Diversity of critical behavior within a universality class

Volker Dohm
Institute of Theoretical Physics, RWTH Aachen University, D-52056 Aachen, Germany
(Received 25 January 2008; published 19 June 2008)

We study spatial anisotropy effects on the bulk and finite-size critical behavior of the O(n) symmetric anisotropic φ^4 lattice model with periodic boundary conditions in a d-dimensional hypercubic geometry above, at, and below T_c. The absence of two-scale factor universality is discussed for the bulk order-parameter correlation function, the bulk scattering intensity, and for several universal bulk amplitude relations. The anisotropy parameters are observable by scattering experiments at T_c. For the confined system, renormalization-group theory within the minimal subtraction scheme at fixed dimension d for $2<d<4$ is employed. In contrast to the $\varepsilon=4-d$ expansion, the fixed-d finite-size approach keeps the exponential form of the order-parameter distribution function unexpanded. For the case of cubic symmetry and for $n=1$, our perturbation approach yields excellent agreement with the Monte Carlo (MC) data for the finite-size amplitude of the free energy of the three-dimensional Ising model at T_c by Mon [Phys. Rev. Lett. **54**, 2671 (1985)]. The ε expansion result is in less good agreement. Below T_c, a minimum of the scaling function of the excess free energy is found. We predict a measurable dependence of this minimum on the anisotropy parameters. The relative anisotropy effect on the free energy is predicted to be significantly larger than that on the Binder cumulant. Our theory agrees quantitatively with the nonmonotonic dependence of the Binder cumulant on the ferromagnetic next-nearest-neighbor (NNN) coupling of the two-dimensional Ising model found by MC simulations of Selke and Shchur [J. Phys. A **38**, L739 (2005)]. Our theory also predicts a nonmonotonic dependence for small values of the *antiferromagnetic* NNN coupling and the existence of a Lifshitz point at a larger value of this coupling. The nonuniversal anisotropy effects in the finite-size scaling regime are predicted to satisfy a kind of restricted universality. The tails of the large-L behavior at $T\neq T_c$ violate both finite-size scaling and universality even for isotropic systems as they depend on the bare four-point coupling of the φ^4 theory, on the cutoff procedure, and on subleading long-range interactions.

DOI: 10.1103/PhysRevE.77.061128 PACS number(s): 05.70.Jk, 64.60.−i, 75.40.−s

I. INTRODUCTION AND SUMMARY

A major achievement of the renormalization-group (RG) theory is the proof that critical phenomena can be divided into distinct *universality classes* (for a review, see, e.g., [1]). They are characterized by the spatial dimension d and the symmetry of the ordered state, which, for simplicity, we assume in the following to be $O(n)$ symmetric with an n component order parameter. (For other universality classes, see, e.g., [2].) Within a given (d,n) universality class, all bulk systems (with finite-range interactions and with subleading long-range interactions of the van der Waals type) have the same critical exponents and the same thermodynamic functions near criticality in terms of universal scaling functions that are obtained after a rescaling of two amplitudes: that of the singular part of the bulk free-energy density $f_{s,b}$ and that of the field h conjugate to the order parameter. This is summarized in the asymptotic [small $t=(T-T_c)/T_c$, small h] scaling form (below $d=4$ dimensions)

$$f_{s,b}(t,h) = A_1|t|^{d\nu}W_{\pm}(A_2h|t|^{-\beta\delta}) \tag{1.1}$$

with universal critical exponents ν,β,δ and the universal scaling function $W_{\pm}(z)$ above (+) and below (−) T_c. Once the universal quantities are known, one knows the asymptotic thermodynamic critical behavior of all members of the universality class provided that only the *two* nonuniversal amplitudes A_1 and A_2 are specified. (For the application to real systems, additional experimental information is necessary to identify the order parameter and the appropriate thermodynamic path tangential to the coexistence line.) We refer to this property as *thermodynamic two-scale factor universality*. Here universality means the independence of all microscopic details such as lattice structure, lattice spacing, and the specific form and magnitude of the finite-range or subleading long-range interaction. This implies that both fluids and anisotropic solids within the same universality class have the same scaling function $W_{\pm}$.

This important concept of scaling and thermodynamic two-scale factor universality was extended to the distance ($\mathbf{r}$) dependence of bulk correlation functions [3] and to the size (L) dependence of quantities of confined systems [4–6] (for reviews see, e.g., [8,7]). It is this *extended* hypothesis that is the focus of the present paper. We shall present results for the finite-size critical behavior of the free energy above, at, and below T_c that demonstrate a considerable degree of diversity within a given (d,n) universality class primarily due to spatial anisotropy in lattice systems with noncubic symmetry, but also due to the lattice spacing $\tilde{a}$ in systems with cubic symmetry and due to the bare four-point coupling u_0 of the φ^4 theory even in the isotropic case. In this context, we also discuss nonuniversal effects related to the cutoff and to subleading long-range (van der Waals type) interactions. This diversity suggests to distinguish subclasses of interactions within a given universality class where the subclasses have different bulk amplitude relations, different bulk correlation functions, and, for given geometry and boundary conditions (b.c.), different finite-size scaling functions. All of these nonuniversal differences exist in the *asymptotic* critical region

TABLE I. Subclasses of asymptotic critical behavior within a (d,n) universality class for $O(n)$ symmetric systems in a cubic volume $V=L^d$ with periodic boundary conditions for general n above T_c and $n=1$ below T_c. All subclasses have the same fixed point value $u^*(d,n)$ of the renormalized four-point coupling, the same critical exponents, and the same bulk thermodynamic scaling functions. This table complements Table IV of [1].

Classes of interactions $\delta\hat{K}(\mathbf{k})$ in Eq. (2.7)	Basic lengths, nonuniversal parameters	Bulk amplitude relations	Bulk correlation functions	Finite-size effects
isotropic short range[a] $\mathbf{k}^2+O(k^4)$	correlation length[b] $\xi_\pm$, two nonuniversal amplitudes C_1, C_2, four-point coupling u_0	two-scale factor universality	$r/\xi_\pm \lesssim O(1)$: universal isotropic power-law scaling form; $r \gg \xi_\pm$: exponential form with nonuniversal tails	$L/\xi_\pm \lesssim O(1)$: universal power-law scaling form; $L \gg \xi_\pm$: exponential form with nonuniversal tails
anisotropic short range[c] $\sum_{\alpha,\beta=1}^{d} A_{\alpha\beta}k_\alpha k_\beta$ det $\mathbf{A}>0$ $A_{\alpha\beta}=A_{\beta\alpha}$	d principal correlation lengths $\xi_\pm^{(\alpha)}$, up to $d(d+1)/2+1$ nonuniversal parameters[d] $C_1', C_2', \bar{A}_{\alpha\beta}$, four-point coupling u_0	multiparameter universality	$r/\xi_\pm^{(\alpha)} \lesssim O(1)$: universal power-law scaling form with $d(d+1)/2+1$ nonuniversal parameters in the scaling arguments; $r \gg \xi_\pm^{(\alpha)}$: exponential form with nonuniversal tails	$L/\xi_\pm^{(\alpha)} \lesssim O(1)$: nonuniversal power-law scaling form, restricted universality; $L \gg \xi_\pm^{(\alpha)}$: exponential form with nonuniversal tails
isotropic subleading long range[e] $\mathbf{k}^2-b\lvert\mathbf{k}\rvert^\sigma$ $2<\sigma<4$	correlation length $\xi_\pm$, interaction length scale $b^{1/(\sigma-2)}$, five nonuniversal parameters C_1, C_2, b, σ, u_0	two-scale factor universality	$r/\xi_\pm \lesssim O(1)$: universal power-law scaling form; $r/\xi_\pm > O(1)$: nonuniversal power-law form depending on b, σ	$L/\xi_\pm \lesssim O(1)$: universal power-law scaling form; $L/\xi_\pm > O(1)$: nonuniversal power-law form depending on b, σ

[a]References [1,8–11].
[b]For isotropic systems, ξ_+ and ξ_- denote the second-moment bulk correlation lengths above and below T_c, with a universal ratio ξ_+/ξ_-. For anisotropic systems, $\xi_\pm^{(\alpha)}$ are the principal bulk correlation lengths with universal ratios $\xi_+^{(\alpha)}/\xi_-^{(\alpha)}, \alpha=1,2,\ldots,d$.
[c]References [12,13].
[d]The reduced anisotropy matrix $\bar{\mathbf{A}}=\mathbf{A}/(\det \mathbf{A})^{1/d}$ has $d(d+1)/2-1$ independent matrix elements $\bar{A}_{\alpha\beta}$.
[e]References [11,14–18].

$\lvert t\rvert \ll 1$, $L \gg \tilde{a}$, and $r \gg \tilde{a}$ where corrections to scaling in the sense of Wegner [19] are negligible. A summary of these properties is given in Table I. The basic framework of RG theory is fully compatible with this diversity of critical behavior.

Spatially anisotropic systems such as magnetic materials, alloys, superconductors [20], and solids with structural phase transitions [21,22] represent an important class of systems with cooperative phenomena. One may distinguish between long-range anisotropic interactions (such as dipolar, Ruderman-Kittel-Kasuya-Yosida, and effective elastic interactions) and short-range anisotropic interactions, which include the Dzyaloshinskii-Moriya-type antisymmetric exchange [23] and the spatially anisotropic Heisenberg exchange interactions, which, in the long-wavelength limit, are described by a $d\times d$ anisotropy matrix $\mathbf{A}$ [12,13]. We shall confine ourselves to a detailed study of the latter type of systems, but the general aspects of our results have an impact also on the former type of anisotropic systems and on systems of other universality classes [2], for example on the range of validity of universality for anisotropic spin glasses [24] or for anisotropic surface critical phenomena [25].

A characteristic feature of spatial anisotropy with noncubic symmetry is the fact that there exists no unique bulk correlation-length amplitude but rather d different amplitudes $\xi_{0\pm}^{(\alpha)}$ in the directions $\alpha=1,\ldots,d$ of the d principal axes. Such systems still have a single correlation-length exponent ν provided that $\det \mathbf{A}>0$. [We do not consider *strongly* anisotropic systems with critical exponents different from those of the usual (d,n) universality classes; see, e.g., [26].] Noncubic anisotropy effects in crystals with cubic symmetry can be easily generated by applying shear forces. In earlier work on two-scale factor universality [5,8,27–30], isotropic systems with a single bulk correlation length ξ_∞ were considered and important universal bulk amplitude relations were derived that depend on only two nonuniversal parameters. Recently, some of these relations were reformulated for anisotropic systems within the same universality class [12,13]. In Sec. III of this paper, we give a derivation of these and other relations above and below T_c and express them in terms of universal scaling functions. The physical quantities entering these relations depend, in general, on $d(d+1)/2+1$ nonuniversal parameters. We also present the appropriate formulation of the bulk scattering intensity of anisotropic systems near criticality in terms of the eigenvalues of the anisotropy matrix and discuss the nonuniversal properties of bulk correlation functions.

For *confined* systems with a characteristic length L, the hypothesis of two-scale factor universality is summarized by the asymptotic (large L, small t, small h) scaling form for the singular part of the free-energy density (divided by k_BT) [5,7,8],

$$f_s(t,h,L) = L^{-d}\mathcal{F}(C_1 t L^{1/\nu}, C_2 h L^{\beta\delta/\nu}), \tag{1.2}$$

where $\mathcal{F}(x,y)$, for given geometry and b.c., is a universal scaling function and where the two constants C_1 and C_2 are universally related to the bulk constants A_1 and A_2 of Eq. (1.1). For simplicity, we shall confine ourselves to a hypercubic shape with volume $V=L^d$ and with periodic b.c. Calculations of $f_s(t,0,L)$ for this case were carried out within the spherical model [31], which supported the form of Eq. (1.2). For $n=1$, the scaling form (1.2) was discussed in the framework of the $\varepsilon=4-d$ expansion [32,33]. No theoretical prediction for the function $\mathcal{F}(x,y)$ is available as of yet for finite n in cubic geometry, except in the large-n limit [11]. Monte Carlo (MC) simulations [34–36] for three-dimensional Ising models with nearest-neighbor (NN) couplings on different lattices of cubic symmetry were consistent with the universality of the amplitude $\mathcal{F}(0,0)$. These models belong to the subclass of (asymptotically) isotropic systems.

