method of momentum space renormalization relies upon the epsilon expansion. Power series expansions work well only when the expansion parameter is small, but in two dimensions epsilon is equal to two.

The following argument, although it is highly simplified, should indicate how the real-space renormalization procedure is related to the previous renormalization procedure that used continuous magnetization variables. We consider a rectangular 2D lattice in which we have introduced only two magnetization variables, M_1 and M_2, which represent the sums of the spins in the respective squares. It is assumed that the number of spins is so large that M_1 and M_2 can be treated as continuous variables, ranging from $-\infty$ to ∞. Under a single renormalization, the system is converted to a larger system with corresponding magnetization variables, M_1' and M_2'. (See Fig. 9.18.) When the possibility of scaling is taken into account, the existence of a fixed point would imply that

$$\mathbf{P}[M_1 = a, M_2 = b] = \mathbf{P}[M_1' = \gamma a, M_2' = \gamma b] \tag{9.145}$$

Discrete block spin variables, σ_1, σ_2, σ_1', and σ_2', defined by majority rule, are related to the magnetization variables by $\sigma(M) = \text{sgn}(M)$. (With continuous variables, we can ignore the possibility of M being exactly zero.) The joint probability distribution of σ_1 and σ_2 is related to that for M_1 and M_2 by

$$\mathbf{P}[\sigma_1 = +1, \sigma_2 = +1] = \mathbf{P}[M_1 > 0, M_2 > 0] \tag{9.146}$$

with similar equations for the other three possible values of σ_1 and σ_2. It is now easy to verify that, if Eq. (9.145) is satisfied with any positive value of the scaling parameter γ, then

$$\mathbf{P}[\sigma_1 = +1, \sigma_2 = +1] = \mathbf{P}[\sigma_1' = +1, \sigma_2' = +1] \tag{9.147}$$

because the scaling parameter will have no effect on the integrated probability that M_1 and M_2 are positive. Thus the equality of the continuous probability distribution, *with scaling*, implies the simple equality of the discrete probability distributions. The search for fixed points in the block spin formalism is basically equivalent to the search for fixed points in the scaled magnetization formalism.
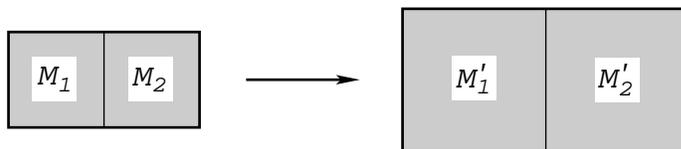
Fig. 9.18   Under renormalization, the magnetization variables of the smaller system are mapped into those of the larger one.

PROBLEMS

9.1 Equation (8.100) is the basic equation of the mean-field approximation applied to the 3D Ising model. With no external field, it states that the energy of a configuration is

$$E(C) = 3NV\bar{\sigma}^2 - 6V\bar{\sigma}\sum\sigma(\mathbf{r}) \tag{9.148}$$

It is not at all obvious that this approximation is equivalent to the Landau theory, which states that the conditional canonical potential for a fixed value of the uniform magnetization M is

$$\phi(T, M) = \phi_o - VatM^2 - VbM^4 \tag{9.149}$$

The objects of this problem are to show that, close to the critical point of the mean-field approximation $(kT_c = 6V)$, for small values of M, the value of $\phi(T, M)$ calculated from Eq. (9.148) agrees with the Landau theory and to identify the Landau parameters ϕ_o, a, and b. In comparing the two theories, the Landau order parameter M is identified with the average spin polarization $\bar{\sigma}$. (a) Replace $\bar{\sigma}$ by M in Eq. (9.148) and evaluate $\phi(M)$ by summing $\exp(-\beta E(C))$ over all 2^N configurations. (b) Using the definition, $t = (T - T_c)/T_c$, and the fact that $kT_c = 6V$, eliminate β in the expression you obtained in (a), in favor of t. (c) Expand the expression obtained in (b) as a power series in the small quantities, M^2 and t, retaining all terms through second-order. [That is, one keeps the second-order terms, $M^2 t$ and $(M^2)^2$, but drops the third order terms, $M^2 t^2$ and $(M^2)^2 t$. At the critical point, $M \sim (-t)^{1/2}$, so that M^2 and t are of the same order.] (d) Comparing the result obtained in (c) with Eq. (9.149), determine the Landau parameters ϕ_o, a, and b for the 3D Ising model.

