# First-order phase transitions, the Maxwell construction, and the momentum-space renormalization group

A. Parola
*Dipartimento di Fisica, Università di Catania, Catania, Italy*

D. Pini and L. Reatto
*Dipartimento di Fisica, Università di Milano, Milano, Italy*

(Received 25 May 1993)

The behavior of a nonperturbative momentum-space renormalization group (RG) is analyzed both above and below the critical temperature. The case of a scalar order parameter and of the Ising model is studied in detail by analytical and numerical means. It is shown that this RG transformation is always well defined even inside the coexistence curve. van der Waals loops are suppressed by long-wavelength fluctuations which enforce the convexity of the free energy. The RG description emerging from this study is then compared with exact results and other approximate theories.

PACS number(s): 64.60.Fr, 64.60.Cn, 64.60.Ak, 05.70.Fh

## I. INTRODUCTION

Although first-order phase transitions underlie many important phenomena in different fields of physics through the quite general mechanism of spontaneous symmetry breaking, they have received limited attention from the theoretical point of view, compared to the widespread interest raised by critical phenomena. A possible explanation is that usual mean-field descriptions giving rise to the van der Waals loop and Maxwell construction provide a qualitative picture of the transition, and in fact reproduce the exact solution of models with suitably chosen long-range interactions [1]. A phenomenological picture of the liquid-vapor phase transition is provided by the celebrated *droplet model* which describes the physical mechanisms leading to phase separation and predicts the occurrence of some *universal* features at the transition [2]. In particular, the free energy is shown to have an essential singularity on the coexistence curve, a result which goes beyond all mean-field treatments and was later confirmed by rigorous analysis, at least for the Ising model in arbitrary dimension [3]. Unfortunately, the simplest mean-field theories devised for first-order phase transitions are not suited for dealing with long-range fluctuations which characterize the critical point and therefore they do not match with the known properties of critical points which should instead be recovered as the temperature approaches its critical value. On the other hand, the droplet model does predict scaling laws in the critical region but does not provide a quantitative framework for calculating critical exponents and scaling functions.

The possibility to apply renormalization-group (RG) ideas to the description of first-order transitions has been a matter of debate since RG's were first studied. The original proposal of a particular "discontinuity" fixed point [4] which should describe the universal features at the transition was later confirmed by approximate real-space renormalization-group calculations which also showed the presence of the same essential singularity predicted by the droplet model [5]. However, this promising description of first-order transitions was never analyzed beyond approximate calculations and never reached the same degree of confidence attained by critical phenomena through $\epsilon=4-d$ or $1/n$ expansions [6]. On the other hand, recent numerical studies suggested that both real- and momentum-space renormalization groups might show pathologies near first-order phase boundaries [7], and in fact singularities and nonanalyticities in RG transformation were reported by several groups [8]. The presence of this kind of anomalies in an exact implementation of RG was later excluded by rigorous results which, however, suggested that, near phase boundaries, the renormalized Hamiltonian might not exist at all even after a *single* RG step [9]. This theorem was explicitly proven in the framework of real-space RG but it was conjectured to hold also for momentum-space RG.

The problem of the description of first-order transitions within RG's is therefore still open and a theory able to consistently describe both phase separation and critical points is lacking. Here we analyze the momentum-space RG formalism and we consider an approximation, the so-called "local potential approximation" (LPA), which is known to give a correct picture of critical phenomena to lowest order of the $\epsilon$ expansion [10]. Contrary to previous results, our analysis does not show any anomaly even inside the coexistence region where all the derivatives of the chemical potential identically vanish, and shows how nonperturbative effects are crucial for a correct description of the phenomenon of phase separation.

In Sec. II, we sketch the derivation of the exact momentum-space renormalization transformation for the lattice-gas model in the framework of the hierarchical theory of fluids [11]. This method allows for a twofold interpretation of the renormalized Hamiltonian which turns out to be useful for getting physical insight on the evolution of the RG flow. Then we discuss the simple

1063-651X/93/48(5)/3321(12)/$06.00  

LPA approximation to the exact hierarchy, which arises quite naturally in this context.

Section III is devoted to the analysis of the possible asymptotic behaviors of the differential equation previously obtained. The asymptotic analysis is then compared with the numerical solution for a $\phi^4$ theory in Sec. IV. Both numerical and analytical results show that LPA is free of any singularity at any finite value of the momentum cutoff and successfully describes the coexistence region by reproducing rigorously flat isotherms at convergence. No *ad hoc* Maxwell construction has to be used but the integration over long-wavelength modes is responsible for the correct thermodynamic behavior in the two-phase region. In fact, the isotherms progressively flatten but a constant chemical potential at coexistence is recovered only after fluctuations of arbitrary long wavelengths have been taken into account. The first-order phase boundary correctly matches with the critical region when the temperature is raised but the description of the coexistence curve, within the LPA, is not satisfactory because, in three dimensions, it predicts diverging compressibility at coexistence for all temperatures below the critical point. This situation improves for dimensions larger than 4 where the same approximation is shown to give rise to a finite compressibility at coexistence, in agreement with known exact results. In this case, numerical results indicate the presence of an essential singularity on the coexistence curve.

In Sec. V we apply our method directly to the three-dimensional Ising model in order to extract both the universal and the nonuniversal properties of the model and we discuss how these findings compare with known results in that system. The implications of a correct short distance behavior in the correlation functions are also analyzed.

A discussion about the possible occurrence of a "discontinuity fixed point" within our formalism, together with more elaborate extensions of the theory can be found in Sec. VI.

## II. MOMENTUM-SPACE RG FOR THE LATTICE-GAS MODEL

For future reference, we give a short derivation of the full set of RG differential equations in the framework of the hierarchical theory of fluids (HRT) [11]. Here we consider a lattice gas on a hypercubic lattice in $d$ dimensions with nearest-neighbor attraction and on-site hard-core respulsion. As is well known, this model can be mapped into the ferromagnetic Ising model by associating the presence of a particle on a given lattice site with an *up* spin. The thermodynamics of the model is given by the grand partition function

$$\Xi=\sum_{N\geq 0}\frac{z^N}{N!}\sum_{r_1}\cdots\sum_{r_N}e^{-\beta H} , \tag{2.1}$$

where $\beta=1/k_BT$, $z=\exp(\beta\mu)$ is the fugacity, the sum labels $r_j$ run over all the lattice sites and the Hamiltonian $H$ is

$$H=\frac{1}{2}\sum_{\substack{r_1,r_2\\ r_1\neq r_2}} v(r_1-r_2) . \tag{2.2}$$

Here the two-body interaction $v(r)$ corresponding to the usual nearest-neighbor ferromagnetic Ising model is defined by

$$v(r)=\begin{cases}\infty , & \text{for } r=0\\ -w , & \text{for nearest neighbors}\\ 0 , & \text{elsewhere}\end{cases} \tag{2.3}$$

but its precise form will never be needed in the following. As a first step we split the interaction in the sum of two terms:

$$v(r)=v^R(r)+w(r) , \tag{2.4}$$

where the reference part $v^R$ coincides with the hard-core contribution while $w(r)$ is the nearest-neighbor attraction. In this particular case, all correlation functions of the reference system are known: the many-particle direct correlation functions [12] are extremely local vanishing everywhere except if all their arguments coincide. Conversely, in momentum space, they are wave vector independent and their value can be obtained via the generalized compressibility sum rule:

$$c_n^R(k_1,\ldots,k_n)\equiv\frac{\delta^n \ln Z^R}{\delta\rho(k_1)\cdots\delta\rho(k_n)} \tag{2.5a}$$

$$=\frac{\partial^n(\ln Z^R/V)}{\partial\rho^n}=-\frac{\partial^n}{\partial\rho^n}[(1-\rho)\ln(1-\rho)+\rho\ln\rho] , \tag{2.5b}$$

where $\rho$ and $V$ are, respectively, the density and the volume of the system. Notice that in our definition (2.5a) the direct correlation functions include the ideal-gas contribution. $Z$ is the canonical partition function which can be obtained from $\Xi$ by a Legendre transform:

$$\ln Z=\ln\Xi-\int \ln z(r)\rho(r)d^dr , \qquad \rho(r)=\frac{\delta\ln\Xi}{\delta\ln z(r)} , \tag{2.6}$$

and the label $R$ identifies the reference system. For the lattice model we are dealing with, spatial integrations must be interpreted as series over lattice sites. In such a case, functional derivatives just correspond to partial derivatives. Then, we expand the logarithm of the grand partition function in a diagrammatic series in powers of the attractive part of the interaction $w$ and formally perform the Legendre transform (2.6) on the *full* partition function order by order in the diagrammatic expansion.