It was already noted in [5,8,37] that lattice anisotropy is a marginal perturbation in the RG sense, thus it was not obvious *a priori* to what extent two-scale factor universality is valid in the presence of anisotropic couplings [8]. It was also known that, for most anisotropic systems, (asymptotic) isotropy can be restored by an anisotropic scale transformation [38,39] (for further references, see [12]). Recently, it was pointed out [12] that, in systems with anisotropic interactions of noncubic symmetry, the scaling function $\mathcal{F}$ is indeed affected by anisotropy. In particular, it was shown [13] that by means of an appropriate rescaling of lengths, a transformation to an (asymptotically) isotropic system is always possible provided that the anisotropy matrix $\mathbf{A}$ is positive definite and that the rescaling is performed along the d *nonuniversal* directions of the *principal* axes which, in general, differ from the symmetry axes of the system. This rescaling is equivalent to a shear transformation that distorts the shape, the lattice structure, and the boundary conditions in a nonuniversal way (e.g., from a cube to a parallelepiped, from an orthorhombic to a triclinic lattice, and from periodic b.c. in rectangular directions to those in nonrectangular directions). This nonuniversality is reflected in a dependence of the scaling function $\mathcal{F}$ on the anisotropy matrix $\mathbf{A}$, in addition to the dependence on C_1 and C_2.

Specifically, on the basis of the results of renormalized perturbation theory in Secs. IV–VI we propose that, for anisotropic systems with the shape of a cube, Eq. (1.2) is to be replaced by [40]

$$f_s(t,h,L) = L^{-d}\mathcal{F}_{\text{cube}}(C_1' t L'^{1/\nu}, C_2' h' L'^{\beta\delta/\nu}; \bar{\mathbf{A}}), \tag{1.3}$$

with $L'=L(\det \mathbf{A})^{-1/(2d)}$, $h'=h(\det \mathbf{A})^{1/4}$, and with the reduced anisotropy matrix $\bar{\mathbf{A}}=\mathbf{A}/(\det \mathbf{A})^{1/d}$, $\det \mathbf{A}>0$. The nonuniversal constants C_1' and C_2' will be specified in Sec. VI in terms of the asymptotic amplitudes ξ_{0+}' and ξ_c' of the second-moment bulk correlation lengths for $T>T_c$, $h'=0$ and for $T=T_c$, $h'\neq 0$, respectively, of the transformed isotropic system. The free-energy density $f_s'=f_s(\det \mathbf{A})^{1/2}$ of the parallelepiped with the volume $V'=V(\det \mathbf{A})^{-1/2}$ and with $\bar{\mathbf{A}}'=\mathbf{A}'/(\det \mathbf{A}')=\mathbf{1}$ (isotropy) then attains the scaling form

$$f_s'(t,h',L') = L'^{-d}\mathcal{F}_{\text{iso},\bar{\mathbf{A}}}(C_1' t L'^{1/\nu}, C_2' h' L'^{\beta\delta/\nu}), \tag{1.4}$$

where the characteristic length $L'=V'^{1/d}$ determines the overall size of the parallelepiped and

$$\mathcal{F}_{\text{iso},\bar{\mathbf{A}}}(x,y) = \mathcal{F}_{\text{cube}}(x,y;\bar{\mathbf{A}}). \tag{1.5}$$

Equation (1.4) has the structure of the isotropic Privman-Fisher scaling form (1.2) with a rescaled length L' and with only two nonuniversal constants C_1' and C_2', which, superficially, appears to be in agreement with two-scale factor universality. The remaining $d(d+1)/2-1$ nonuniversal parameters, however, are hidden in the index "iso, $\bar{\mathbf{A}}$." This index is the notation for a system with the shape of a parallelepiped whose interaction $\delta\hat{K}'(\mathbf{k}')=\mathbf{k}'^2+O(k'^4)$ is (asymptotically) isotropic and whose $d(d-1)/2$ angles and $d-1$ length ratios are determined by the $d(d+1)/2-1$ nonuniversal parameters of the reduced anisotropy matrix $\bar{\mathbf{A}}$. These parameters appear in the calculation of $\mathcal{F}_{\text{iso},\bar{\mathbf{A}}}$ via the summation over the discrete $\mathbf{k}'$ vectors in the Fourier space of the parallelepiped system since the $\mathbf{k}'$ vectors depend explicitly on $\bar{\mathbf{A}}$, unlike the $\mathbf{k}$ vectors of the cubic system. Thus for the calculation of $\mathcal{F}_{\text{iso},\bar{\mathbf{A}}}$, the same nonuniversal information is required as for the calculation of $\mathcal{F}_{\text{cube}}(x,y;\bar{\mathbf{A}})$.

For general $\mathbf{A}$, the function $\mathcal{F}_{\text{cube}}(x,0;\bar{\mathbf{A}})$ was presented in [12] for $t\geq 0$ in the large-n limit. Furthermore, quantitative predictions were made for the nonuniversal dependence of the critical Binder cumulant [8,41],

$$U_{\text{cube}}(\bar{\mathbf{A}}) = \frac{1}{3}\left[\frac{\partial^4 \mathcal{F}_{\text{cube}}(0,y;\bar{\mathbf{A}})/\partial y^4}{(\partial^2 \mathcal{F}_{\text{cube}}(0,y;\bar{\mathbf{A}})/\partial y^2)^2}\right]_{y=0} \tag{1.6}$$

for $n=1,2,3$ both in three [12,13] and two [13] dimensions. MC simulations [42,43] for the anisotropic three-dimensional Ising model indeed showed nonuniversal anisotropy effects, which, however, did not agree with the theoretical prediction. More accurate MC simulations [44] for the anisotropic two-dimensional Ising model demonstrated the nonuniversality of the critical Binder cumulant, but no comparison with a quantitative theoretical prediction was available for this two-dimensional case. Thus the anisotropic finite-size theory of [12,13] is as yet unconfirmed.

In Secs. IV–VI of this paper, we derive the finite-size scaling function $\mathcal{F}^{\text{ex}}_{\text{cube}}(x,0;\bar{\mathbf{A}})$ of the singular part of the excess free-energy density $f_s^{\text{ex}}=f_s-f_{s,b}$ at $h=0$ above, at, and below T_c for the $n=1$ universality class in $2<d<4$ dimensions on the basis of the anisotropic φ^4 lattice model. For the isotropic case at T_c we find excellent agreement with the MC data of Mon [34,35]. Slightly below T_c we find a minimum of the scaling function that is similar to the minimum of the scaling function of the critical Casimir force for the $d=3$ Ising model in slab geometry with periodic boundary conditions [45,46]. For future tests of our theory by MC simulations, we consider both three- and two-dimensional anisotropies. In both cases, we predict a measurable dependence of the minimum on the anisotropy parameters, thus demonstrating the nonuniversality of the finite-size scaling function of the excess free-energy density. The magnitude of this anisotropy effect is predicted to be considerably larger than that on the Binder cumulant.

We believe that a similar nonuniversal dependence can be derived for the critical Casimir force by means of our perturbation approach. For $n \to \infty$ and at $T = T_c$, the nonuniversality of the Casimir amplitude due to anisotropy was already demonstrated within the φ^4 theory in [12]. This suggests that, for given geometry and b.c., the existing theoretical [11,47–54] and MC [45,46,48,55] results for the Casimir force scaling function are not universal within the *entire* universality class but are restricted to the subclass of isotropic systems. Extensions to the subclass of anisotropic systems are, in general, not straightforward and cannot be obtained just by transformations but require new nonuniversal input, new analytical and numerical calculations, and new MC simulations. Experiments, e.g., in anisotropic superconducting films [20,56] could, in principle, demonstrate the nonuniversality in real systems.

Our present results for the φ^4 theory cannot be applied directly to two-dimensional critical phenomena. Nevertheless, we are able to study two-dimensional anisotropy effects within a three-dimensional model. For the purpose of a comparison with the two-dimensional MC data [44], we consider (in Sec. VIII) a three-dimensional φ^4 lattice model with the same two-dimensional anisotropy in the horizontal planes as in the two-dimensional Ising model studied by Selke and Shchur [44]. Our theory agrees quantitatively with the nonmonotonicity of the Binder cumulant as a function of the anisotropiy *ferromagnetic* next-nearest-neighbor (NNN) coupling found in [44]. We also predict a nonmonotonicity for small *antiferromagnetic* couplings and the existence of a Lifshitz point at a larger value of this coupling. Very recent preliminary MC data by Selke [57] for the *two*-dimensional Ising model indeed reveal such a nonmonotonicity that was not yet detected in [44]. We predict a similar anisotropy effect for the excess free-energy density of the anisotropic two-dimensional Ising model. This effect can become quite large if one of the eigenvalues of $\bar{\mathbf{A}}$ approaches zero, in particular if a Lifshitz point is approached (Sec. VIII).

An important property of the scaling form (1.3) is that it depends on $\bar{\mathbf{A}}$ but not on other nonuniversal parameters such as the bare four-point coupling, the lattice spacing, and the cutoff of φ^4 field theory. This is a kind of *restricted universality* since it implies that the same finite-size scaling functions exist for the large variety of those systems within a universality class that have the same reduced anisotropy matrix $\bar{\mathbf{A}}$ (and the same geometry and boundary conditions). In Sec. IX, we propose two examples for testing this hypothesis of restricted finite-size universality by MC simulations for spin models with *anisotropic* interactions. For recent tests of finite-size universality of two-dimensional Ising models with (asymptotically) *isotropic* interactions, see [58,59] (see also Table 10.1 of [8]).

Unlike the bulk scaling function $W_{\pm}(z)$, Eq. (1.1), which is valid in the entire range $-\infty \le z \le \infty$ of the scaling argument z, the finite-size scaling functions such as $\mathcal{F}_{\rm cube}(x,y;\bar{\mathbf{A}})$ are valid only in a limited range of x and y, above the shaded region in Fig. 1. In the shaded region, nonuniversal nonscaling effects become non-negligible and even dominant for sufficiently large $|x|$ and $|y|$ for both short-range and subleading long-range interactions. In this region, not only the correlation lengths are relevant, but also additional nonuniversal length scales such as the lattice spacing $\tilde{a}$, the inverse cutoff Λ^{-1}, the length scale $u_0^{-1/\varepsilon}$ set by the four-point coupling, and the van der Waals interaction length $b^{1/(\sigma-2)}$, as discussed in Sec. X.

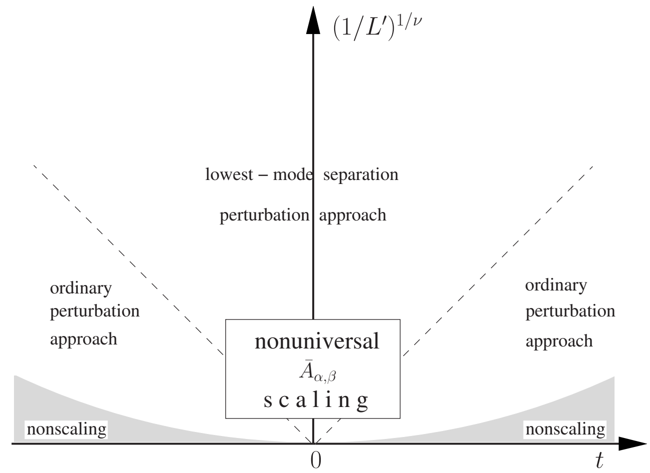

FIG. 1. Asymptotic part of the $L'^{-1/\nu}$-t plane at $h=0$ for the anisotropic φ^4 theory in a cubic geometry with periodic boundary conditions. In the central finite-size region (above the dashed lines), the lowest mode must be separated, whereas outside this region ordinary perturbation theory is applicable. Above the shaded region, finite-size scaling is valid but with scaling functions that depend on the anisotropy parameters $\bar{A}_{\alpha\beta}$, see Eq. (1.3). In the large - L' regime at $t \neq 0$ (shaded region), finite-size scaling and universality are violated for both short-range and subleading long-range interactions and for both isotropic and anisotropic systems. A similar plot is valid for the $L'^{-\beta\delta/\nu}$-h' plane at $T=T_c$.