9.2 Consider a two-dimensional Ising system in the form of an $L \times L$ square. We assume that the lattice spacing is so small in comparison with L that the state of the system can be described by a continuous magnetization variable $M(x, y)$, where x and y have the range 0 to L. The conditional canonical potential associated with any magnetization pattern $M(x, y)$ is assumed to have the two-dimensional equivalent of the form given in Eq. (9.37).

$$\phi(M) = \phi_o - \int\int\left[atM^2(x, y) + bM^4 + c|\nabla M(x, y)|^2\right]dx\,dy \tag{9.150}$$

We also assume that the values of $M(x, y)$ at the boundaries are some known, fixed, functions, let us say

$$M(0, y) = M_o \quad\text{and}\quad M(x, 0) = M(x, L) = M(L, y) = 0 \tag{9.151}$$

Since the probability of obtaining any particular magnetization pattern is proportional to $\exp\phi(M)$ and, away from the critical point, the fluctuations from the most probable pattern are negligible, the pattern that would actually be observed is the one that maximizes $\phi(M)$. We call the function that maximizes $\phi(M)$ and also satisfies the boundary conditions [Eq. (9.151)] $\bar{M}(x, y)$. Let $\Delta M(x, y)$ be any function that is zero on all of the boundaries. Then $M(x, y, \lambda) = \bar{M}(x, y) + \lambda\Delta M(x, y)$ is a function that satisfies the boundary conditions for any value of the parameter λ and

$$\phi(\lambda) \equiv \phi_o - \int\int\left[atM^2(x, y, \lambda) + bM^4(x, y, \lambda) + c|\nabla M(x, y, \lambda)|^2\right]dx\,dy \tag{9.152}$$

has a maximum at $\lambda = 0$. (a) Using the condition that $\Delta M(x, y)$ vanishes on all the boundaries, prove the identity

$$\int\int\nabla M(x, y)\cdot\nabla[\Delta M(x, y)]\,dx\,dy = -\int\int\nabla^2 M(x, y)\Delta M(x, y)\,dx\,dy \tag{9.153}$$

(b) Using the identity proved in (a), show that the condition that $d\phi(\lambda)/d\lambda = 0$ at $\lambda = 0$ for any $\Delta M(x, y)$ that vanishes on all the boundaries implies that $\bar{M}(x, y)$ satisfies the equation

$$-c\nabla^2 \bar{M}(x, y) + at\bar{M}(x, y) + 2b\bar{M}^3(x, y) = 0 \tag{9.154}$$

9.3 (a) Repeat the calculation described in Problem 8.26 for the values, $\beta V = 0.3$, 0.35, and 0.4. (b) For a 2D Ising model, the critical value of βV is known from the Onsager solution to be $(\beta V)_c = 0.4407\ldots$. Assume that, as $\beta V \to (\beta V)_c$, the correlation length goes to infinity as some negative power of $(\beta V)_c - \beta V$, that is, that

$$\ell = \ell_o (0.4407 - \beta V)^{-\nu}$$

Plotting $\log \ell$ versus $\log(0.4407 - \beta V)$, try to determine the value of ν for a 2D Ising model.

9.4 (a) Using Eq. (9.122), derive a scaling formula that gives the specific heat exponent α [see Eq. (9.4)], in terms of the fixed point parameters y_t and y_B. (b) Use the epsilon expansion formulas given in Exercise 9.4, to estimate α for a 3D Ising model. Because of the fact that α is quite small for the 3D Ising model, the result you obtain will have a large fractional error. The exponent α, because of its small size, is difficult to determine accurately, both experimentally and theoretically.

9.5 In deriving the scaling laws in Section 9.21, explicit use was made of the fact that, as the dimensions of a system are scaled by a factor s, the volume increases as $s^3 V$. This is true only in three dimensions, and therefore the conclusions drawn there are restricted to 3D systems. (a) Rederive the scaling formulas for β and γ for the general case of a D-dimensional system. (b) In Exercise 9.4, an expansion is given, through second-order in $\varepsilon = 4 - D$, of the fundamental exponents y_t and y_B. Use that expansion, and the results of (a), to show that in four dimensions one obtains mean-field (that is, simple Landau theory) values for β and γ.