The result, valid both for the lattice gas and for ordinary fluids, reads as

$$\ln Z = \ln Z^R - \tfrac{1}{2} V\rho\phi(0) + \tfrac{1}{2} V\rho^2 \int d^d r\, \phi(r) + \mathcal{D}_1 , \qquad (2.7)$$

where $\mathcal{D}_1$ represents all connected diagrams built with $n$-point vertices $c_n^R$ ($n \geq 3$), $F^R$ bonds, and $\phi$ bonds satisfying the following conditions: (1) There is at least a $\phi$ bond in each diagram. (2) The end point of a $\phi$ bond must be connected to the end point of a $F^R$ bond. (3) The end point of a $F^R$ bond may be connected either to a $\phi$ bond or to a $c_n^R$ vertex. (4) There is at most one "reference path" (i.e., a path of $F^R$ bonds and $c_n^R$ vertices) between each pair of points in the diagram. (5) The diagram remains connected after cutting a single bond.

Here $\phi(r) = -\beta w(r)$, the $n$-particle direct correlation functions $c_n^R(r_1, \ldots, r_n)$ are defined as functional derivatives analogously to Eq. (2.5a) and $F(k) \equiv -1/c_2(k)$ is just $\rho$ times the usual structure factor. We have been forced to obtain the diagrammatic expansion of the Helmholtz free energy starting from the *grand canonical* ensemble and performing a Legendre transformation, in order to eliminate some "anomalous diagrams" present in the canonical formalism for any finite system [13,14].

Analogous expansions for the $n$-particle direct correlation functions can be immediately obtained from Eq. (2.7) by functional differentiation with respect to the density profile $\rho(r)$. The diagrammatic expansion (2.7) can be arranged in the form of a loop expansion by summing up the chains of $F^R$ and $\phi$ bonds which are allowed by the rules (2.7). By defining the new bond $\Delta$

$$\Delta(k) = \frac{\phi(k)}{1 - F^R(k)\phi(k)} \qquad (2.8)$$

in place of $\phi$, the expansion for the Helmholtz free energy becomes

$$\ln Z = \ln Z^R - \tfrac{1}{2} V\rho\phi(0) + \tfrac{1}{2} V\rho^2 \int d^d r\, \phi(r) + \mathcal{S} + \mathcal{D}_2 , \qquad (2.9)$$

where $\mathcal{S}$ represents the sum of chains of $\phi$ and $F^R$ bonds explicitly given by

$$-\tfrac{1}{2} V \int \frac{d^d p}{(2\pi)^d} \ln[1 - F^R(p)\phi(p)]$$

and $\mathcal{D}_2$ represents all connected diagrams built with $n$-point vertices $c_n^R$ ($n \geq 3$), $F^R$ bonds, and $\Delta$ bonds satisfying the previous conditions (1)–(5) with the two additional conditions: (6) there is at least one vertex $c_n^R$; (7) a diagram cannot contain a chain of $F^R$ and $\Delta$ bonds with two or more $\Delta$ bonds.

Notice that the zero-loop term reproduces the well-known mean-field approximation to the free energy of the interacting system $\ln Z_{\mathrm{MF}} = -\beta A_{\mathrm{MF}}$, the sum of chains formally coincides with the random-phase approximation [13], while the other diagrams can be thought of as a formal way to include higher-order fluctuations. Due to the strong similarity of (2.9) with the analogous expansion of a scalar field theory, we can interpret each bond as a propagator and each $n$-particle direct correlation function of the reference system as representing an "interaction" in the field theory [15].

The first step in Wilson's momentum-space RG [15] is just to integrate the short-wavelength fluctuations, i.e., to define a sequence of systems where fluctuations over long wavelengths are inhibited. In our expansion, each loop, i.e., each integration in momentum space, is associated to the introduction of fluctuations. Therefore, if *all* the momentum integrations in the diagrammatic expansion are cutoff at a given infrared scale $Q$, we expect that fluctuations over length scales $L \geq 1/Q$ are formally inhibited. We define $-k_B T \mathcal{A}_Q$ as the free energy per unit volume given by the full expansion where all integrations in momentum space are limited to a domain $\Omega_Q$ which excludes a neighborhood of the $k=0$ point of the Brillouin zone. Clearly, the free energy of the fully interacting system is reproduced in the $Q \to 0$ limit, when $\Omega_Q$ coincides with the full zone, while the mean-field approximation is recovered when the domain of integration $\Omega_Q$ vanishes. Physically $\mathcal{A}_Q$ includes fluctuations up to a minimum wave vector $Q$ and we do not expect any singularity in the modified free energy $\mathcal{A}_Q$, related to the $k=0$ mode, as long as $Q$ is different from zero: The effects of this infrared cutoff are somehow similar to confining our system into a box of size $L \sim 1/Q$.

According to the rules (2.9), each loop in the expansion must contain at least one $\Delta$ bond which is proportional to the Fourier transform of the original two-body interaction of the lattice gas. Then, a cutoff in the momentum integration is reproduced, to all orders, by cutting off the long-wavelength components of $\phi(k)$: A convenient way to inhibit long-wavelength fluctuations in the system is then to consider a sequence of models, that will be called *Q systems,* characterized by a two-body potential with a hard core on site plus a tail $w_Q(r)$ whose Fourier components coincide with those of $w(r)$ in $\Omega_Q$ and are set identically to zero in the remaining of the Brillouin zone. Strictly speaking, this procedure also modifies the zero-loop (mean-field) part of the free energy and therefore we cannot identify the free energy $A_Q$ of the $Q$ system with the modified free energy previously defined, but the relationship between the two quantities is easily obtained:

$$\mathcal{A}_Q = \frac{-\beta A_Q}{V} - \frac{\rho}{2}[\phi(0) - \phi_Q(0)] + \frac{\rho^2}{2} \int d^d r [\phi(r) - \phi_Q(r)] . \qquad (2.10)$$

Analogously, the two-particle direct correlation function, and hence the structure factor, acquires a discontinuity at wave vectors lying on the boundary of $\Omega_Q$. This discontinuity is due only to the zero-loop diagrams in the expansion of $c_2^Q$ and can be removed by defining the corresponding modified quantity:

$$\mathcal{C}_Q(k) = c_2^Q(k) + \phi(k) - \phi_Q(k) . \qquad (2.11)$$

Higher-order correlation functions do not have zero-loop diagrams and are therefore continuous in the whole Brillouin zone.

Within the framework of Wilson's RG, fluctuations of shorter wavelengths are iteratively integrated out and the Hamiltonian governing the dynamics of the remaining degrees of freedom is related to the original Hamiltonian through a set of differential equations for the coupling constants. In our language, this corresponds to relating the set of correlation functions of the $Q$ system with those of a system infinitesimally close to it characterized by a cutoff $Q-dQ$, which includes fluctuations in a wider wave-vector range. The exact relationship can be easily found on the basis of the perturbation expansion (2.9) where the "reference system" now is taken as the $Q$ system and the "perturbation potential" $\phi(r)$ has Fourier components only in the region $[k\in\Omega_{Q-dQ}, k\notin\Omega_Q]$ of vanishing measure. Therefore, the perturbation potential vanishes almost everywhere in the Brillouin zone, and only one-loop diagrams survive in the $dQ\to 0$ limit. A differential equation governing the "evolution" of the free energy can be immediately found from the previous loop expansion (2.9) with the result

$$-\frac{d\mathcal{A}_Q}{dQ}=\frac{1}{2}\int_{\Sigma_Q}\frac{dp}{(2\pi)^d}\ln[1+\mathcal{F}_Q(p)\phi(p)] , \qquad (2.12)$$

where $\Sigma_Q$ is the boundary of $\Omega_Q$ ($\Sigma_Q=d\Omega_Q/dQ$) and the modified correlation function $\mathcal{F}_Q(k)\equiv -1/\mathcal{C}_Q(k)$ is related, in the long-wavelength limit, to the modified free energy by a compressibility sum rule [13]

$$\mathcal{F}_Q(k=0)=-\left[\frac{\partial^2\mathcal{A}_Q}{\partial\rho^2}\right]^{-1} . \qquad (2.13)$$

The exact evolution equation (2.12) describes the effects of introducing fluctuations of wave vector $Q$ into the free energy of the system. It should be integrated starting from an initial wave vector $Q_0$ characterized by the condition $\Omega_{Q_0}=\emptyset$ where the modified free energy coincides with the mean-field approximation.