We briefly comment on the methodological aspects of our finite-size calculations. As far as the field-theoretic [60] renormalization of the φ^4 lattice model is concerned, we use the minimal subtraction scheme [61] not within the ε expansion but at fixed dimension d, as introduced in [62] and further developed in [63]. As far as finite-size theory is concerned, we further develop earlier approaches [32,64–66] that have been successfully used to solve several finite-size problems in the past [67–70]. After the transformation from the anisotropic to an isotropic system, the same renormalization constants (Z factors) and the same fixed-point value u^* of the renormalized four-point coupling are obtained as for the standard isotropic φ^4 Hamiltonian. For this reason, the same fixed-point Hamiltonian and the same critical exponents govern isotropic and (weakly) anisotropic systems—they belong to the same universality class. The crucial point, however, is that not only the fixed-point value u^* but also the orientation of the eigenvectors (principal axes) of the fixed-point Hamiltonian relative to the orientation of the given boundaries of the *confined* anisotropic system determine the finite-size scaling functions. This is a physical fact that introduces a source of nonuniversality that cannot be elimi-

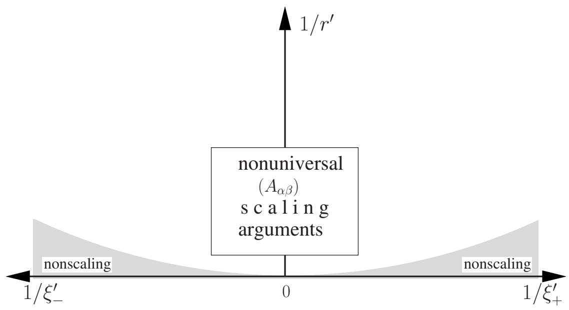

FIG. 2. Asymptotic part of the r'^{-1}-$\xi_{\pm}'^{-1}$ plane at $h=0$ for anisotropic bulk systems. Above the shaded region, there exists a universal scaling function $\Phi_{\pm}(r'/\xi'_{\pm},0)$ of the bulk correlation function G_b, Eq. (3.19). The scaling argument, however, contains the spatial variable $r'\equiv|\mathbf{x}'|$, Eq. (3.23), that depends on the anisotropy matrix $(A_{\alpha\beta})$ with $d(d+1)/2$ nonuniversal parameters. In the large-r' regime at $t\neq 0$ (shaded region), scaling and universality are violated for both short-range and subleading long-range interactions and for both isotropic and anisotropic systems. A similar plot is valid in the r'^{-1}-$\xi_h'^{-1}$ plane at $T=T_c, h'\neq 0$, with $\xi'_h=\xi'_c|h'|^{-\nu/(\beta\delta)}$.

nated by transformations and that makes anisotropic confined systems distinctly different from isotropic confined systems within the same universality class.

The main result for f_s^{ex} will be obtained in the central finite-size regime (above the dashed lines in Fig. 1) where the finite-size effects are most significant and where it is necessary to separate the lowest mode from the higher modes. In this regime, finite-size scaling is valid in the form of Eq. (1.3). We compare the result of our fixed-d perturbation approach [62,63,65,66] with that of the ε-expansion approach. The advantage of the former approach is that it keeps the exponential structure of the order-parameter distribution function unexpanded. This leads to a result at T_c in excellent agreement with the MC data in the isotropic case [34,35] and lends credibility also to the quantitative features of our predictions of anisotropy effects. The ε-expansion result at T_c turns out to be in less good agreement.

The separation of the lowest mode is inadequate in the limit of large $L'\gg\xi'_{\pm}$ at fixed $T\neq T_c$. In order to capture the exponential structure of finite-size effects for large L', we complement (in Sec. X) our results by ordinary perturbation theory outside the central finite-size regime (below the dashed lines in Fig. 1). This includes a small but finite region where finite-size scaling is violated (shaded region in Fig. 1). There exists diversity rather than universality of finite-size critical behavior in this region depending on all microscopic details of the interactions such as the lattice spacing, the bare four-point coupling, the cutoff of the φ^4 theory, and the amplitude of subleading long-range interactions. This diversity can be traced back to a corresponding diversity of the large-distance ($r'\gg\xi'_{\pm}$) behavior of the *bulk* order-parameter correlation function G_b [10], where r' is the distance in the transformed isotropic bulk system, as discussed in Sec. III. For G_b, there exists a region of the $r'^{-1}-\xi_{\pm}'^{-1}$plane (shaded region in Fig. 2) that is the analogue of the shaded region of Fig. 1. In the isotropic case, this region is of physical relevance for fluids with van der Waals interactions [11,14–18,50,52].

II. ANISOTROPIC φ^4 LATTICE MODEL

A. Hamiltonian with spatial anisotropy

We start from the $O(n)$ symmetric φ^4 lattice Hamiltonian (divided by k_BT),

$$H = v\left[\sum_{i=1}^{N}\left(\frac{r_0}{2}\varphi_i^2 + u_0(\varphi_i^2)^2 - h\varphi_i\right) + \sum_{i,j=1}^{N}\frac{K_{i,j}}{2}(\varphi_i-\varphi_j)^2\right], \tag{2.1}$$

$r_0(T)=r_{0c}+a_0t$, $t=(T-T_c)/T_c$ with $a_0>0$, $u_0>0$. The variables $\varphi_i\equiv\varphi(\mathbf{x}_i)$ are n-component vectors on N lattice points $\mathbf{x}_i\equiv(x_{i1},x_{i2},\ldots,x_{id})$ of a d-dimensional Bravais lattice with the finite volume $V=Nv$ with the characteristic length $L=V^{1/d}$, where v is the volume of the primitive cell. The components $\varphi_i^{(\mu)}$, $\mu=1,2,\ldots,n$ of φ_i vary in the continuous range $-\infty\leq\varphi_i^{(\mu)}\leq\infty$. The couplings $K_{i,j}=K_{j,i}\equiv K(\mathbf{x}_i-\mathbf{x}_j)$ and the temperature variable $r_0(T)$ have the dimension of L^{-2}, whereas the variables φ_i have the dimension of $L^{(2-d)/2}$ such that H is dimensionless. The free energy per unit volume divided by k_BT is

$$f(t,h,L) = -V^{-1}\ln Z, \tag{2.2}$$

$$Z(t,h,L) = \left[\prod_{i=1}^{N}\frac{\int d^n\varphi_i}{v^{n(2-d)/(2d)}}\right]\exp(-H), \tag{2.3}$$

where Z is the dimensionless partition function. The total excess free-energy density is defined as

$$f^{\text{ex}}(t,h,L) = f(t,h,L) - f_b(t,h), \tag{2.4}$$

where $f_b(t,h)=\lim_{L\to\infty}f(t,h,L)$ is the bulk free-energy density. Following [6–8], we shall decompose f, for large L, into singular and nonsingular parts,

$$f(t,h,L) = f_s(t,h,L) + f_{\text{ns}}(t,L), \tag{2.5}$$

where $f_{\text{ns}}(t,L)$ has a regular t dependence around $t=0$. In earlier work on finite-size effects, it was supposed [5,7,11] that, *for periodic boundary conditions*, one can assume that there exists no L dependence of the nonsingular part f_{ns}. Adopting this assumption leads to a misinterpretation [11] of the singular part f_s of the free-energy density and of the Casimir force in the presence of a sharp cutoff of φ^4 field theory. Here we shall not exclude the possibility of an L-dependent nonsingular part $f_{\text{ns}}(t,L)$ even for periodic boundary conditions if long-range correlations are present. As will be shown in Sec. X, this will reconcile the earlier results [11] with the concepts of finite-size scaling.

For periodic b.c., the Fourier representations are $\varphi(\mathbf{x}_j)=V^{-1}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}_j}\hat{\varphi}(\mathbf{k})$ and

$$K(\mathbf{x}_i-\mathbf{x}_j) = N^{-1}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}\hat{K}(\mathbf{k}), \tag{2.6}$$

where the summations $\Sigma_{\mathbf{k}}$ run over the N discrete vectors $\mathbf{k}$ of the first Brillouin zone of the reciprocal lattice. We assume finite-range interactions $K_{i,j}$ with a finite value

$\hat{K}(\mathbf{0})=N^{-1}\Sigma_{i,j=1}^{N}K_{i,j}$. In terms of the Fourier components, the Hamiltonian reads

$$H = V^{-1}\sum_{\mathbf{k}} \frac{1}{2}[r_0 + \delta\hat{K}(\mathbf{k})]\hat{\varphi}(\mathbf{k})\hat{\varphi}(-\mathbf{k}) - h\hat{\varphi}(\mathbf{0}) + u_0 V^{-3}\sum_{\mathbf{kpq}} [\hat{\varphi}(\mathbf{k})\hat{\varphi}(\mathbf{p})][\hat{\varphi}(\mathbf{q})\hat{\varphi}(-\mathbf{k}-\mathbf{p}-\mathbf{q})], \quad (2.7)$$

where $\delta\hat{K}(\mathbf{k})=2[\hat{K}(\mathbf{0})-\hat{K}(\mathbf{k})]$. In perturbation theory, $r_0 + \delta\hat{K}(\mathbf{k})$ plays the role of an inverse propagator.

The Hamiltonian H is isotropic in the vector space of the n-component variables φ_i and $\hat{\varphi}(\mathbf{k})$ but may be anisotropic in real space and $\mathbf{k}$ space. A variety of anisotropies may arise both through the lattice structure and through the couplings $K_{i,j}$. They manifest themselves on macroscopic length scales via the $d\times d$ anisotropy matrix $\mathbf{A}=(A_{\alpha\beta})$ and the anisotropy tensor $\mathbf{B}=(B_{\alpha\beta\gamma\delta})$ that appear in the long-wavelength form

$$\delta\hat{K}(\mathbf{k}) = \sum_{\alpha,\beta=1}^{d} A_{\alpha\beta}k_\alpha k_\beta + \sum_{\alpha,\beta,\gamma,\delta}^{d} B_{\alpha\beta\gamma\delta}k_\alpha k_\beta k_\gamma k_\delta + O(k^6). \quad (2.8)$$

Odd powers of k_α are excluded because of inversion symmetry of the Bravais lattice. (For the case of non-Bravais lattices, see the discussion in Sec. II.C of Ref. [71].) For cubic symmetry, $\mathbf{A}$ has the isotropic form $A_{\alpha\beta}=c_0\delta_{\alpha\beta}$ while the $O(k^4)$ terms of cubic systems differ from those of isotropic systems. In Secs. III and X, we shall consider the model (2.7) also in a fully isotropic form with the short-range interaction $\delta\hat{K}(\mathbf{k})=\mathbf{k}^2$ including a finite cutoff Λ and, for $n=1$, with the subleading long-range interaction [11,14–18,50,52]

$$\delta\hat{K}(\mathbf{k}) = \mathbf{k}^2 - b|\mathbf{k}|^\sigma + O(k^4), 2 < \sigma < 4 \quad (2.9)$$

with $b>0$. The second term of the interaction (2.9) is usually classified as "irrelevant" in the renormalization-group sense [50] since it leaves *some* (but not all) of the universal quantities unchanged: critical exponents and bulk thermodynamic scaling functions. This terminology is somewhat misleading as the term $-b|\mathbf{k}|^\sigma$ changes not only the leading *finite-size* critical behavior at $T\neq T_c$ (in the shaded region of Fig. 1) but it also destroys the universality of the leading *bulk* critical behavior of the order-parameter correlation function G_b (and of other bulk correlation functions): G_b attains an interaction-dependent power-law structure [14,16] in the large-distance regime at $T\neq T_c$ (in the shaded region of Fig. 2) whereas systems with purely short-range interaction in the same universality class have an *exponentially* decaying G_b in this regime (this decay has, in addition, a nonuniversal exponential tail; see Sec. X).

The expression for $A_{\alpha\beta}$ and $B_{\alpha\beta\gamma\delta}$ in terms of the microscopic couplings $K_{i,j}$ is given by the second moments [13]

$$A_{\alpha\beta} = A_{\beta\alpha} = N^{-1}\sum_{i,j=1}^{N} (x_{i\alpha}-x_{j\alpha})(x_{i\beta}-x_{j\beta})K_{i,j} \quad (2.10)$$

and the fourth-order moments of $K_{i,j}$, respectively. They have been classified and studied in the context of the bulk correlation function in Ref. [71]. The symmetric matrix $\mathbf{A}$ depends only on the lattice structure and on the pair interactions $K_{i,j}$ and is independent of the boundary conditions and the geometry of the system. Its eigenvalues $\lambda_\alpha, \alpha=1,2,\ldots,d$, and eigenvectors $\mathbf{e}^{(\alpha)}$ are determined by the eigenvalue equation $\mathbf{A}\mathbf{e}^{(\alpha)}=\lambda_\alpha\mathbf{e}^{(\alpha)}$ with $\mathbf{e}^{(\alpha)}\cdot\mathbf{e}^{(\beta)}=\delta_{\alpha\beta}$. In order to have an ordinary critical point of the usual (d,n) universality classes, we assume positive eigenvalues λ_α, $\det\mathbf{A}=\Pi_{\alpha=1}^{d}\lambda_\alpha>0$, and that the fourth-order moments $B_{\alpha\beta\gamma\delta}$ enter only the corrections to scaling. The critical point occurs at $h=0$ and at $T=T_c$ corresponding to some critical value $r_0(T_c)=r_{0c}$ that is defined implicitly by $\lim_{t\to0+}\chi_b(t,0)^{-1}=0$, where $\chi_b(t,h)=-\lim_{L\to\infty}\partial^2 f(t,h,L)/\partial h^2$ is the bulk susceptibility for $t>0$. This implies that $r_0(T_c)=r_{0c}(K_{i,j},v,u_0)$ depends on the lattice structure, on v, on u_0, and on all couplings $K_{i,j}$.