9.6 (a) Use Eq. (9.121) and the thermodynamic relation $\partial\phi/\partial B = \beta\langle M \rangle$ to derive a scaling formula for the critical isotherm exponent δ for a 3D system. (b) Use the epsilon expansion given in Exercise 9.4 to estimate the value of δ for a 3D uniaxial ferromagnet.

9.7 The aim of this problem is to show that the sharp spike in the magnetic susceptibility per spin at the critical temperature, $\tau_c \approx 4.511$, appears only in the thermodynamic limit. Using the Fortran program Ising_3D.for, with $H = 0$ and $V = 1$, calculate and plot the magnetic susceptibility per spin for an $L \times L \times L$ lattice in the range $4 < \tau < 5$ for lattices of size $L = 2$, 4, and 8.

9.8 Calculate the constant $I_{\mathbf{K}}$ defined in Eq 9.55.

9.9 Extend the renormalization flow diagram shown in Exercise 9.7 to negative values of K and "explain" your result.

9.10 Using the program Ising_2.for, with $V = 1$, on an 8×8 lattice, plot the magnetic susceptibility per spin between $\tau = 1$ and 4 for the external field values, $H = 0$, 0.05, and 0.1. Use at least 10,000 sweeps for each point.

9.11 In this problem, we will investigate the number of iterations needed for a Monte Carlo process to come to equilibrium. In the program Ising_2.for, after each sweep through the lattice, the current values of $|M|$, M^2, E, and E^2 are added to Sum_M, Sum_M2, Sum_E, and Sum_E2, to be used later in calculating $\langle |M| \rangle$, $\langle M^2 \rangle$, $\langle E \rangle$, and $\langle E^2 \rangle$. (a) Modify the program in the following ways: (1) Drop all instructions used in calulating $\langle |M| \rangle$, $\langle M^2 \rangle$, $\langle E \rangle$, and $\langle E^2 \rangle$. (2) Add an integer array, Mag(1),..., Mag(10000). (3) Let $N_{\text{sweeps}} = 10000$ and, after the kth sweep, store the total magnetization in Mag(k). (3) For each value of K from 0 to 1000, calculate the *magnetization autocorrelation function*

$$C(K) = \left(\sum \text{Mag}(i)\text{Mag}(i + K) \right) \Big/ (10000 - K) \tag{9.155}$$

where the sum on i is from 1 to $10000 - K$. (b) For an 8×8 lattice, with $H = 0$ and $V = 1$, calculate and plot $C(k)$ for the temperatures, $\tau = 3$, 2.5, and 2.25. (c) Explain why and how the function $C(k)$ is related to the number of sweeps necessary to bring the lattice to equilibrium.

9.12 This problem will illustrate some of the difficulties one encounters in trying to determine τ_c, the transition temperature for an Ising system, by making Monte Carlo calculations. It will also illustrate two of the methods used to circumvent those difficulties. For an $L \times L$ Ising lattice, the specific heat per spin C is given by $L^2 C = (\langle E^2 \rangle - \langle E \rangle^2)/\tau^2$. We also define a quantity Q by $L^2 Q = 2L^2 C - (\langle E^3 \rangle - 3 \langle E^2 \rangle \langle E \rangle + 2 \langle E \rangle^3)/\tau^3$. In the limit $L \to \infty$, $C(\tau)$ becomes infinite at the critical temperature τ_c but for finite L, C only develops a finite maximum at some temperature $\tau_{\max}(L)$, which depends on the size of the lattice. Of course, $\tau_{\max}(L) \to \tau_c$ as $L \to \infty$. (a) Modify the program Ising_2.for so that it calculates and saves the values of C and Q for each value of τ. (It may be helpful to take out the instructions that calculate and save the values of $\langle M \rangle$ and χ.) (b) With $L = 8$, $H = 0$, $V = 1$, $\tau_{\min} = 2$, $\tau_{\max} = 3$, $N_{\mathrm{runs}} = 11$, and $N_{\mathrm{sweeps}} = 10000$, run the program and show that statistical fluctuation in $C(\tau)$ prevent one from determining $\tau_{\max}(8)$ with reasonable accuracy. (c) By taking first, second, and third derivatives of the canonical potential $\phi(\beta)$, prove that another criterion for $\tau_{\max}$ is that $Q(\tau_{\max}) = 0$ and show that this criterion does allow a reasonably accurate determination of $\tau_{\max}(8)$ by interpolation. In a similar way, determine $\tau_{\max}(4)$ and $\tau_{\max}(6)$. (d) It can be proved that, for large values of L, $\tau_{\max}(L) \approx \tau_c + A/L$ for some constant A. Plotting the three values of $\tau_{\max}$ that you have determined as a function of $x = 1/L$, try to determine the value of τ_c for a two-dimensional Ising model. (The exact value is about 2.2692.)