Analogous "evolution" equations can be written for the many-particle direct correlation functions and together they form an exact hierarchy of differential equations for the structure and the thermodynamics of the model [11].

This set of equations, in the critical region and at long wavelengths, becomes completely equivalent to momentum-space RG. In fact, in this regime, $\mathcal{F}_Q(0)$ becomes large and the argument of the logarithm in Eq. (2.12) can be approximated by $\mathcal{F}_Q(p)$. The attractive potential thereby disappears from the equation which explicitly shows the universal character of long-wavelength fluctuations:

$$\frac{d\mathcal{A}_Q}{dQ}=\frac{1}{2}\int_{\Sigma_Q}\frac{dp}{(2\pi)^d}\ln[-\mathcal{C}_Q(p)] . \qquad (2.14)$$

From the structure of this equation we see that a RG for a scalar field theory is recovered within the formalism of HRT, the role of renormalized propagator on a wave-vector scale $Q$ being played by the (modified) direct correlation function $\mathcal{C}_Q(k)$ of the previously defined $Q$ system. Analogous simplifications occur in the equations governing the evolution of the other correlation functions. The full hierarchy of RG differential equations can then be recovered by a simple change of variable, i.e., by rescaling the $n$-particle correlation function with suitably chosen powers of the cutoff $Q$. In this way, we can identify, apart from a scaling factor, the $n$-particle correlation functions of the previously defined $Q$ system with the coefficients of the RG effective Hamiltonian, when the fluctuations at momenta larger than $Q$ have been integrated out [11]. On the other hand, our derivation of the exact hierarchy of differential equations shows that the direct correlation functions at cutoff $Q$ are defined for all wave vectors $k$ and keep complete information about the short, as well as the long, range behavior of the system. Therefore they provide a comprehensive description of the equilibrium properties of the model.

This correspondence is, in fact, quite useful in the discussion of possible approximation schemes to the full hierarchy. A natural ansatz is to maintain that the modified direct correlation function of the $Q$ system can be represented in an Ornstein-Zernike (OZ) form also in the neighborhood of a phase transition. In this approximation, the long-wavelength limit of $\mathcal{C}_Q(k)$ is

$$\mathcal{C}_Q(k)\underset{k\to 0}{\sim}\mathcal{C}_Q(0)-bk^2 . \qquad (2.15)$$

This hypothesis is actually justified in dimension larger than 4 where the asymptotic form (2.15) is valid also at the critical point. In three dimensions, the small value of the critical exponent $\eta$ suggests that (2.15) might be a reasonable first approximation which already includes the correct lowest order in an $\epsilon=4-d$ expansion [11]. If the zero-momentum limit of the pair correlation function is related to the modified free energy via the compressibility sum rule (2.13), the first equation of the hierarchy becomes a closed partial differential equation equivalent to the local potential approximation of the RG approach:

$$\frac{\partial\mathcal{A}_Q}{\partial Q}=\frac{K_d}{2}Q^{d-1}\ln\left[-\frac{\partial^2\mathcal{A}_Q}{\partial\rho^2}+bQ^2\right] , \qquad (2.16)$$

where $K_d$ is a geometric dimensionless factor and we have assumed that the chosen volume $\Omega_Q$ in the $Q\to 0$ limit contains all wave vectors in the Brillouin zone except those contained into a small sphere of radius $Q$ centered around $k=0$. We stress that Eq. (2.16) represents the evolution of the free energy at long wavelength and in the critical region within the Ornstein-Zernike approximation implied by Eq. (2.15). The full evolution at all length scales is instead given by the exact differential equation (2.12) which can also be applied far from the critical region or at short distances.

If the density variable $\rho$ is identified with the scalar field $\psi(x)$, the modified free energy $\mathcal{A}_Q(\rho)$ becomes the potential $U_Q(\psi(x))$ of the effective Hamiltonian at length scales $1/Q$. This statement can be proved either by comparing our equation with usual RG equations in LPA [10] or by expanding the modified free energy in powers of the density, starting from the critical density $\rho_c$, and writing the full hierarchy of differential equations for the expansion coefficients which comes out of our approximate equation. All the terms (diagrams) of this approximate hierarchy can be shown to keep the topological structure of the exact hierarchy, and the OZ ansatz (2.15) has the only effect to approximate the momentum dependence [15] of the $n$-particle correlations $c_n^Q$. Here we just want to stress that this OZ approximation of the HRT, or equivalently the LPA in the RG, is *nonperturbative in nature* and keeps all orders in the field theory interactions generated by the renormalization-group flow.

## III. SCALING BEHAVIOR OF THE RG EQUATION

In order to analyze the general features of the solution to Eq. (2.16) in the $Q \to 0$ limit, it is convenient to put it into a dimensionless form by suitably normalizing both density and free energy:

$$x=(\rho-\rho_c)\left[\frac{b}{K_d}\right]^{1/2},$$
$$\Psi_Q=[\mathcal{A}_Q(\rho_c)-\mathcal{A}_Q(\rho)]\frac{1}{K_d}. \tag{3.1}$$

By use of these new variables, the evolution equation (2.16) can be written in a universal form, independent of the particular system we are considering. Therefore, it is an appropriate starting point for studying how LPA describes the growth of correlations and the spontaneous symmetry breaking in models with scalar order parameter. Equation (2.16) then becomes

$$\frac{\partial\Psi_Q}{\partial Q}=-\frac{1}{2}Q^{d-1}\ln\left[\frac{\dfrac{\partial^2\Psi_Q}{\partial x^2}+Q^2}{\left[\dfrac{\partial^2\Psi_Q}{\partial x^2}\right]_0+Q^2}\right], \tag{3.2}$$

where subscript 0 labels quantities evaluated at the critical density $x=0$. Let us consider the main features of the solution to Eq. (3.2) above and below the critical temperature.

### A. $T \geq T_c$

The critical properties described by Eq. (3.2) have been the subject of several studies both in $d=3$ and near four dimensions, where this approximation reproduces the correct first order in the $\epsilon$ expansion. Here we recall that by "renormalizing" Eq. (3.2) through the rescaling

$$t=-\ln Q,$$
$$z=xQ^{-(d-2)/2}, \tag{3.3}$$
$$H_t=\Psi_Q Q^{-d},$$

the scale factor $Q$ can be eliminated from Eq. (3.2) and our equation acquires a scale-invariant form suitable for fixed point analysis:

$$\frac{\partial H_t}{\partial t}+\frac{d-2}{2}z\frac{\partial H_t}{\partial z}-dH_t=\frac{1}{2}\ln\left[\frac{\dfrac{\partial^2 H_t}{\partial z^2}+1}{\left[\dfrac{\partial^2 H_t}{\partial z^2}\right]_0+1}\right]. \tag{3.4}$$

This equation, mathematically equivalent to Eq. (2.16), should be integrated from an ultraviolet cutoff up to $t\to\infty$. The appropriate cutoff for a given physical model is consistently included in the more general Eq. (2.12) but is lost in the long-wavelength approximation leading to Eq. (2.16). In this section we will specialize to the study of a scalar $\phi^4$ field theory postponing the discussion of the Ising model to Sec. V. In this case, the appropriate initial condition is imposed at $t=0$ and is characterized by a mass $r$ and a quartic coupling $u$:

$$H_{t=0}(z)=rz^2+uz^4. \tag{3.5}$$

Physical quantities at a given cutoff $t$ can be obtained from Eq. (3.4) by performing the correct rescaling implied by (3.3). In particular, the inverse compressibility at the critical density is proportional to

$$[\chi_t]^{-1}\sim e^{-2t}\left[\frac{\partial^2 H_t}{\partial z^2}\right]_0. \tag{3.6}$$

Therefore, a finite compressibility in the physical, $t\to\infty$ limit, corresponds to a diverging solution, while, in $d<4$, the critical point is characterized by a finite asymptotic value $H^*(z)$ which can be computed by looking for stationary solutions to Eq. (3.4), i.e., by solving the RG fixed point equation. As usual, critical exponents can be obtained by linearizing the evolution equation near its fixed point solution and searching for the eigenvalues of the relevant perturbations. The odd (i.e., the "magnetic") eigenfunction is exactly given by the first derivative of the fixed point function with respect to the variable $z$ and corresponds to a critical exponent $\delta=(d+2)/(d-2)$ below four dimensions. Instead, the evaluation of the even (i.e., the "thermal") eigenfunction must be carried out numerically with the result $\gamma=1.378$ for the compressibility critical exponent in three dimensions [11]. In two dimensions, the OZ assumption (2.15) leading to the evolution equation (2.16) is no longer justified and a nonzero value of $\eta$ is crucial for reproducing the correct physics at the lower critical dimension.