The matrix $\mathbf{A}$ affects the observable bulk critical behavior: the eigenvalues λ_α enter the amplitudes of the bulk correlation lengths $\xi^{(\alpha)}$ in the direction of the *principal axes*; the latter are determined by the eigenvectors $\mathbf{e}^{(\alpha)}$ of $\mathbf{A}$, which provide the reference axes for the spatial dependence of the anisotropic bulk order-parameter correlation function

$$G_b(\mathbf{x_i}-\mathbf{x_j};t,h) = \lim_{V\to\infty}\{\langle\varphi_i\varphi_j\rangle - \langle\varphi\rangle^2\}, \quad (2.11)$$

where $\langle\varphi\rangle(t,h,L)=-\partial f(t,h,L)/\partial h$. Correspondingly, the matrix $\mathbf{A}$ determines the anisotropy of the $\mathbf{k}$ dependence of the Fourier transform

$$\hat{G}_b(\mathbf{k};t,h) = v\sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}}G_b(\mathbf{x};t,h), \quad (2.12)$$

which is proportional to the observable scattering intensity. The *principal* axes must be distinguished from the *symmetry* axes of the Bravais lattice. The latter depend only on the lattice points $\mathbf{x}_i$ but not on the couplings $K_{i,j}$. Below, an example is given where the principal axes differ from the symmetry axes.

The long-wavelength approximation takes into account only the leading $O(k_\alpha k_\beta)$ term of $\delta\hat{K}(\mathbf{k})$. In real space, this is equivalent to using the φ^4 continuum Hamiltonian for the vector field $\varphi(\mathbf{x})$

$$H_{\text{field}} = \int_V d^d x\left[\frac{r_0}{2}\varphi^2 + \sum_{\alpha,\beta=1}^{d}\frac{A_{\alpha\beta}}{2}\frac{\partial\varphi}{\partial x_\alpha}\frac{\partial\varphi}{\partial x_\beta} + u_0(\varphi^2)^2 - h\varphi\right] \quad (2.13)$$

with some cutoff Λ.

Various types of anisotropies may result not only from pair interactions on rectangular lattice structures but also from nonrectangular lattice structures, from effective many-body interactions, as well as from distortions of the lattice structure, e.g., due to external shear forces. The semimacroscopic continuum model (2.13) is expected to be of general significance in that it provides a complete long-wavelength description of a large class of real systems near criticality whose nonuniversal properties can be condensed into the $d(d+1)/2$ parameters of the anisotropy matrix $\mathbf{A}$, in addition to the nonuniversal parameters r_0, u_0, h, Λ. The quantities $A_{\alpha\beta}$ depend on all microscopic details (lattice structure, electronic structure, many-body interactions), which, in general,

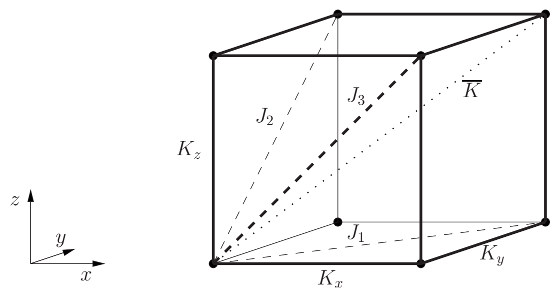

FIG. 3. Lattice points $\mathbf{x}_j$ of the primitive cell (cube) of the anisotropic simple-cubic lattice model (2.1) and (2.7) with $\bar{\mathbf{A}} \neq \mathbf{1}$. Solid, dashed, and dotted lines indicate the NN couplings K_α, the NNN couplings J_i, and the third-NN coupling $\bar{K}$.

are not known *a priori* for a given material. Thus the matrix elements $A_{\alpha\beta}$ represent phenomenological parameters of a truly nonuniversal character. Consequently, physical quantities depending on $A_{\alpha\beta}$ [such as $\mathcal{F}_{\text{cube}}(0,0;\bar{\mathbf{A}})$, the Binder cumulant $U_{\text{cube}}(\bar{\mathbf{A}})$, and the critical Casimir amplitude] are nonuniversal as well.

For an appropriate formulation of the bulk order-parameter correlation function (see Sec. III) and of finite-size scaling functions (see Sec. VI), it will be important to employ the reduced anisotropy matrix $\bar{\mathbf{A}}=\mathbf{A}/(\det \mathbf{A})^{1/d}$, $\bar{\mathbf{A}}\mathbf{e}^{(\alpha)}=\bar{\lambda}_\alpha \mathbf{e}^{(\alpha)}$ with the eigenvalues $\bar{\lambda}_\alpha=\lambda_\alpha/(\det \mathbf{A})^{1/d}>0$ and with $\det \bar{\mathbf{A}}=\prod_{\alpha=1}^{d}\bar{\lambda}_\alpha=1$. The matrix $\bar{\mathbf{A}}$ is independent of the kind of variables φ_i on the lattice points and independent of the number n of components of φ_i. It is well defined,e.g., also for models with fixed-length spin variables $\mathbf{S_i}$ with $|\mathbf{S_i}|=1$ and for Ising models with discrete spin variables $\sigma_i=\pm 1$ instead of the continuous vector variables φ_i. Thus the *XY* and Ising Hamiltonians $H_{XY}=-\Sigma_{i,j}J_{i,j}\mathbf{S_i}\cdot\mathbf{S_j}$ and $H_{\text{Ising}}=-\Sigma_{i,j}J_{i,j}\sigma_i\sigma_j$ have the same reduced anisotropy matrix $\bar{\mathbf{A}}$ and the same reduced eigenvalues $\bar{\lambda}_\alpha$ as the φ^4 lattice Hamiltonian if these models are defined on the same lattice points $\mathbf{x}_i$ and if the couplings $J_{i,j}$ are proportional to $K_{i,j}$.

As an illustration, we consider an $L\times L\times L$ simple-cubic lattice model (Fig. 3) with a lattice constant $\tilde{a}$ and with the following couplings: nearest-neighbor (NN) couplings K_x,K_y,K_z along the cubic symmetry axes, next-nearest-neighbor (NNN) couplings J_1,J_2,J_3 only in the $\pm(1,1,0)$, $\pm(0,1,1)$, $\pm(1,0,1)$ directions [but not in the $\pm(-1,1,0),\pm(0,-1,1),\pm(-1,0,1)$ directions], and a third-NN coupling $\bar{K}$ only in the diagonal $\pm(1,1,1)$ direction (Fig. 3). The corresponding anisotropy matrix is obtained from Eq. (2.10) as

$$\mathbf{A} = 2\tilde{a}^2\begin{pmatrix} D_x & J_1+\bar{K} & J_3+\bar{K} \\ J_1+\bar{K} & D_y & J_2+\bar{K} \\ J_3+\bar{K} & J_2+\bar{K} & D_z \end{pmatrix}, \tag{2.14}$$

with the diagonal elements $D_x=K_x+J_1+J_3+\bar{K}$, $D_y=K_y+J_2+J_1+\bar{K}$, and $D_z=K_z+J_3+J_2+\bar{K}$. For quantitative analytical and numerical studies, this model with seven different couplings would, of course, be much too complicated. We shall present explicit quantitative results only for two nontrivial cases:

(i) Model with *three-dimensional anisotropy*: isotropic ferromagnetic NN couplings $K_x=K_y=K_z\equiv K>0$ and three equal anisotropic NNN couplings $J_1=J_2=J_3\equiv J$. MC simulations for three-dimensional Ising models with this type of anisotropy (with $\bar{K}=0$) have been performed by Schulte and Drope [42] and by Sumour *et al.* [43]. The corresponding reduced anisotropy matrix (with $\bar{K}\neq 0$) is

$$\bar{\mathbf{A}} = (1-3w^2+2w^3)^{-1/3}\begin{pmatrix} 1 & w & w \\ w & 1 & w \\ w & w & 1 \end{pmatrix}, \tag{2.15}$$

which depends only on the single anisotropy parameter

$$w = \frac{J+\bar{K}}{K+2J+\bar{K}}. \tag{2.16}$$

The eigenvalues of $\mathbf{A}$ and $\bar{\mathbf{A}}$ are $\lambda_1=2\tilde{a}^2(K+4J+3\bar{K})$, $\lambda_2=\lambda_3=2\tilde{a}^2(K+J)$ and $\bar{\lambda}_1=(1-3w^2+2w^3)^{-1/3}(1+2w)$, $\bar{\lambda}_2=\bar{\lambda}_3=(1-3w^2+2w^3)^{-1/3}(1-w)$, respectively. The eigenvectors

$$\mathbf{e}^{(1)}=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}, \quad \mathbf{e}^{(2)}=\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\end{pmatrix}, \quad \mathbf{e}^{(3)}=\frac{1}{\sqrt{6}}\begin{pmatrix}1\\1\\-2\end{pmatrix} \tag{2.17}$$

defining the principal axes are not parallel to the cubic symmetry axes. The possible range of w consistent with $\det \bar{\mathbf{A}}(w)>0$ is $-\frac{1}{2}<w<1$. In the limit $K\to 0, J\to 0$ at fixed $\bar{K}\neq 0$ corresponding to $w\to 1$, the model describes a system of variables φ_i on decoupled one-dimensional chains with NN interactions $\bar{K}$. In the previous version [12] of this model with $\bar{K}=0$, the range of w was restricted to $-\frac{1}{2}<w\leq\frac{1}{2}$. A vanishing of λ_2 andλ_3 occurs for $J\to -K$. At some value $w=w_{\text{LP}}$ near $-\frac{1}{2}$ (corresponding to $\lambda_1=0$), our model is predicted to have a Lifshitz point with a wave-vector instability in the direction of $\mathbf{e}^{(1)}$, i.e., in the $(1,1,1)$ direction (see also Sec. VIII E).

(ii) Model with *two-dimensional anisotropy*: An anisotropic NNN coupling $J_1\equiv J$ is taken into account only in the *x-y* planes of the three-dimensional sc lattice, whereas all other anisotropic couplings J_2,J_3 and $\bar{K}$ vanish. This model is of interest for comparison with the MC data by Selke and Shchur [44] for the *two-dimensional* anisotropic Ising model as will be discussed in Sec. VIII. For further recent studies of the anisotropic two-dimensional Ising model, see also [72].

The bulk critical behavior of both models (i) and (ii) belongs to the same $d=3$ universality class as that of the isotropic model with $K_x=K_y=K_z=K>0$ and $J_1=J_2=J_3=\bar{K}=0$ provided that $\lambda_\alpha>0, \alpha=1,2,3$.