9.13 Use the program LatGas.for to obtain data for the curves shown in Fig. 9.3.

9.14 The spin–spin correlation function in the x direction on an Ising lattice is defined as

$$C(n) = \left\langle \sum_x \sum_y \sigma(x, y)\sigma(x + n, y) \right\rangle / L_x L_y - \left(\langle \sum \sigma \rangle / L_x L_y \right)^2 \qquad (9.156)$$

where the expectation value is taken over a canonical ensemble or, in Monte Carlo calculations, over a long Monte Carlo run. (a) Modify Ising_2.for so that it can take different values for L_x and L_y. Take $L_x = 20$ and $L_y = 15$. With $H = 0$, $V = 1$, and $N_{\mathrm{sweeps}} = 10,000$, calculate $C(3)$, $C(5)$, and $C(7)$ for the temperatures, $\tau = 2.0$, 2.25, and 2.5. (b) At the critical temperature, $C(n)$ has the form $C(n) = A/n^\lambda$ for some constants A and λ. In that case $\log C(n) = a - \lambda \log n$. That is, $\log C(n)$ is a linear function of $\log n$. For each temperature, determine values of a and λ that minimize the error E, defined as

$$E = \sum_n [\log C(n) - a - \lambda \log n]^2 \qquad (9.157)$$

where n is summed over the values 3, 5, and 7. The value of E is a measure of how far $C(n)$ deviates from having a power-law form. For what temperature is E smallest?

9.15 Using the display program AB Model, describe qualitatively the equilibrium phases for the nine combinations of α and βV that occur by taking $\alpha = -1$, 0, and $+1$ and $\beta V = -0.5$, 0, and $+0.5$.

9.16 For the AB Model, we define an observable Γ by

$$\Gamma = \sum_m \sum_n mn \, \mathrm{Lat}(m, n) \qquad (9.158)$$

Modify the program AB.for so that it calculates $\langle \Gamma^2 \rangle$ and, with $\beta V = 0.5$, $L = 20$, and $N_{\mathrm{sweeps}} = 10,000$, plot $\langle \Gamma^2 \rangle$ as a function of α in the range $-2 < \alpha < 2$ and give a physical interpretation of your results.

9.17 Using Ising_4.for with $L = 16$, plot the magnetic susceptibility, with $V = 1$ and τ going from 2 to 3, for the vacancy rates 0, 0.1, and 0.2. Qualitatively describe the effects of random vacancies on the magnetic properties of this finite system.

9.18 The program Ising_4.for can be used to study the effects of randomly distributed vacancies on the thermodynamic properties of a two-dimensional Ising model and, one hopes, on real magnetic solids. Regarding the effects of random defects, such as vacancies, there are two seemingly reasonable arguments that lead to contradictory conclusions. They are:
Argument 1. The randomness of the vacancy distribution will cause different parts of the system to have

different critical temperatures. Thus the magnetic phase transition in an infinite system will be rounded over, as it is for a finite-size lattice. There will be no perfectly sharp critical temperature.

Argument 2. As the critical temperature is approached, the fluctuations that are important in the phase transition are of such long wavelength that they sample very large portions of the system. On those large scales, the vacancy distribution is effectively uniform, due to the law of large numbers. Thus, although the vacancies may cause quantitative shifts in the properties of the system, such as the value of the critical temperature or the critical exponents, at least for low enough density, they will have no qualitative effect on the phase transition—it will still be perfectly sharp.

Try to use the program Ising_4.for to obtain some useful information about this fundamental qualitative question on the effects of random defects on phase transitions. Warning: This is a very difficult assignment.