According to the RG picture, the initial evolution of the free energy (3.5) in the critical region leads $H_t(z)$ close to the fixed point solution $H^*(z)$. In such a regime, the evolution (3.4) is well represented by the linearized form and the most relevant contribution comes from the leading thermal eigenvalue. If the temperature is slightly above the critical value, the linear evolution drives the renormalized zero-field compressibility $(\partial^2 H_t/\partial z^2)_0$ towards growing positive values:

$$\frac{\partial^2 H_t(z)}{\partial z^2}\sim\frac{d^2H^*(z)}{dz^2}+\tau e^{\lambda t}\frac{d^2h_T(z)}{dz^2}, \tag{3.7}$$

where $\tau$ is a measure of the reduced temperature and $h_T(z)$ is the relevant thermal eigenfunction and $\lambda=2/\gamma$. The nonlinear evolution then generates a finite value for the physical compressibility (3.6) in the $t\to\infty$ limit.

### B. $T < T_c$

The RG flow (3.7) is quite different slightly *below* the critical temperature: In this case $\tau$ is negative, the linear evolution (3.7) drives the compressibility towards *negative* values [16] and we might expect that the argument of the logarithm in the fully nonlinear evolution equation (3.4) goes negative thereby generating singularities at finite cutoff $Q=\exp(-t)$. This scenario, advocated in Ref. [7], is forbidden, however, by a general theorem in the case of the *exact* RG transformation [9] and does not occur even for the approximate RG-LPA evolution (3.4) as we are going to show. By taking the second derivative of Eq. (3.2) with respect to $x$ and defining the variable

$$u_Q(x)\equiv\ln\left[\frac{\partial^2\Psi_Q(x)}{\partial x^2}+Q^2\right] \tag{3.8}$$

we cast the evolution equation for the logarithm of the dimensionless inverse compressibility in quasilinear form:

$$e^{u_Q}\frac{\partial u_Q}{\partial Q}=2Q-\frac{1}{2}\frac{\partial^2 u_Q}{\partial x^2}Q^{d-1} . \tag{3.9}$$

In the region where $u_Q(x)$ is negative and large, this equation can be simplified by neglecting exponentially small terms and the resulting evolution can be easily integrated giving

$$u_Q=2(x^2-x_0^2)Q^{-(d-2)} \tag{3.10}$$

which is clearly free of any singularity at finite cutoff. The same analysis can be equivalently carried out for the renormalized equation (3.4). This asymptotic solution describes the behavior of the compressibility within LPA inside the coexistence curve and in fact has been obtained by assuming that the evolution drives the logarithm of the inverse compressibility to negative values. We see that fluctuations inhibit van der Waals loops and instead, the inverse compressibility tends to zero in the whole region $|x|<x_0$ thereby reproducing flat isotherms, i.e., the phenomenological Maxwell construction in the $Q\to 0$ limit. Equation (3.10) is consistent with our assumption of large and negative $u_Q(x)$ in the region $|x|<x_0$ for $d>2$. The solution, however, breaks down at $x=\pm x_0$ where our analysis is not valid any more and the compressibility should attain a finite value. Therefore, we are led to identify $x_0$ as the coexistence density measured from $\rho_c$.

The way in which the solution inside the coexistence curve (3.10) matches with the external solution, is a delicate issue which can be solved by a careful analysis of the evolution equation (3.9). In order to extract this information, it is convenient to look more carefully at the region $x\sim x_0$, i.e., at the behavior of the compressibility near the coexistence curve. The form of Eq. (3.10) suggests a density rescaling of the form:

$$z=(x-x_0)Q^{-(d-2)} . \tag{3.11}$$

The relevant dependence on $Q$ can be eliminated from the exact evolution equation (3.9) by the shift

$$U_Q=u_Q-(4-d)\ln Q . \tag{3.12a}$$

By use of these variables, the equation becomes

$$e^{U_Q}\left[Q\frac{\partial U_Q}{\partial Q}-(d-2)z\frac{\partial U_Q}{\partial z}+(4-d)\right]=-\frac{1}{2}\frac{\partial^2 U_Q}{\partial z^2}+2Q^{d-2} . \tag{3.12b}$$

By neglecting the last term, which vanishes in the $Q\to 0$ limit, we obtain an asymptotic evolution equation, valid in the neighborhood of the coexistence curve. If $d<4$, for every value of $x_0$, i.e., at any point of the coexistence curve, this equation admits a fixed point solution satisfying the boundary conditions:

$$U_Q(z)\underset{z\to-\infty}{\sim}4x_0 z , \tag{3.13a}$$

$$U_Q(z)\underset{z\to+\infty}{\sim}\frac{4-d}{d-2}\ln z . \tag{3.13b}$$

Equation (3.13a) is required by the correct matching with the solution (3.10) in the two-phase region while (3.13b) guarantees finite compressibility outside the coexistence curve.

This fixed point solution has the unphysical feature to give a diverging compressibility at coexistence: the coexistence curve therefore merges with the spinodal curve in this approximation [17]. The asymptotic behavior predicted by our solution is

$$\chi\sim(x-x_0)^{-(4-d)/(d-2)} \tag{3.14}$$

near the phase boundary. This solution, as pointed out before, is consistent with our evolution equation (2.16) only for $d<4$ and in fact the "critical exponent" in Eq. (3.14) vanishes when the dimensionality tends to the upper critical dimension 4. Therefore we conclude that the basic OZ ansatz (2.15) cannot be justified, at least for dimensionality lower than four but we expect that a more realistic description of the behavior near coexistence can be obtained for sufficiently high dimensions.

The reason for such a different behavior in $d>4$ can be traced back to the relevance of the fluctuation corrections to the position of the phase boundary when the dimensionality is increased. In fact, if we assume that the coexistence density $x_0$ moves with $Q$ as

$$x_0(Q)\sim x_0-aQ^2+\cdots \tag{3.15}$$

and we rescale the density according to Eq. (3.11), we get the asymptotic solution

$$u_Q\sim u_0-\ln[1+\exp(-4aze^{u_0}+b)] \tag{3.16}$$

with the correct behavior at $z\to\pm\infty$. Contrary to the solution (3.14), this form shows the expected discontinuity of the inverse compressibility at coexistence [proportional to $\exp(u_0)$] and suggests that momentum-space RG in LPA is able to describe, at least qualitatively, the phenomenon of spontaneous symmetry breaking for scalar field theories in $d>4$.

## IV. NUMERICAL RESULTS

The asymptotic analysis presented in Sec. III on the possible behaviors of the evolution equation (3.2) near phase transitions must be supplemented by the accurate numerical solution of the partial differential equation in order to be fully convincing. We have carried out such a numerical study starting from an initial condition of the form (3.5) for a fixed value of the "interaction" $u=0.05$ and different "temperatures" $r$ and spatial dimensions

$d > 2$. We have solved Eq. (3.9) using a fully implicit, predictor corrector, finite difference method [18] which we found particularly convenient for equations of quasilinear structure. Some numerical isotherms below the critical temperature are shown in Fig. 1 for $d < 4$ and compare quite favorably with the predictions of the asymptotic analysis. A flat portion of the isotherms is clearly visible in the figure, in agreement with the analytical results of Sec. III. The coexistence curve can be identified without ambiguities from the numerical data, due to the exponential character (3.10) of the divergence of the compressibility in the two-phase region. The numerical solution is stable with respect to a substantial refinement of the numerical mesh and the predicted power-law divergence (3.14) of the compressibility at coexistence can be accurately extracted from the data. A plot of the coexistence density in the neighborhood of the critical point for $d = 3$, as a function of the reduced temperature (Fig. 2) shows the expected power-law behavior

$$x_0(r) \sim |r - r_c|^\beta \tag{4.1}$$

consistent with the scaling laws and the critical exponents obtained above $T_c$ ($\beta = 0.345$) [11].