B. Rotation and rescaling: Shear transformation

In order to derive an appropriate representation of the anisotropic bulk order-parameter correlation function (see

Sec. III), to develop an appropriate formulation of finite-size perturbation theory (see Sec. IV), and to treat the anisotropic Hamiltonian H by RG theory (see Sec. V), it is necessary to first transform H such that the $O(k_\alpha k_\beta)$ terms of $\delta\hat{K}(\mathbf{k})$ attain an isotropic form. This is a shear transformation that consists of a rotation and rescaling of lengths in the direction of the principal axes [13]. The rotation is provided by the orthogonal matrix $\mathbf{U}$ with matrix elements $U_{\alpha\beta}=e_\beta^{(\alpha)}$, $(\mathbf{U}^{-1})_{\alpha\beta}=e_\alpha^{(\beta)}$, where $e_\beta^{(\alpha)}$ denote the Cartesian components of the eigenvectors $\mathbf{e}^{(\alpha)}$. The rescaling is provided by the diagonal matrix $\boldsymbol{\lambda}=\mathbf{U}\mathbf{A}\mathbf{U}^{-1}$ with diagonal elements $\lambda_\alpha>0$. In $\mathbf{k}$ space, the transformation is $\mathbf{k}'=\boldsymbol{\lambda}^{1/2}\mathbf{U}\mathbf{k}$ such that the $O(k'_\alpha k'_\beta)$ term of $\delta\hat{K}$ is brought into an isotropic form with $\mathbf{A}'=\mathbf{1}$,

$$\delta\hat{K}(\mathbf{k}) = \delta\hat{K}(\mathbf{U}^{-1}\boldsymbol{\lambda}^{-1/2}\mathbf{k}') \equiv \delta\hat{K}'(\mathbf{k}') = \sum_{\alpha=1}^{d} k_\alpha'^2 + O(k'^4). \tag{2.18}$$

In real space, the transformed lattice points are $\mathbf{x}'_\mathbf{j}=\boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x}_\mathbf{j}$. This transformation leaves the scalar product $\mathbf{k}'\cdot\mathbf{x}'_\mathbf{j}=\mathbf{k}\cdot\mathbf{x}_\mathbf{j}$ invariant. Thereby the volume of the primitive cells is changed to $v'=(\det\mathbf{A})^{-1/2}v$. Correspondingly, the total volume of the transformed system is $V'=Nv'=(\det\mathbf{A})^{-1/2}V$ with the characteristic length $L'=V'^{1/d}$.

Our transformation is defined such that the values of the couplings $K_{i,j}$ on the transformed lattice as well as the temperature variable $r_0(T)$ including the values of r_{0c}, a_0, and t are invariant [see also Eq. (4.32) below]. This requires us to perform the additional transformations $\varphi'_j=(\det\mathbf{A})^{1/4}\varphi_j, u'_0=(\det\mathbf{A})^{-1/2}u_0$, and

$$h' = (\det\mathbf{A})^{1/4}h. \tag{2.19}$$

In terms of the Fourier transform $\hat{\varphi}'(\mathbf{k}')=v'\sum_{j=1}^{N}e^{-i\mathbf{k}'\cdot\mathbf{x}'_j}\varphi'_j$, the transformed lattice Hamiltonian reads

$$H' = V'^{-1}\sum_{\mathbf{k}'}\frac{1}{2}[r_0+\delta\hat{K}'(\mathbf{k}')]\hat{\varphi}'(\mathbf{k}')\hat{\varphi}'(-\mathbf{k}') + u'_0V'^{-3} \times \sum_{\mathbf{k}'\mathbf{p}'\mathbf{q}'}[\hat{\varphi}'(\mathbf{k}')\hat{\varphi}'(\mathbf{p}')][\hat{\varphi}'(\mathbf{q}')\hat{\varphi}'(-\mathbf{k}'-\mathbf{p}'-\mathbf{q}')] - h'\hat{\varphi}'(\mathbf{0}). \tag{2.20}$$

We illustrate this transformation by the example of the simple-cubic lattice model shown in Fig. 3. The primitive cell with the volume $v'=(\det\mathbf{A})^{-1/2}\tilde{a}^3$ of the transformed system is shown in Fig. 4. It has the shape of a parallelepiped whose lengths and angles are determined such that the transformed second-moment matrix $\mathbf{A}'=\mathbf{1}$ is the unity matrix although there are still the *same* NN couplings K_α, NNN couplings J_i, and third-NN coupling $\bar{K}$ as in the simple-cubic lattice model of Fig. 3.

Working with H' rather than H will be of advantage in the context of *bulk* properties and bulk renormalizations in Sec. V. This is not the case for the confined system. Although the $O(\mathbf{k}'^2)$ term of $\delta\hat{K}'(\mathbf{k}')$ in Eqs. (2.18) and (2.20) looks quite simple, namely $\mathbf{k}'\cdot\mathbf{k}'$ with a trivial anisotropy matrix $\mathbf{A}'=\mathbf{1}$, the summations $\Sigma_{\mathbf{k}'}$ are nontrivial.

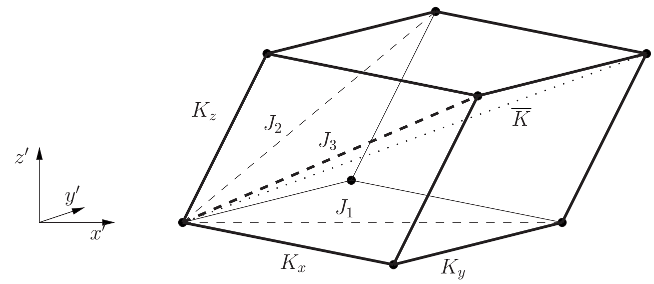

FIG. 4. Lattice points $\mathbf{x}'_j$ of the primitive cell (parallelepiped) of the transformed lattice model (2.20) and (2.23) with the volume $v'=(\lambda_1\lambda_2\lambda_3)^{-1/2}\tilde{a}^3$. Solid, dashed, and dotted lines indicate the NN couplings K_α, the NNN couplings J_i, and the third-NN coupling $\bar{K}$. The couplings are the same as in Fig. 3 but $\mathbf{A}'=\mathbf{1}$ (compare Figs. 1 and 2 of [13]).

For concreteness, consider the simplified example (i) with the matrix (2.15) and the eigenvectors (2.17). While the $\mathbf{k}$ vectors of the sc lattice have the simple form

$$\mathbf{k} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = \frac{2\pi}{L}\begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix} \tag{2.21}$$

with the integer numbers $m_i=0,\pm1,\pm2,\ldots$, the $\mathbf{k}'$ vectors are considerably more complicated,

$$\mathbf{k}' = \begin{pmatrix} k'_1 \\ k'_2 \\ k'_3 \end{pmatrix} = \frac{2\pi}{L\sqrt{6}}\begin{pmatrix} (m_1+m_2+m_3)\sqrt{2\lambda_1} \\ (m_2-m_1)\sqrt{3\lambda_2} \\ (m_1+m_2-2m_3)\sqrt{\lambda_3} \end{pmatrix}. \tag{2.22}$$

These $\mathbf{k}'$ vectors reflect the shape and lattice structure of the transformed system. Thus the price paid for transforming $\mathbf{A}\neq\mathbf{1}$ to $\mathbf{A}'=\mathbf{1}$ is to work with more complicated $\mathbf{k}'$ vectors. This example demonstrates that the effect of anisotropy cannot be eliminated for *confined* systems. In our applications, the summations in finite-size perturbation theory will be performed in the simpler $\mathbf{k}$ space whereas *bulk* integrals (with infinite cutoff) are simplified in $\mathbf{k}'$ space.

In real space, the Hamiltonian H' reads

$$H' = v'\left[\sum_{i=1}^{N}\left(\frac{r_0}{2}\varphi_i'^2 + u'_0(\varphi_i'^2)^2 - h'\varphi'_i\right) + \sum_{i,j=1}^{N}\frac{K_{i,j}}{2}(\varphi'_i-\varphi'_j)^2\right]. \tag{2.23}$$

By substituting the transformations defined above, one easily verifies

$$H(r_0,h,u_0,K_{i,j},v,L) = H'(r_0,h',u'_0,K_{i,j},v',L'). \tag{2.24}$$

The measure for the temperature distance from criticality $r_0-r_{0c}=a_0t$ is the same for both H and H'. Defining the free-energy density f' (divided by k_BT) as

$$f'(t,h',L') = -V'^{-1}\ln Z'(t,h',L'), \tag{2.25}$$

$$Z'(t,h',L') = \left[\prod_{j=1}^{N} \frac{\int d^n \varphi_j'}{(v')^{n(2-d)/(2d)}} \right] \exp(-H'), \quad (2.26)$$

one obtains the exact relations

$$Z(t,h,L) = (\det \mathbf{A})^{-nN/(2d)} Z'(t,h',L'), \quad (2.27)$$

$$f(t,h,L) = (\det \mathbf{A})^{-1/2} f'(t,h',L') + [n/(2dv)] \ln(\det \mathbf{A}). \quad (2.28)$$

The last term is a bulk contribution, i.e., independent of L. Furthermore, it is independent of t, i.e., a nonsingular bulk contribution, thus the singular bulk parts of $f_b(t,h) = f(t,h,\infty)$ and of $f_b'(t,h') = f'(t,h',\infty)$ as well as the total singular parts of $f(t,h,L)$ and of $f'(t,h',L')$ are related by

$$f_{s,b}(t,h) = (\det \mathbf{A})^{-1/2} f_{s,b}'(t,h'), \quad (2.29)$$

$$f_s(t,h,L) = (\det \mathbf{A})^{-1/2} f_s'(t,h',L'). \quad (2.30)$$

The bulk correlation function of the transformed system is

$$G_b'(\mathbf{x}_i' - \mathbf{x}_j'; t,h') = \lim_{V' \to \infty} \{ \langle \varphi_i' \varphi_j' \rangle' - (\langle \varphi' \rangle')^2 \}, \quad (2.31)$$

where $\langle \cdots \rangle'$ denotes the average with the weight $\sim \exp(-H')$. It is related to G_b by

$$G_b(\mathbf{x};t,h) = (\det \mathbf{A})^{-1/2} G_b'(\boldsymbol{\lambda}^{-1/2} \mathbf{U}\mathbf{x}; t, (\det \mathbf{A})^{1/4} h). \quad (2.32)$$

The corresponding relation between the Fourier transforms is

$$\hat{G}_b(\mathbf{k};t,h) = \hat{G}_b'(\boldsymbol{\lambda}^{1/2} \mathbf{U}\mathbf{k}; t, (\det \mathbf{A})^{1/4} h). \quad (2.33)$$

[In the arguments of Eqs. (2.27)–(2.33), we have, for simplicity, not indicated explicitly the additional transformations of $u_0 = (\det \mathbf{A})^{1/2} u_0'$ and of $v' = (\det \mathbf{A})^{-1/2} v$.] In terms of the transformed field $\varphi'(\mathbf{x}') = (\det \mathbf{A})^{1/4} \varphi(\mathbf{U}^{-1} \boldsymbol{\lambda}^{1/2} \mathbf{x}')$, the Hamiltonian (2.13) attains the form of the standard isotropic Landau-Ginzburg-Wilson Hamiltonian,

$$H_{\text{field}} = H_{\text{field}}' = \int_{V'} d^d x' \left(\frac{r_0}{2} \varphi'(\mathbf{x}')^2 + \frac{1}{2} (\nabla' \varphi')^2 + u_0' (\varphi'^2)^2 - h' \varphi' \right), \quad (2.34)$$

where $\nabla' \varphi' \equiv (\partial \varphi' / \partial x_1', \ldots, \partial \varphi' / \partial x_d')$ with a transformed cutoff.

III. BULK CRITICAL BEHAVIOR OF ANISOTROPIC SYSTEMS

Before turning to finite-size theory of anisotropic systems, it is necessary to first discuss the bulk critical behavior of anisotropic systems and its relation to that of isotropic systems. We are not aware of such a discussion in the literature. It is well known that anisotropic systems and isotropic systems have the same critical exponents (in a limited range of the anisotropy; see, e.g., [73], and references therein). Within the φ^4 theory this is immediately seen from the relation of dimensionally regularized bulk integrals (at infinite cutoff) such as

$$u_0 \int_{\mathbf{k}}^{\infty} (r_0 + \mathbf{k} \cdot \mathbf{A}\mathbf{k})^{-1} = u_0' \int_{\mathbf{k}'}^{\infty} (r_0 + \mathbf{k}' \cdot \mathbf{k}')^{-1} = -\frac{A_d}{\varepsilon} r_0^{(d-2)/2} u_0', \quad (3.1)$$

$$\int_{\mathbf{k}'}^{\infty} = (\det \mathbf{A})^{1/2} \int_{\mathbf{k}}^{\infty} \equiv (\det \mathbf{A})^{1/2} \prod_{\alpha=1}^{d} \int_{-\infty}^{\infty} \frac{dk_\alpha}{2\pi}, \quad (3.2)$$

provided that $\det \mathbf{A} > 0$. We see that the $\mathbf{A}$ dependence is completely absorbed by the coupling u_0' and that the $d=4$ pole term $\sim \varepsilon^{-1}$ does not depend on the matrix $\mathbf{A}$. This leads to identical field-theoretic functions for anisotropic and isotropic systems (as functions of the renormalized couplings u' and u, respectively) and yields the same critical exponents and fixed-point value $u'^* = u^*$ for anisotropic and isotropic systems (see Sec. V). (The $d=2$ pole of the integral (3.1), which has nothing to do with the critical behavior in $d>2$ dimensions, can be incorporated in the geometric factor A_d [62], which is finite in $2<d\leq 4$ dimensions [see Eq. (5.2) below].)