The results at and above dimension 4 are instead reported in Fig. 3 and show the expected dramatic difference with respect to the cases previously discussed. The inverse compressibility still vanishes exponentially in the coexistence region but is characterized by a sharp discontinuity at the phase boundary. This discontinuity is clearly visible from the numerical output, because there is always exactly one mesh point at an intermediate value of the compressibility no matter which is the mesh spacing.

Therefore, as anticipated, we must conclude that above four dimensions, momentum space RG in LPA is able to reproduce both a flat isotherm in the two-phase region and the correct discontinuity of the compressibility across the coexistence curve. Then, we can ask whether the free energy as a function of the density is analytic outside the coexistence curve or presents an essential singularity at coexistence. It is quite difficult to extract this information from the numerical results because essential singularities are rather elusive and cannot be easily detected. A stringent condition for the occurrence of essential singularities is the vanishing of the radius of convergence of the Taylor expansion about the singularity. For the Ising model the expected behavior for the $n$th derivative of the thermodynamic potential with respect to the external magnetic field [3] is

$$F_n \equiv \left. \frac{d^n \ln \Xi}{dh^n} \right|_{h=0^+} \sim K^n (n!)^{d/(d-1)} \tag{4.2}$$

in agreement with the droplet model predictions [2]; we recall that in the lattice-gas picture the magnetic field $h$ in (4.2) is replaced by the chemical potential. The actual

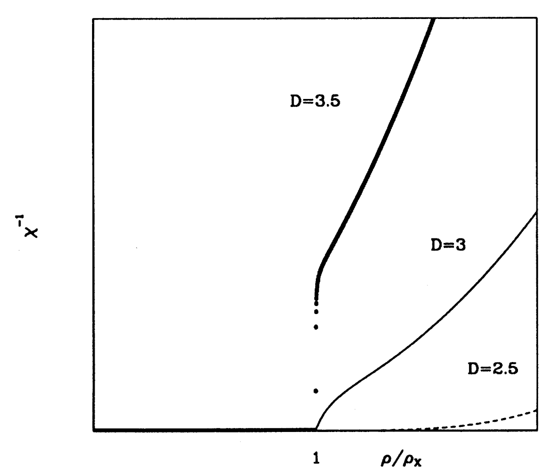


FIG. 1. Inverse compressibility (in arbitrary units) as a function of density normalized to its value at coexistence. The results of the numerical integration of the evolution equation (2.16) are shown for three different space dimensionalities $D = 2.5, 3, 3.5$.

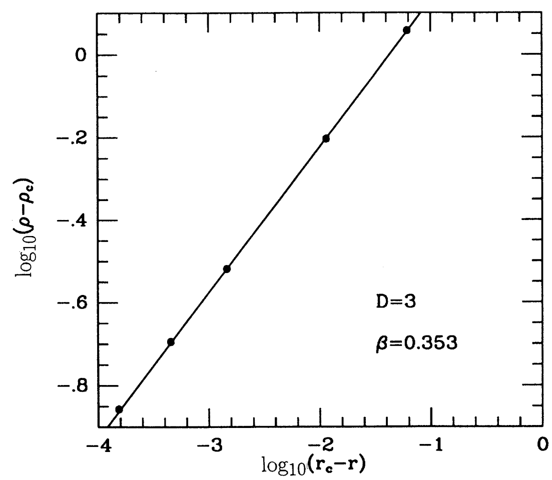


FIG. 2. Density-temperature plot of the coexistence curve close to the critical point in $D = 3$. Dots are the results of Eq. (2.16) while the continuous line is a power-law fit corresponding to the critical exponent $\beta = 0.353$.

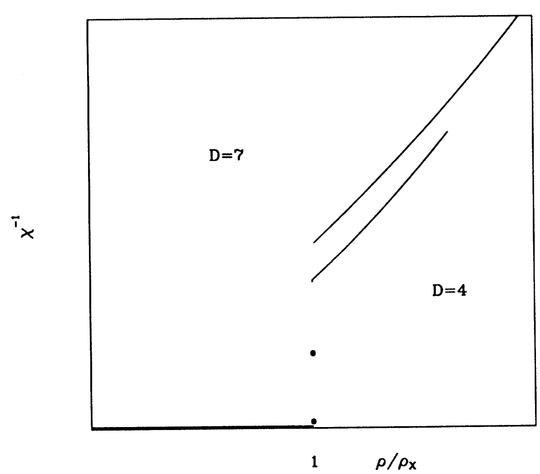


FIG. 3. Same as Fig. 1 for space dimensions $D = 4, 7$.

computation of these high-order derivatives of the numerical solution of our partial differential equation is rather delicate but can be pursued at least for the first ten derivatives. The results in $d=4$ and $d=5$ are shown in Fig. 4 as a function of $\ln(n!)$ and strongly suggest a rapid increase of $F_n$ with $n!$ at an approximate rate $F_n \sim (n!)^2$. Such a behavior would imply that the presence of an essential singularity at coexistence is reproduced by this RG treatment. However, the form of the singularity indicated by the numerical fit does not agree with the Ising model exact result (4.2) pointing out a quantitative inadequacy of our equation.

Notice that both the discontinuous behavior of our solution across the coexistence curve and the numerical indication of an essential singularity of the inverse compressibility are features generated by the strong nonlinearities of the evolution equation (2.16). In fact, in order to reproduce these results, it is crucial to keep track of all the correlation functions of arbitrarily high order, i.e., to introduce an infinite number of coupling constants in the renormalized field theory. Any truncation, e.g., keeping only the mass term and a quartic interaction in the renormalized Hamiltonian [16], drastically changes the long-wavelength evolution and a mean-field-like free energy is recovered: the flat portion of the isotherms disappears while the van der Waals loop and the spinodal curve survive in the $Q \to 0$ limit. Therefore, even if a renormalization procedure which takes into account just quartic interactions shows a qualitatively correct critical behavior, it fails in describing some important features of the symmetry-breaking phenomenon in any space dimensionality, $d>4$ included. The standard analysis of momentum-space RG equations within the framework of $\epsilon$ expansion [16], amounts to solving the differential equations up to a given length scale, usually chosen by requiring that the renormalized correlation length is of the same order as the lattice spacing. Then, the RG flow has driven the Hamiltonian into a noncritical region and mean-field approximation can be used to evaluate thermodynamics and correlations. In the language of HRT, it means that the integration of Eq. (2.16) (which is exact to order $\epsilon$) is not carried out up to zero wave vector $Q$ as it should but it is arbitrarily stopped at a minimum $Q$. Beyond this momentum cutoff, the standard RG procedure assumes that the free energy is not affected by the inclusion of fluctuations of longer wavelength. This can actually be checked *above the critical temperature* by explicitly solving the RG equation up to zero cutoff wave vector: The resulting free energy does not appreciably differ from the RG estimate and the critical properties are correctly reproduced by the matching prescription. The picture, however, drastically changes below the critical temperature where the matching prescription allows one to correctly describe the shape of the coexistence curve and the universal amplitude ratio $C_+/C_-$ between the values of the compressibility on the critical isochore and on the coexistence curve, respectively, above and below the critical temperature. Instead, as we have shown, the correct integration of the evolution equation (2.16) predicts an infinite compressibility on the coexistence curve (i.e., $C_+/C_-=0$) for all dimensions below four. From this point of view, such a behavior is actually unexpected because Eq. (2.16) contains the correct first term in the $\epsilon$ expansion and therefore is expected to reproduce the exact critical properties at least in $d=4-\epsilon$. A possible explanation is that during the RG evolution beyond the matching point the approximation (2.15), the only approximation in our theory, breaks down near the coexistence curve and a more complicate momentum dependence of the direct correlation function is generated by the RG flow within the coexistence curve. We will further elaborate on this point in Sec. VI.

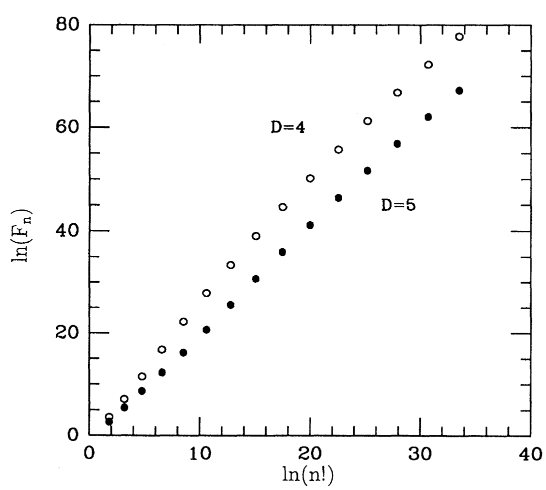


FIG. 4. Plot of the absolute value of the $n$th derivative of the free energy at coexistence as a function of $n!$. Data are obtained by solving numerically Eq. (2.16) for space dimensions $D=4$, 5.

## V. APPLICATION TO THE THREE-DIMENSIONAL ISING MODEL

In the two previous sections the asymptotic form (2.16) of the evolution equation for the free energy, which contains the universal features of the phase transition, has been analyzed in detail. If we want to extract also the nonuniversal properties of the system we must, however, integrate the full evolution equation (2.12). To this end, we need a closure relation involving the direct correlation function $\mathcal{C}_Q(\mathbf{k})=-1/\mathcal{F}_Q(\mathbf{k})$. In order to match with the above description in the critical region, the OZ form (2.15) for $\mathcal{C}_Q(\mathbf{k})$ must be recovered in the long-wavelength limit. A natural way to extend the relation (2.15) outside the critical region is to assume that $\mathcal{C}_Q(\mathbf{k})$ depends on the wave vector $\mathbf{k}$ only through the Fourier transform of the attractive part $w(\mathbf{r})$ of the interaction [19] (we recall that in our case the direct correlation function of the reference system, in momentum space, does not depend on $\mathbf{k}$). For the three-dimensional, nearest-neighbor lattice gas we have [see (2.3)]

$$\phi(\mathbf{k})=6\beta w\gamma(\mathbf{k}) , \quad (5.1)$$

where we have introduced the nearest-neighbor Fourier transform

$$\gamma(\mathbf{k})=\tfrac{1}{3}(\cos k_x+\cos k_y+\cos k_z) . \quad (5.2)$$

The form (2.15) for the direct correlation function in the limit $\mathbf{k}\to\mathbf{0}$ and the compressibility sum rule (2.13) are then obtained if we state

$$\mathcal{C}_Q(\mathbf{k})=\frac{\partial^2\mathcal{A}_Q}{\partial\rho^2}+B_Q(\rho,T)[1-\gamma(\mathbf{k})] \ . \quad (5.3)$$

We note that with this choice the integrand at the right-hand side of Eq. (2.12) is a function of $\gamma(\mathbf{k})$, so that the integration surfaces $\Sigma_Q$ can be conveniently taken as the equipotential surfaces in momentum space $\gamma(\mathbf{k})=\text{const}$. The coefficient $B_Q(\rho,T)$ in (5.3) is chosen so as to ensure that the radial distribution function at zero separation $g_Q(\mathbf{r}=\mathbf{0})$ vanishes for every $Q$ due to the singular on-site repulsion $v_R(\mathbf{r})$ which prevents each lattice site from being occupied by more than one particle. If we turn to the picture of the model as a system of interacting spins $s_j=\pm 1$ on each lattice site $j$, this amounts to requiring that our choice for the direct correlation function correctly implies the relation $\langle s_j^2\rangle=1$ for the mean value of the spin squared. Since the radial distribution function $g_Q(\mathbf{r})$ is related to the Fourier transform of the structure factor $S_Q(\mathbf{k})=-1/\rho c_2^Q(\mathbf{k})$, the constraint $g_Q(\mathbf{r}=\mathbf{0})=0$—the so-called *core condition*— gives rise to an integral condition for the direct correlation function. The closure relation (5.3) then resembles the well-known optimized random-phase approximation (ORPA) of liquid state, which in turn is equivalent to the lowest order of the $\Gamma$-ordered approximation in a lattice gas [20]. However, in our case, the coefficient $B_Q$ is not given by its high-temperature limit $-6\beta w$ but instead is free to adjust itself in order to satisfy both the core condition *and* the evolution equation (2.12). Since the core condition involves the short-range behavior of the system, we expect that it does not affect the universal features of the theory in the critical region. In fact, according to Sec. III, the critical behavior is uniquely determined by the asymptotic equation (2.16), which in turn depends only on the OZ approximation (2.15) and on the compressibility sum rule (2.13) fixing the behavior of $\mathcal{C}_Q(\mathbf{k})$ in the long-wavelength limit. Nevertheless, this condition must be taken into account if we want to achieve an accurate description of the system over the whole phase plane.

The evolution equation (2.12) and the core condition supported by the closure relation (5.3) give rise to a closed system of two integrodifferential equations. A detailed derivation has been reported elsewhere [21]. The integration of these equations has been performed numerically starting from the reference system—namely, the hard-core lattice gas without nearest-neighbor attraction—to end up with the fully interacting one. The results are in agreement with those given in Secs. III–IV. In the present case, also the nonuniversal properties of the model can be obtained; here they are reported in terms of the usual magnetic quantities. In particular, we get for the critical temperature the value $kT_c/6J=0.7553$, where $J=w/4$ is the usual ferromagnetic coupling constant of the Ising model. This result is to be compared with the "exact" one $kT_c/6J=0.7518$, obtained by extrapolation of series expansions [22]: we see that the agreement is quite good (within less than 0.5%). It is worthwhile noticing that this value can be obtained either looking for the divergence of the isothermal susceptibility $\chi$ (the compressibility in the lattice-gas description) above $T_c$ or for the vanishing of the spontaneous magnetization $m_0$ below $T_c$; this shows that in the present approach the critical point is recovered starting both from the ordered and the disordered phase. The value of the critical exponents $\gamma$ and $\beta$ are in agreement with those reported in Secs. III–IV $\gamma=1.378,\beta=0.345$. We recall that these values are expected for any closure which satisfies the OZ approximation (2.15). They differ from the correct values by about 10%.

The inverse reduced susceptibility $1/\chi_{\text{red}}=1/kT\chi$ below the critical temperature as a function of the magnetization $m$ is shown in Fig. 5. As expected on the basis of the analysis developed in the two previous sections, the susceptibility is indeed infinite over a finite interval, which can be then unambiguously identified as the coexistence region. Moreover, for the three-dimensional system under study, the inverse susceptibility remains continuous when one crosses the coexistence region, in contrast with the true behavior of the model. In the figure we also show the value of $1/\chi_{\text{red}}$ obtained by summing a large number of terms in the low-temperature expansion [23]. By plotting the amplitude of the coexistence region as a function of temperature we get the spontaneous magnetization curve, which is shown in Fig. 6 together with a Padé approximant.

The behavior inside the coexistence region deserves some more attention. In this region the function $u_Q$ defined in (3.8) diverges as the fully interacting system is approached due to the vanishing of the inverse susceptibility. It can then be seen that in the rather elaborate structure of our equations several cancellations occur; if we take them carefully into account, we are able to satisfy the core condition within numerical accuracy even at

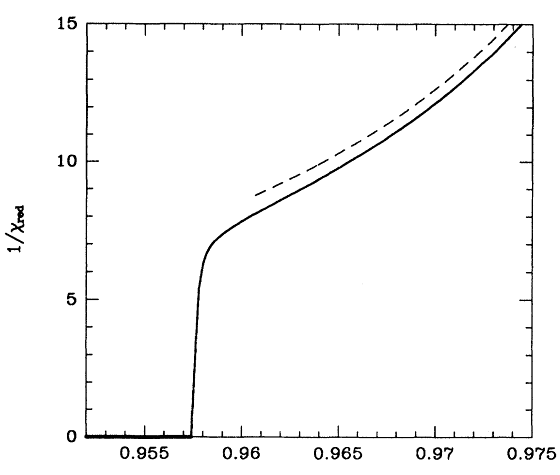


FIG. 5. Inverse reduced susceptibility as a function of magnetization for the Ising model in $D=3$ below the critical temperature ($kT/6J=0.47$). Continuous line: present theory; dashed line: data from low-temperature expansions.