For this reason, not much attention has been paid to the role played by anisotropy in bulk critical phenomena. This is not justified, however, in the context of the important feature of two-scale factor universality [3,8]. Its validity has been established by the RG theory only for *isotropic* systems at $h=0$ with short-range interactions [27–30]. A brief derivation was also given by Privman and Fisher [5] and by Privman *et al.* [8] using scaling assumptions at $h \neq 0$. Their ansatz for the order-parameter correlation function, however, is not valid for anisotropic systems since they assumed the existence of a *single* bulk correlation length ξ_∞. Recently it was pointed out that two-scale factor universality is absent in anisotropic systems [12] and that anisotropy has an effect on several universal bulk amplitude combinations [13] but no derivation was given. In particular, two important universal amplitude relations derived by Privman and Fisher [5] [Eqs. (3.10) and (3.11) below] have not been discussed in the context of anisotropic systems. Furthermore, the bulk order-parameter correlation function of anisotropic systems was discussed only for $h=0$ and $T \geq T_c$ [12]. Here we extend this discussion to $h \neq 0$ and $T < T_c$ and provide an appropriate formulation of the order-parameter correlation function and of the scattering intensity in terms of both the eigenvalues λ_α and the reduced eigenvalues $\bar{\lambda}_\alpha$ of the anisotropic system. We also present the derivation of several amplitude combinations for anisotropic systems in terms of universal scaling functions.

All of the *thermodynamic* bulk relations given in Secs. III A and III B remain valid also in the presence of subleading long-range interactions of the type (2.9). This is not the case, however, for bulk correlation functions at $T \neq T_c$, $h=0$ and $h \neq 0$, $T=T_c$ in the large-distance regime corresponding to the shaded region in Fig. 2.

A. Two-scale factor universality in isotropic bulk systems

First we summarize the bulk critical behavior of systems described by the (asymptotically) isotropic lattice Hamiltonian H' and the continuum Hamiltonian $H'_{\rm field}$. Near T_c, the bulk free-energy density can be decomposed uniquely into singular and nonsingular parts as $f'_b(t,h') = f'_{s,b}(t,h') + f'_{{\rm ns},b}(t)$, where $f'_{{\rm ns},b}(t)$ has a regular t dependence. It is well established that $f'_{s,b}$ has the asymptotic (small t, small h') scaling form below $d=4$ dimensions,

$$f'_{s,b}(t,h') = A'_1|t|^{d\nu}W_\pm(A'_2h'|t|^{-\beta\delta}) \tag{3.3}$$

with the universal scaling function $W_\pm(z)$, $\infty \le z \le \infty$. This function is independent of the cutoff procedure of $H'_{\rm field}$. We use the normalization $W_+(0)=1$. The two amplitudes A'_1 and A'_2 are nonuniversal.

Because of isotropy, it is justified to define a *single* (second-moment) bulk correlation length

$$\xi'_\pm(t,h') = \left(\frac{1}{2d} \frac{\sum_{\mathbf{x}'} \mathbf{x}'^2 G'_b(\mathbf{x}';t,h')}{\sum_{\mathbf{x}'} G'_b(\mathbf{x}';t,h')} \right)^{1/2} \tag{3.4}$$

above and below T_c, respectively. In Eq. (3.4), we have assumed sufficiently rapidly decaying correlations, i.e., general n for $T \ge T_c$ but $n=1$ for $T<T_c$. We assume, in the asymptotic region $|\mathbf{x}'| \gg (v')^{1/d}, \xi'_\pm \gg (v')^{1/d}$ and for $|\mathbf{x}'|/\xi'_\pm \lesssim O(1)$ and small h', the asymptotic *isotropic* scaling form

$$G'_b(\mathbf{x}';t,h') = D'_1|\mathbf{x}'|^{-d+2-\eta}\Phi_\pm(|\mathbf{x}'|/\xi'_\pm, D'_2h'|t|^{-\beta\delta}), \tag{3.5}$$

$$\xi'_\pm(t,h') = \xi'_{0+}|t|^{-\nu}X_\pm(D'_2h'|t|^{-\beta\delta}), \tag{3.6}$$

with universal scaling functions $\Phi_\pm(x,y)$ and $X_\pm(y)$. We use the normalization $X_+(0)=1$, thus $\xi'_+(t,0)=\xi'_{0+}t^{-\nu}$ above T_c. The length ξ'_{0+} will be needed as a reference length in the formulation of renormalized finite-size theory in Sec. V. The corresponding scaling form of the Fourier transform $\hat{G}'_b$ of Eq. (3.5) is

$$\hat{G}'_b(\mathbf{k}';t,h') = D'_1|\mathbf{k}'|^{-2+\eta}\hat{\Phi}_\pm(|\mathbf{k}'|\xi'_\pm, D'_2h'|t|^{-\beta\delta}), \tag{3.7}$$

$$\hat{\Phi}_\pm(x',y') = 2\pi^{(d-1)/2}\Gamma[(d-1)/2]^{-1}\int_0^\infty ds\, s^{1-\eta} \times \int_{-1}^{1} d(\cos\vartheta)(\sin\vartheta)^{d-3}e^{-is\cos\vartheta}\Phi_\pm(s/x',y'). \tag{3.8}$$

The three amplitudes D'_1, D'_2, and ξ'_{0+} in Eqs. (3.5)–(3.7) are nonuniversal. The basic content of two-scale factor universality is that all of these amplitudes are universally related to the two thermodynamic amplitudes A'_1 and A'_2. The relations read

$$(\xi'_{0+})^d A'_1 = Q_1(d,n) = \text{universal}, \tag{3.9}$$

$$A'_2/D'_2 = P_2(d,n) = \text{universal}, \tag{3.10}$$

$$D'_1(A'_2)^{-2}(A'_1)^{-1-\gamma/(d\nu)} = P_3(d,n) = \text{universal}. \tag{3.11}$$

In Ref. [5], the universal constants P_2 and P_3 were denoted by Q_2 and Q_3. In order to conform with Refs. [8,74] and to avoid confusion, we reserve the notation Q_2 and Q_3 for the *different* universal constants in Eqs. (3.13) and (3.14) below. For the sake of clarity, we present the explicit expressions for Q_i and P_i in terms of universal scaling functions in Appendix A. An equivalent formulation of Eq. (3.9) is

$$\lim_{t\to 0+}[f'_{s,b}(t,0)\xi'_+(t,0)^d] = Q_1(d,n) = \text{universal}. \tag{3.12}$$

The validity of Eqs. (3.9) and (3.12) has been established by the RG theory [27,30].

Furthermore, the amplitude ratios

$$(\Gamma'_+/\Gamma'_c)(\xi'_c/\xi'_{0+})^{2-\eta} = Q_2(d,n) = \text{universal}, \tag{3.13}$$

$$\hat{D}'_\infty(\xi'_{0+})^{2-\eta}/\Gamma'_+ = Q_3(d,n) = \text{universal} \tag{3.14}$$

have been proposed [74] to be universal. The constants Γ'_+, Γ'_c, and ξ'_c are defined as follows: $\chi'_b(t,0)=\Gamma'_+t^{-\gamma}$ for $t>0$, $\chi'_b(0,h')=\Gamma'_c|h'|^{-\gamma/(\beta\delta)}$, where $\chi'_b(t,h') = -\partial^2 f'_b(t,h')/\partial h'^2$, and $\xi'_\pm(0,h') \equiv \xi'_h = \xi'_c|h'|^{-\nu/(\beta\delta)}$. The length ξ'_h with the amplitude ξ'_c is a natural reference length of finite-size theory at $t=0$, $h'\neq 0$ [see Eq. (6.11) below]. $\hat{D}'_\infty$ is the asymptotic (small-$\mathbf{k}'$) amplitude of $\hat{G}'_b(\mathbf{k}';0,0) \approx \hat{D}'_\infty|\mathbf{k}'|^{-2+\eta}$. Alternatively, Eq. (3.14) can be formulated as $D'_\infty(\xi'_{0+})^{2-\eta}/\Gamma'_+ = \tilde{Q}_3(d,n)$, or, equivalently,

$$\lim_{|\mathbf{x}'|\to\infty}\{G'_b(\mathbf{x}';0,0)(|\mathbf{x}'|/\xi'_{0+})^{d-2+\eta}\}(\xi'_{0+})^d/\Gamma'_+ = \tilde{Q}_3(d,n) = (D'_\infty/\hat{D}'_\infty)Q_3(d,n) = \text{universal}, \tag{3.15}$$

where D'_∞ is the asymptotic (large-$\mathbf{x}'$) amplitude of $G'_b(\mathbf{x}';0,0) \approx D'_\infty|\mathbf{x}'|^{-d+2-\eta}$. The derivation of Eqs. (3.13)–(3.15) is sketched in Appendix A. Again, all of the constants on the left-hand sides of Eqs. (3.13)–(3.15) are universally related to A'_1 and A'_2.

Below T_c at $h'=0$ we have, for $n=1$, $\xi'_- = \xi'_{0-}|t|^{-\nu}$ with the universal ratio

$$\xi'_{0-}/\xi'_{0+} = X_-(0) = \text{universal}. \tag{3.16}$$

Previously the bulk relations (3.9)–(3.16) were expected to be universal for all systems *within a given universality class* [8]. Consistency with the universality of Eqs. (3.13) and (3.14) was found [74] for two-dimensional (square and triangular) Ising lattices and three-dimensional (sc and bcc) Ising lattices with *isotropic* nearest-neighbor interactions (see also [75]). All of these systems, however, belong to the subclass of asymptotically isotropic systems with an anisotropy matrix $\mathbf{A}=c_0\mathbf{1}$ or $\bar{\mathbf{A}}=\mathbf{1}$ and with an isotropic scattering intensity [74]. Also the honeycomb-lattice Ising model considered in [5] belongs to that subclass, with a constant c_0 different from that for the triangular lattice or the square lattice. As will be shown in Sec. III B, Eqs. (3.9) and (3.12)–(3.16) must be reformulated for anisotropic systems with noncubic anisotropy at $O(k_\alpha k_\beta)$, whereas Eqs. (3.10) and (3.11) remain valid also for anisotropic systems provided that A_1', A_2', D_1', and D_2', are transformed appropriately.

It has been shown [9–11,16] that the universal scaling form (3.5), (3.6) is not valid in the regime $r' \equiv |\mathbf{x}'| \gg \xi_+'$ above T_c. The same can be shown for $n=1$ in the regime $r' \gg \xi_-'$ below T_c. Note that this regime is part of the *asymptotic* critical region $r' \gg \tilde{a}$ and $\xi_\pm' \gg \tilde{a}$ corresponding to the shaded area in the r'^{-1} - $\xi_\pm'^{-1}$ plane in Fig. 2. In this regime, corrections to scaling in the sense of Wegner [19]are still negligible. One must distinguish at least four cases. (i) For the φ^4 lattice model with short-range interactions, the exponential decay above T_c depends explicitly on the lattice spacing $\tilde{a}$ via the *exponential correlation length* $\xi_{\mathbf{e}}$ [11,92]; in Sec. X, we shall show that it also depends on the bare four-point coupling u_0. (ii) For the φ^4 continuum theory with a *smooth* cutoff Λ, the exponential decay depends explicitly on Λ via $\xi_{\mathbf{e}}(\Lambda)$ [9,10] (see also Sec. X). (iii) For the φ^4 continuum theory with a *sharp* cutoff Λ, a nonuniversal oscillatory power-law decay dominates the exponential decay [11,99]. (iv) In the presence of subleading long-range interactions of the type (2.9), the power law $\sim b|\mathbf{x}'|^{-d-\sigma}$[14,16] dominates the exponential short-range behavior. For $T>T_c$, this has been shown explicitly for the mean spherical model where the asymptotic structure for $|\mathbf{x}'|/\xi_+ \gg 1$ at $h=0$ is [16]

$$G_b'(\mathbf{x}';t,0) = \frac{D_1'}{|\mathbf{x}'|^{d-2}}\left[\Phi_+\left(\frac{|\mathbf{x}'|}{\xi_+}\right) + \frac{b}{|\mathbf{x}'|^{\sigma-2}}\mathcal{D}\left(\frac{|\mathbf{x}'|}{\xi_+}\right)\right] \tag{3.17}$$

with $\mathcal{D}(|\mathbf{x}'|/\xi_+) \sim (|\mathbf{x}'|/\xi_+)^{-4}$. In cases (i)–(iv), scaling in the sense of Eqs. (3.5) and (3.6) and two-scale factor universality are violated in the regime $|\mathbf{x}'| \gg \xi_\pm'$ (shaded area in Fig. 2) because, in addition to the reference length ξ_{0+}', the nonuniversal lengths $\tilde{a}$, $u_0^{-1/\varepsilon}$, Λ^{-1}, and $b^{1/(\sigma-2)}$ govern the leading large $|\mathbf{x}'|$ behavior.