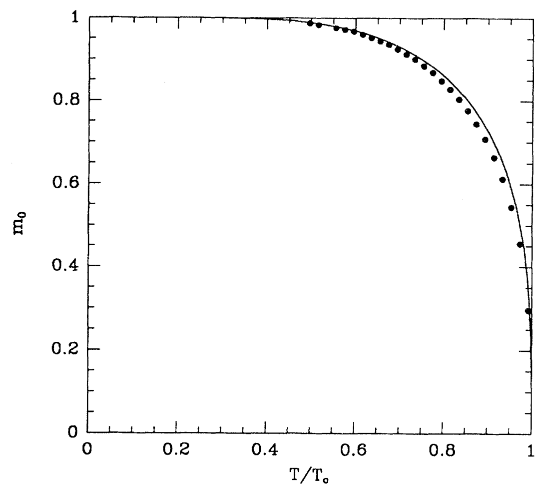


FIG. 6. Coexistence curve for the Ising model in $D=3$. Dots: present theory; continuous line: Padé approximant.

coexistence. It is found that as $u_Q$ diverges the core condition can be verified for finite $B_Q$ if one has $u_Q \sim 1/Q$ for $Q \rightarrow 0$, which is consistent with (3.10) for $d=3$. In Fig. 7 we report $B_Q$ for the completely interacting system as a function of the magnetization $m$ on an isotherm below $T_c$. We note that, as we cross the coexistence region, $B_Q$ varies very sharply, although continuously. The value of $B_Q$ on the boundary of the coexistence region can be directly extracted from the core condition by setting the inverse susceptibility to zero; this gives $B_Q = -24W_0/(1-m^2)$ for every temperature, where $W_0 \simeq 0.252\,731$ is the Watson function $W(x)$ in three dimensions evaluated at $x=0$ [24]. However, it can be seen that as we move inside the coexistence region, i.e., as the magnetization $m$ is decreased, $B_Q$ does not depend on $m$ any more, being locked to its boundary value instead of decreasing in modulus as predicted by the above expression. This surprising feature shows that at the interior of the coexistence region the limit with respect to $Q$ in the core condition, which reads as an integral condition in momentum space, cannot be moved inside the integral, so that the limiting behavior of $B_Q$ does not coincide with the result obtained naively by setting $1/\chi=0$ in the core condition itself, although the two values match at the boundary of the coexistence region. As the temperature is lowered, the absolute value of $B_Q$ rapidly increases due to the corresponding increase in the spontaneous magnetization $m_0$. Since $B_Q$ determines the curvature of the direct correlation function $\mathcal{C}_Q(\mathbf{k})$, this causes the direct correlation function below $T_c$ to be very steep near $\mathbf{k}=0$ *for each point inside the coexistence region.* The physical meaning of this momentum dependence will be analyzed in the next section.

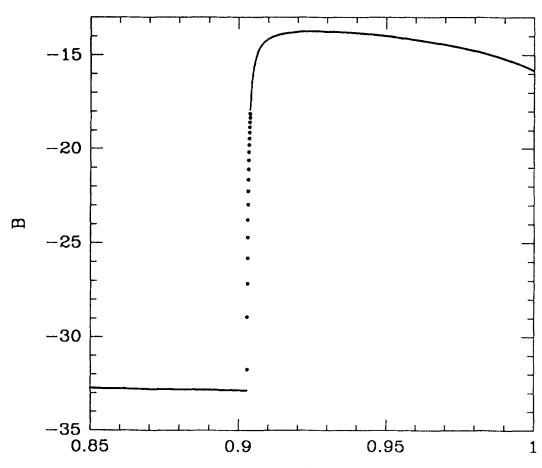


FIG. 7. Curvature $B$ of the direct correlation function [see Eq. (5.3)] at convergence for the Ising model in $D=3$ as a function of magnetization below the critical temperature ($kT/6J=0.55$). Notice the sharp flattening in the two-phase region.

## VI. CRITICAL DISCUSSION

In the previous sections we have provided analytical and numerical evidence showing that the local potential approximation to momentum-space RG equations for the Ising model is free of singularity for any finite cutoff $Q$ above and below the critical temperature and correctly predicts flat isotherms in the two-phase region. However, the same analysis has pointed out some severe deficiencies of this approximation particularly for space dimensionality $d<4$ where an infinite susceptibility along the coexistence curve has been found. The character of the approximation used to derive the RG equations is more clearly discussed within the framework of the hierarchical reference theory of fluids [11] which shows that LPA is exactly equivalent to an Ornstein-Zernike approximation (2.15) for the direct correlation function of the $Q$ system, a system where fluctuations of a wave vector smaller than $Q$ remain bounded. Moreover, the study of the Ising model, where a short distance condition (the core condition) is introduced for determining the range of the direct correlation function $\mathcal{C}_Q(k)$, shows the tendency of $\mathcal{C}_Q$ to acquire a rapidly varying momentum dependence across the coexistence curve (see Fig. 7) and to substantially modify its range in the two-phase region. This suggests that the origin of the spurious behavior we find resides in the oversimplified OZ approximation (2.15) which misses some important feature of the $k$ dependence of the direct correlation function below the critical temperature. As long as we stay outside the two-phase region, we have no reason to believe that Eq. (2.15) is qualitatively incorrect and in fact the extrapolations for the correlation function of the Ising model based on low-temperature expansions [19] confirm this approximate behavior at long wavelengths. However, Eq. (2.15) is obviously incorrect inside the two-phase region, at least in the physical, $Q=0$, limit where the direct correlation function is known to have a discontinuity at $k=0$ due to the occurrence of long-range order in the system [25]. This is an immediate consequence of the long distance behavior of the spin-spin correlation function when a nonzero spontaneous magnetization $m_0$ is present in the model which, in zero field, reads as

$$\langle S_0 S_R \rangle \underset{R\to\infty}{\longrightarrow} m_0^2 \ . \tag{6.1}$$

A spontaneous magnetization generates a δ-function singularity at $k=0$ in the structure factor which, via the Ornstein-Zernike relation, implies a vanishing direct correlation function at zero momentum. However, if the momentum is finite the structure factor is regular and the direct correlation function is expected to have a smooth dependence on the wave vector $k$ with a finite limit for $k\to 0$ related to the susceptibility of the model at coexistence. Then we see that Eq. (2.15) cannot be a qualitatively correct approximation at least at $Q=0$ because it forces the direct correlation function to remain continuous in $k$ also in the two-phase region. In order to better investigate the expected momentum dependence of $\mathcal{C}_Q(k)$ at nonzero $Q$, we notice that the effect of the cutoff $Q$ is qualitatively analogous to enclosing the system in a box of size $L\sim 1/Q$. In fact both procedures eliminate the phase transition by inhibiting fluctuations at long wavelengths. Therefore we may estimate the $k$ dependence of $\mathcal{C}_Q$ by using the long distance behavior, Eq. (6.1), of the spin-spin correlation function only for distances smaller than the "correlated box size" $1/Q$. In this way we find that $\mathcal{C}_Q(k)$ scales like

$$\mathcal{C}_Q(k)=Q^d m_0^{-2}F(k/Q)\ , \tag{6.2}$$

where the scaling function $F(x)$ is analytic at small $x$ and depends on the details of the "box." In particular, if we specialize to $k=Q$ (i.e, the value entering the evolution equation of the free energy) we get $\mathcal{C}_0(k=Q)\sim Q^d$ inside the coexistence curve, a behavior which agrees with the scaling result based on the hypothesis of a "discontinuity fixed point" governing first-order transitions [6]. Let us explore the consequence of such an expected $k$ dependence within momentum-space RG by replacing Eq. (2.15) inside the two-phase region with the simple analytical form

$$\mathcal{C}_Q(k)\underset{k\to 0}{\sim}\mathcal{C}_Q(0)-bk^d \tag{6.3}$$

which satisfies the compressibility sum rule in the $k\to 0$ limit and also introduces the $Q^d$ scaling expected in the $Q\to 0$ limit. According to the previous analysis, the range $b$ of the direct correlation function should scale as $m_0^{-2}$ which diverges as the spontaneous magnetization vanishes, i.e., when the critical point is approached from below. Of course the specific form of Eq. (6.3) has no microscopic justification and has been adopted here just to investigate the effects of a $Q^d$ scaling within the momentum-space RG. By substituting Eq. (6.3) into our asymptotic evolution equation (2.14) we get the following equation for the free energy replacing Eq. (2.16):