B. Absence of two-scale factor universality in anisotropic bulk systems

Now we turn to the anisotropic system. According to Eqs. (2.19), (2.29), and (3.3), the asymptotic scaling form of $f_{s,b}$ is given by Eq. (1.1) with the nonuniversal amplitudes

$$A_1 = A_1'(\det \mathbf{A})^{-1/2}, \quad A_2 = A_2'(\det \mathbf{A})^{1/4}. \tag{3.18}$$

In order to represent the order-parameter correlation function (2.11) in an appropriate asymptotic scaling form, it is necessary to employ both of the diagonal matrices $\boldsymbol{\lambda}$ and $\bar{\boldsymbol{\lambda}}$ with diagonal elements λ_α and $\bar{\lambda}_\alpha$. Using Eqs. (2.32), (2.33), (3.5), and (3.7), we write G_b and $\hat{G}_b$ as

$$G_b(\mathbf{x};t,h) = D_1|\bar{\boldsymbol{\lambda}}^{-1/2}\mathbf{U}\mathbf{x}|^{-d+2-\eta} \times \Phi_\pm(|\boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x}|/\xi_\pm, D_2 h|t|^{-\beta\delta}), \tag{3.19}$$

$$\hat{G}_b(\mathbf{k};t,h) = D_1|\bar{\lambda}^{1/2}\mathbf{U}\mathbf{k}|^{-2+\eta}\hat{\Phi}_\pm(|\boldsymbol{\lambda}^{1/2}\mathbf{U}\mathbf{k}|\xi_\pm, D_2 h|t|^{-\beta\delta}) \tag{3.20}$$

with the nonuniversal amplitudes

$$D_1 = D_1'(\det \mathbf{A})^{(-2+\eta)/(2d)}, \tag{3.21}$$

$$D_2 = D_2'(\det \mathbf{A})^{1/4}. \tag{3.22}$$

Here we identify the spatial variable r' in the scaling argument of $\Phi_\pm(r'/\xi_\pm', 0)$ used in Fig. 2 as

$$r' \equiv |\mathbf{x}'| = |\boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x}|, \tag{3.23}$$

which, for given $\mathbf{x}$, depends on all of the $d(d+1)/2$ parameters contained in $\mathbf{A}$.

While the simple transformations (3.18) and (3.22) follow immediately from the transformations of h, φ_i, and V, the transformation of D_1 is less trivial. Using Eqs. (3.18), (3.21), and (3.22), we find that the universal amplitude relations (3.10) and (3.11) of isotropic systems remain valid also for anisotropic systems,

$$A_2/D_2 = P_2(d,n) = \text{universal}, \tag{3.24}$$

$$D_1 A_2^{-2} A_1^{-1-\gamma/(d\nu)} = P_3(d,n) = \text{universal} \tag{3.25}$$

with the same universal constants P_2 and P_3 as in Eqs. (3.10) and (3.11). Equation (3.19) differs from the representation of G_b of [12] at $h=0$ where, instead of D_1, an overall amplitude $A_G' = D_1'(\det \mathbf{A})^{-1/2}$ was employed. The latter representation is inappropriate as A_G' is not universally related to A_1 and A_2. The relations (3.10) and (3.24) follow from the sum rule (see Appendix A)

$$\begin{aligned}\chi_b'(t,h') &= -\partial^2 f_b'(t,h')/\partial h'^2 \\ &= v'\sum_{\mathbf{x}'} G_b'(\mathbf{x}';t,h') = \chi_b(t,h) = -\partial^2 f_b(t,h)/\partial h^2 \\ &= v\sum_{\mathbf{x}} G_b(\mathbf{x};t,h).\end{aligned} \tag{3.26}$$

Less obvious are the relations (3.11) and (3.25). Their derivation is, in fact, based on an additional assumption about the *unsubtracted* order-parameter correlation function (see Appendix A). The physical significance of Eq. (3.25) is that, at criticality, the bulk correlation function and its Fourier transform, if expressed in terms of $\boldsymbol{\lambda}$,

$$G_b(\mathbf{x};0,0) = D_1\Phi_\pm(0,0)|\boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x}|^{-d+2-\eta}, \tag{3.27}$$

$$\hat{G}_b(\mathbf{k};0,0) = D_1\hat{\Phi}_\pm(0,0)|\boldsymbol{\lambda}^{1/2}\mathbf{U}\mathbf{k}|^{-2+\eta}, \tag{3.28}$$

have an overall amplitude D_1 that is universally determined by the *thermodynamic* amplitudes A_1 and A_2 of the bulk free energy $f_{s,b}$. Unlike in isotropic systems, however, the spatial dependence of G_b and the $\mathbf{k}$ dependence of $\hat{G}_b$ at criticality are governed by the d reduced nonuniversal eigenvalues $\bar{\lambda}_\alpha$ (with $d-1$ independent parameters). In addition, knowledge of $d(d-1)/2$ nonuniversal parameter is needed in order to specify the orthogonal matrix $\mathbf{U}$, i.e., to specify the directions $\mathbf{e}^{(\alpha)}$ of the principal axes relative to the symmetry axes of the system. Thus $1+(d-1)+d(d-1)/2 = d(d+1)/2$ nonuniversal parameters are needed at $T=T_c$ and $h=0$, and $d(d+1)/2+1$ nonuniversal parameters at finite h. These parameters can be measured by elastic-scattering experiments at bulk criticality of anisotropic solids.

Now we discuss the temperature and h dependence of G_b away from criticality. Along the direction $\mathbf{e}^{(\alpha)}$ of the principal axis α, the spatial dependence of Eq. (3.19) is, for $|\tilde{x}^{(\alpha)}|/\xi_\pm^{(\alpha)} \lesssim O(1)$,

$$G_b(\tilde{\mathbf{x}}^{(\alpha)};t,h) = D_1(|\tilde{x}^{(\alpha)}|/\lambda_\alpha^{1/2})^{-d+2-\eta}\Phi_\pm(|\tilde{x}^{(\alpha)}|/\xi_\pm^{(\alpha)}, D_2 h|t|^{-\beta\delta}) \tag{3.29}$$

with $\tilde{\mathbf{x}}^{(\alpha)} = \tilde{x}^{(\alpha)}\mathbf{e}^{(\alpha)}$ and, because of Eqs. (2.19) and (3.6),

$$\xi_\pm^{(\alpha)}(t,h) = \lambda_\alpha^{1/2}\xi'_\pm(t,(\det \mathbf{A})^{1/4}h) = \xi_{0+}^{(\alpha)}|t|^{-\nu}X_\pm(D_2 h|t|^{-\beta\delta}). \tag{3.30}$$

Thus along the different principal axes [see Fig. 1(b) of Ref. [13]] there exist d different principal correlation lengths $\xi_\pm^{(\alpha)}(t,h)$, which constitute d different nonuniversal reference lengths with d nonuniversal amplitudes $\xi_{0+}^{(\alpha)} = \lambda_\alpha^{1/2}\xi'_{0+}$. Their ratios

$$\xi_{0+}^{(\alpha)}/\xi_{0+}^{(\beta)} = (\lambda_\alpha/\lambda_\beta)^{1/2} \tag{3.31}$$

are also nonuniversal. Below T_c at $h=0$ we have $\xi_-^{(\alpha)} = \xi_{0-}^{(\alpha)}|t|^{-\nu}$ with the universal ratio for each α

$$\xi_{0-}^{(\alpha)}/\xi_{0+}^{(\alpha)} = X_-(0) = \text{universal}, \tag{3.32}$$

but for $\alpha \neq \beta$ the ratios $\xi_{0-}^{(\alpha)}/\xi_{0-}^{(\beta)} = (\lambda_\alpha/\lambda_\beta)^{1/2}$ and $\xi_{0-}^{(\alpha)}/\xi_{0+}^{(\beta)} = (\lambda_\alpha/\lambda_\beta)^{1/2}X_-(0)$ are nonuniversal. Because of $A'_1 = A_1\prod_{\alpha=1}^d \lambda_\alpha^{1/2}$, Eqs. (3.9) and (3.12) imply

$$A_1\prod_{\alpha=1}^{d}\xi_{0+}^{(\alpha)} = \lim_{t\to 0+}\left[f_{s,b}(t,0)\prod_{\alpha=1}^{d}\xi_+^{(\alpha)}(t,0)\right] = Q_1(d,n) = \text{universal}. \tag{3.33}$$

The susceptibility $\chi_b(t,h)$ with $\chi_b(t,0)=\Gamma_+ t^{-\gamma}$ above T_c and $\chi_b(0,h)=\Gamma_c|h|^{-\gamma/\beta\delta}$ have amplitudes $\Gamma_+=\Gamma'_+$ and $\Gamma_c = \Gamma'_c(\det \mathbf{A})^{-\gamma/(4\beta\delta)}$. Here we have used Eqs. (2.19) and (3.26). From Eq. (3.30), we have $\xi_\pm^{(\alpha)}(0,h)=\xi_c^{(\alpha)}|h|^{-\nu/(\beta\delta)}$ with

$$\xi_c^{(\alpha)} = \lambda_\alpha^{1/2}(\det \mathbf{A})^{-\nu/(4\beta\delta)}\xi'_c. \tag{3.34}$$

Equation (3.13) then implies for each $\alpha = 1,\ldots,d$

$$(\Gamma_+/\Gamma_c)(\xi_c^{(\alpha)}/\xi_{0+}^{(\alpha)})^{2-\eta} = Q_2(d,n) = \text{universal}, \tag{3.35}$$

and from Eqs. (3.15) and (3.29) we obtain for each β

$$\lim_{|\tilde{\mathbf{x}}^{(\beta)}|\to\infty}\left\{G_b(\tilde{\mathbf{x}}^{(\beta)};0,0)\left(\frac{|\tilde{\mathbf{x}}^{(\beta)}|}{\xi_{0+}^{(\beta)}}\right)^{d-2+\eta}\right\}\frac{\prod_{\alpha=1}^{d}\xi_{0+}^{(\alpha)}}{\Gamma_+} = \tilde{Q}_3(d,n) = \text{universal}. \tag{3.36}$$

Q_1, Q_2, and $\tilde{Q}_3 = (D_\infty/\hat{D}_\infty)Q_3$ are the same universal numbers for both isotropic and anisotropic systems within the same (d,n) universality class.

Similar reformulations of universal amplitude relations are necessary for $R_{\sigma\xi}$ and R_ξ^T involving the surface tension, Eq. (2.58) of Ref. [8], and the stiffness constant (superfluid density) $\rho_s = \xi_T^{2-d}$, Eqs. (2.17) and (3.54) of Ref. [8], respectively. Corresponding nonuniversal anisotropy effects must be taken into account in the formulation of universal relations involving correction-to-scaling amplitudes (Wegner [19] amplitudes) as well as of universal *dynamic* bulk amplitude combinations [76] such as $R_\lambda, R_2, \tilde{R}_m^-$, and R_Γ defined in Ref. [8].

For completeness, we briefly mention also those universal bulk amplitude relations that do not involve the correlation length, as listed in Eqs. (2.45)–(2.48), (2.51), and (2.52) of Ref. [8]. It is straightforward to show that, as a consequence of the scaling structure of $f'_{s,b}$, Eq. (3.3), and of the universality of the scaling function $W_\pm(z)$, these relations remain valid also for anisotropic systems, i.e., they are independent of the anisotropy parameters $A_{\alpha\beta}$. Consider, for example, the asymptotic amplitudes $A'_\pm$ and $\Gamma'_\pm$ of the bulk specific heat $C'_b = \partial^2 f'_{b,s}/\partial t^2 = (A'_\pm/\alpha)|t|^{-\alpha}$ and of the bulk susceptibility $\chi'_b = -\partial^2 f'_{s,b}/\partial h'^2 = \Gamma'_\pm|t|^{-\gamma}$ of the isotropic system above and below T_c at $h'=0$, respectively, and, correspondingly, $C_b = \partial^2 f_{b,s}/\partial t^2 = (A_\pm/\alpha)|t|^{-\alpha}$, $\chi_b = -\partial^2 f_{s,b}/\partial h^2 = \Gamma_\pm|t|^{-\gamma}$ of the anisotropic system. (For χ'_b and χ_b below T_c, we consider, for simplicity, only $n=1$.) Their amplitude ratios are given by $A'_+/A'_- = A_+/A_- = W_+(0)/W_-(0)$ and by

$$\frac{\Gamma'_+}{\Gamma'_-} = \frac{\Gamma_+}{\Gamma_-} = \left.\frac{\partial^2 W_+(y)/\partial y^2}{\partial^2 W_-(y)/\partial y^2}\right|_{y=0}. \tag{3.37}$$

Thus the nonuniversal parameters $A_{\alpha\beta}$ drop out completely. Corresponding statements hold for the amplitude combinations denoted by R_χ, R_C, R_A in Ref. [8].