$$\frac{d\mathcal{A}_Q}{dQ}=\frac{K_d}{2}Q^{d-1}\ln\left[-\frac{\partial^2\mathcal{A}_Q}{\partial\rho^2}+bQ^d\right] \tag{6.4}$$

which formally corresponds to a scalar field theory with a higher derivative in the kinetic term. The analysis of the long-wavelength solutions of this equation proceeds along the same lines of Sec. III, the only change being the absence of renormalization for the reduced density $x$ of Eq. (3.1) in order to eliminate the explicit occurrence of $Q$ from Eq. (6.4). As a consequence, the RG equation for the renormalized Hamiltonian $H_Q$ in the two-phase region becomes

$$\frac{\partial H_t}{\partial t}-dH_t=\frac{1}{2}\ln\left[\frac{\dfrac{\partial^2 H_t}{\partial x^2}+1}{\left[\dfrac{\partial^2 H_t}{\partial x^2}\right]_0+1}\right]\ , \tag{6.5}$$

where $H$ and $t$ are defined by Eq. (3.3). A line of fixed points of Eq. (6.5) can be found analytically in arbitrary dimension and is given by

$$\int_0^{|H|}dy\left[\frac{\omega}{d}(1-e^{2dy})+2y\right]^{-1/2}=|x| \tag{6.6}$$

in terms of the parameter $\omega<1$ whose nonuniversal value depends on the details of the short-wavelength evolution. Remarkably, the fixed point solution (6.6) is defined only on a finite density domain $|x|<|x_0|$ determined by the positiveness of the radicand at left-hand side of Eq. (6.6). This clearly corresponds to the region of the phase diagram where phase coexistence is allowed and the limiting value of the rescaled density $x_0$ then corresponds to the spontaneous magnetization $m_0$. This result, through Eq. (3.1), implies that $m_0\sim x_0/\sqrt{(b)}$, which is consistent with the proposed scaling $b\sim m_0^{-2}$. The presence of such a solution to the RG equations would imply that also first-order transitions and the phenomenon of phase separation may be described in terms of fixed points and that in the two-phase region all thermodynamical quantities, such as free energy or inverse susceptibility, scale as $Q^d$. This result immediately follows from the adopted scaling of density and free energy. Invoking the qualitative similarity between our momentum cutoff procedure and a finite-size scaling with box length $L\sim 1/Q$, our approach reproduces the known finite-size scaling behavior at first-order transitions derived by use of field theory methods [26]. Moreover, a fixed point like (6,6) can be interpreted as the momentum-space version of the extensively longly sought *discontinuity fixed point* whose actual occurrence has never been convincingly proven within the framework of RG [6,9].

In order to investigate the interesting problem of singularities along the coexistence curve and the matching between the critical domain and the two-phase region, we need a form for the direct correlation function at cutoff $Q$ able to reproduce an Ornstein-Zernike form (2.15) for the homogeneous system and a scaling form of the type (6.2) inside the coexistence curve. This requires a more elaborate ansatz for $\mathcal{C}_Q(k)$ which can be self-consistently determined by explicit use of the second equation of the HRT hierarchy [11]. More specifically, the exact evolution equation for the direct correlation function (or, in field theory language, for the propagator) can be derived in the same way presented in Sec. II and involves the three- and four-point direct correlation functions at cutoff $Q$. If we adopt a closure relating these many-particle correlation functions to $\mathcal{C}_Q(k)$ we obtain new RG equations which, in principle, allow a self-consistent determination of the momentum dependence of the propagator and therefore do not require an *ad hoc* parametrization like Eq. (6.3) for reproducing the correct behavior at coexistence. A possible closure of this type has already been proposed in Ref. [11] and has the further advantage to allow for a nontrivial critical exponent $\eta \neq 0$ which, in fact, turns out to be correct at second order in the $\epsilon$ expansion.

In summary, an accurate analysis of the momentum-space RG for a scalar field theory (or equivalently for the Ising model) shows that the local potential approximation does not generate singularities in the RG flow either above or below the critical temperature. On the contrary, this approximation is able to reproduce rigorously flat isotherms in the two-phase region by suppressing the van der Waals loops present in mean-field treatments. However, the singularity at coexistence is not properly described by LPA and a diverging susceptibility along the phase boundary is found in $d<4$. The origin of this unphysical behavior is clarified by use of the hierarchical reference theory of fluids which provides a different interpretation to the RG equations and suggests the correct scaling which may eliminate the spurious features of LPA in the two-phase region. The resulting approximation also provides a fixed point description of the symmetry-breaking phenomenon quite similar to the discontinuity fixed point picture of first-order transitions. A self-consistent scheme for implementing a momentum-space RG able to reproduce the correct features of phase coexistence has also been proposed.

## ACKNOWLEDGMENTS

We acknowledge financial support by Ministero dell'Università e della Ricerca Scientifica, by Istituto Nazionale di Fisica della Materia, and by Consiglio Nazionale delle Ricerche under Progetto Finalizzato "Sistemi Informatici e Calcolo Parallelo."


[1] P. C. Hemmer and J. L. Lebowitz, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 5b.

[2] M. E. Fisher, in *Critical Phenomena,* Proceedings of the International School of Physics "Enrico Fermi," Course LI, Varenna, 1970, edited by M. S. Green (Academic, New York, 1971); J. D. Gunton, M. San Miguel, and P. S. Shani, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8.

[3] S. N. Isakov, Commun. Math. Phys. **95**, 427 (1984).

[4] B. Nienhuis and M. Nauenberg, Phys. Rev. Lett. **35**, 477 (1975).

[5] W. Klein, D. J. Wallace, and K. P. Zia, Phys. Rev. Lett. **37**, 639 (1976).

[6] M. E. Fisher and A. N. Berker, Phys. Rev. B **26**, 2507 (1982).

[7] R. B. Griffiths and P. A. Pearce, Phys. Rev. Lett. **41**, 917 (1978); A. Hasenfratz and P. Hasenfratz, Nucl. Phys. **B295**, 1 (1988); K. Decker, A. Hasenfratz, and P. Hasenfratz, *ibid.* **B295**, 21 (1988).

[8] H. W. J. Blöte and R. H. Swendsen, Phys. Rev. Lett. **43**, 799 (1979); C. B. Lang, Nucl. Phys. **B280**, 255 (1987).

[9] A. C. D. van Enter, R. Fernandez, and A. D. Sokal, Phys. Rev. Lett. **25**, 3295 (1991).

[10] F. J. Wegner and A. Houghton, Phys. Rev. A **8**, 401 (1973); J. F. Nicoll, T. S. Chang, and H. E. Stanley, *ibid.* **13**, 1251 (1976).

[11] A. Parola and L. Reatto, Phys. Rev. A **31**, 3309 (1985).

[12] See, for instance, G. Stell, in *Phase Transitions and Critical Phenomena* (Ref. [1]).

[13] See, for instance, J. P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Academic, New York, 1986).

[14] R. Zwanzig, J. Chem. Phys. **22**, 1420 (1954).

[15] See, for instance, K. G. Wilson and J. B. Kogut, Phys. Rep. C **12**, 75 (1974).

[16] J. Rudnick and D. R. Nelson, Phys. Rev. B **13**, 2208 (1976); K. Kawasaki *et al.*, in *Perspectives in Statistical Physics,* edited by H. J. Raveché (North-Holland, Amsterdam, 1981).

[17] This result is somehow similar to what is expected in the case of spin models with continuous symmetry, like the *n*-vector model.

[18] W. F. Ames, *Numerical Methods for Partial Differential Equations* (Academic, London, 1977).

[19] M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967).

[20] G. Stell, J. L. Lebowitz, S. Baer, and W. Theumann, J. Math. Phys. **7**, 1532 (1966).

[21] D. Pini, A. Parola, and L. Reatto, J. Stat. Phys. (to be published).

[22] See, for instance, C. Domb, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

[23] G. Bhanot, M. Creutz, and J. Lacki, Phys. Rev. Lett. **69**, 1841 (1992).

[24] See, for instance, G. S. Joyce, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2; A. Parola and L. Reatto, Nuovo Cimento D **6**, 215 (1985).

[25] See, for instance, M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967).

[26] E. Brezin and J. Zinn-Justin, Nucl. Phys. **B257**, 867 (1985); V. Privman and M. E. Fisher, J. Stat. Phys. **33**, 385 (1983).