A Monte Carlo (MC) study [42] of the *anisotropic* three-dimensional Ising model appeared to be at variance with the universality of the bulk susceptibility ratio (3.37). Subsequent MC simulations [43] of the same anisotropic model on larger lattices, however, are consistent with the universality of Eq. (3.37).

The analysis of anisotropy effects near criticality can of course be extended also to the scaling form of other bulk correlation functions such as $\langle\varphi'(\mathbf{x}'_i)^2\varphi'(\mathbf{x}'_j)^2\rangle$. It can also be extended to the case of general n below T_c where one must distinguish between longitudinal and transverse correlations. Furthermore, extensions of this analysis should be applied also to critical dynamics [76] and to boundary critical phenomena [77,78].

In conclusion, all critical exponents and bulk scaling functions $W_\pm(z), \Phi_\pm(x',y')$ with $|x'| \lesssim O(1)$, and $X_\pm(y')$ of anisotropic systems are universal, i.e., they are the same as those of isotropic systems in the same universality class. However, as far as the bulk correlation function $G_b(\mathbf{x};t,h)$ is concerned, the knowledge only of the scaling *function* $\Phi_\pm(x',y')$ is empty unless one knows how the *arguments* x',y' of $\Phi_\pm$ are related to observable properties. In particular, right at criticality, the spatial dependence of $G_b(\mathbf{x};0,0)$ is not at all contained in the scaling function but only in the factor $|\boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x}|^{-d+2-\eta}$ [see Eq. (3.27)]. This requires the knowledge of up to $d(d+1)/2+1$ nonuniversal parameters. As far as the universal bulk amplitude relations are concerned, two-scale factor universality (with only *two* independent nonuniversal amplitudes) is valid only for a subset of such relations, namely for those that do not involve the correlation length [such as Eqs. (3.10), (3.11), (3.24), (3.25), and (3.37), and those of Ref. [8] mentioned above]. The other relations [such as Eqs. (3.33), (3.35), and (3.36)] provide universal relations between quantities depending on up to $d(d+1)/2+1$ independent nonuniversal parameters, thus seven parameters in three dimensions. This is the property of *multiparameter universality* referred to in Table I.

Furthermore, for anisotropic systems there exist nonuniversal anisotropy effects of the large-distance regime of $G_b(\mathbf{x};t,h)$ (corresponding to the shaded region in Fig. 2) at $t\neq 0, h=0$ and $h\neq 0, t=0$ in combination with the nonuniversal nonscaling features of the isotropic cases (i)–(iv) mentioned at the end of Sec. III A.

IV. PERTURBATION APPROACH IN THE CENTRAL FINITE-SIZE REGIME

A. General remarks

Consider the transformed Hamiltonian H' with a one-component order parameter at $h'=0$ in a finite geometry with a characteristic length L' in the presence of periodic boundary conditions. It is expected that, for short-range interactions, there exist three different types of finite-size critical behavior of $f'_s(t,L')-f'_{s,b}(t)$, where $f'_{s,b}(t)$ is the singular bulk part: (a) the exponential L' dependence $\sim\exp(-L'/\xi'_{\mathrm{e}+})$ for large $L'/\xi'_{\mathrm{e}+}\gg 1$ at fixed temperature $T>T_c$ with $\xi'_{\mathrm{e}+}$ being the exponential bulk correlation length above T_c; (b) the power-law behavior $\sim L'^{-d}$ for large L' at fixed $L'/\xi'_\pm, 0\leq L'/\xi'_\pm\leq O(1)$, above, at, and below T_c, where $\xi'_\pm$ is the second-moment bulk correlation length (3.4); (c) the exponential L' dependence $\sim\exp(-L'/\xi'_{\mathrm{e}-})$ for large $L'/\xi'_{\mathrm{e}-}\gg 1$ at fixed temperature $T<T_c$ with $\xi'_{\mathrm{e}-}$ being the exponential bulk correlation length below T_c. For a description of cases (a) and (c), ordinary perturbation theory with respect to u'_0 of the isotropic φ^4 theory is sufficient. For case (b), a separation of the lowest mode and a perturbation treatment of the higher modes is necessary [32,64–66].

For anisotropic systems, the distinction between regimes (a), (b), and (c) remains relevant except that there exist no single correlation lengths $\xi_{\mathrm{e}+}$, ξ_+, ξ_-, and $\xi_{\mathrm{e}-}$. In this and the subsequent sections, we treat case (b) on the basis of the lattice Hamiltonian (2.1) for $n=1$, $h=0$ and defer cases (a) and (c) to Sec. X. Case (b) corresponds to the central finite-size region above the dashed lines in Fig. 1. For simplicity, we assume a cubic shape with volume $V=L^d$ and a simple-cubic lattice with lattice constant $\tilde{a}$. Now the summations $\Sigma_{\mathbf{k}}$ run over N discrete vectors $\mathbf{k}\equiv(k_1,k_2,\ldots,k_d)$ with Cartesian components $k_\alpha=2\pi m_\alpha/L, m_\alpha=0,\pm 1,\pm 2,\ldots,\alpha=1,2,\ldots,d$ in the range $-\pi/\tilde{a}\leq k_\alpha<\pi/\tilde{a}$.

The goal is to derive the finite-size scaling form of the singular finite-size part f_s of the free-energy density of the anisotropic system (2.1) for $n=1$ at $h=0$ with an anisotropy matrix $\mathbf{A}$. We shall show that, for small $|t|$ and large L in regime (b), f_s has the scaling form

$$f_s(t,L;\mathbf{A}) = L^{-d}\mathcal{F}(t(L'/\xi'_{0+})^{1/\nu};\bar{\mathbf{A}}), \tag{4.1}$$

where the scaling argument is expressed in terms of the transformed length $L'=(\det\mathbf{A})^{-1/(2d)}L$, rather than in terms of L, and where ξ'_{0+} is the asymptotic amplitude of the bulk correlation length defined in Eq. (3.4) on the basis of the transformed Hamiltonian H'. Because of Eq. (2.30), $\mathcal{F}$ is identical with the finite-size scaling function of the free-energy density of the transformed system,

$$f'_s(t,L';\bar{\mathbf{A}}) = L'^{-d}\mathcal{F}(t(L'/\xi'_{0+})^{1/\nu};\bar{\mathbf{A}}). \tag{4.2}$$

The advantage of the transformed system is that its bulk renormalizations (see Sec. V) are well known from the standard isotropic φ^4 field theory. Thus, in order to derive the scaling function $\mathcal{F}$, it is most appropriate to develop perturbation theory first within the transformed system with the Hamiltonian H', Eqs. (2.20) and (2.23), with $v'=(\det\mathbf{A})^{-1/2}\tilde{a}^d$.

B. Perturbation approach

It is necessary to reformulate and to further improve the field-theoretic perturbation approach of [66] in the context of our anisotropic lattice model in order to correctly identify the total finite-size part of the free-energy density f'_s including all temperature-independent contributions $\propto L'^{-d}$ and to identify the new parts of the theory that are affected by the anisotropy. The decomposition into the lowest mode and higher modes reads $\varphi'_j=\Phi'+\sigma'_j$,

$$\Phi' = L'^{-d}\hat{\varphi}'(\mathbf{0}) = N^{-1}\sum_j \varphi'_j, \tag{4.3}$$

$$\sigma'_j = L'^{-d}\sum_{\mathbf{k}'\neq\mathbf{0}} e^{i\mathbf{k}'\cdot\mathbf{x}'_j}\hat{\varphi}'(\mathbf{k}'), \tag{4.4}$$

where $L'^d=(\det\mathbf{A})^{-1/2}L^d$. Correspondingly, the lattice Hamiltonian H' and the partition function Z', Eq. (2.26), are decomposed as $H'=H'_0+\tilde{H}'(\Phi',\sigma')$,

$$H'_0(r_0,u'_0,L',\Phi'^2) = L'^d\left(\frac{1}{2}r_0\Phi'^2+u'_0\Phi'^4\right), \tag{4.5}$$

$$\tilde{H}'(\Phi',\sigma') = v'\Bigg\{\sum_{j=1}^N\Bigg[\left(\frac{r_0}{2}+6u'_0\Phi'^2\right)\sigma_j'^2+4u'_0\Phi'\sigma_j'^3 + u'_0\sigma_j'^4\Bigg]+\sum_{i,j=1}^N\frac{K_{i,j}}{2}(\sigma'_i-\sigma'_j)^2\Bigg\}, \tag{4.6}$$

$$Z' = \frac{L'^{d/2}}{(v')^{1/d}}\int_{-\infty}^{\infty}d\Phi'\,\exp\{-[H'_0+\mathring{\Gamma}'(\Phi'^2)]\}, \tag{4.7}$$

$$\mathring{\Gamma}'(\Phi'^2) = -\ln\left[\prod_{\mathbf{k}'\neq\mathbf{0}}\frac{1}{(v')^{1/d}L'^{d/2}}\int d\hat{\sigma}'(\mathbf{k}')\right.\times\left.\exp[-\tilde{H}'(\Phi',\sigma')]\vphantom{\prod}\right] \tag{4.8}$$

where $\hat{\sigma}'(\mathbf{k}')\equiv\hat{\varphi}'(\mathbf{k}')$ for $\mathbf{k}'\neq\mathbf{0}$ and $\tilde{H}'$ is expressed in terms of $\hat{\sigma}'(\mathbf{k}')$. No terms $\sim\Phi'\sigma'_j$ and $\sim\Phi'^3\sigma'_j$ appear in Eq. (4.6) because of $\Sigma_j\sigma'_j=0$. The integration measure $\int d\hat{\sigma}'(\mathbf{k}')$ is defined in Eq. (B2) of AppendixB. [The corresponding (but different) functional integration $\int D\sigma$ of the (cutoff-dependent) continuum model was not explicitly defined in Eq. (2.11) of [66].] The quantity $\overset{\circ}{\Gamma}'(\Phi'^2)$ can be interpreted as a constraint free energy, with the constraint being that the zero-mode amplitude Φ' is fixed. The quantity $\exp[-\overset{\circ}{\Gamma}'(\Phi'^2)]$ is proportional to the order-parameter distribution function of isotropic systems [67], which is a physical quantity in its own right. Therefore, in contrast to the ε-expansion approach of [32] and [64], we shall not expand the exponential form $\exp[-\overset{\circ}{\Gamma}'(\Phi'^2)]$ but only $\overset{\circ}{\Gamma}'(\Phi'^2)$. The advantage of our approach has been demonstrated for the specific heat below T_c in Refs.[66,68].

Following [65,66], we decompose $\widetilde{H}'(\Phi',\sigma')=H_1'+H_2'$ into an unperturbed Gaussian part

$$H_1' = v'\left[\sum_{j=1}^{N}\frac{r_{0L}'}{2}\sigma_j'^2 + \sum_{i,j=1}^{N}\frac{K_{i,j}}{2}(\sigma_i'-\sigma_j')^2\right] \tag{4.9}$$

and a perturbation part

$$H_2' = v'\left\{\sum_{j=1}^{N}[6u_0'(\Phi'^2-M_0'^2)\sigma_j'^2 + 4u_0'\Phi'\sigma_j'^3 + u_0'\sigma_j'^4]\right\}. \tag{4.10}$$

The crucial point is to incorporate the lowest-mode average

$$M_0'^2(r_0,u_0',L') = \frac{\int_{\infty}^{\infty} d\Phi'\Phi'^2\exp(-H_0')}{\int_{\infty}^{\infty} d\Phi'\exp(-H_0')} \tag{4.11}$$

into the parameter

$$r_{0L}'(r_0,u_0',L') = r_0 + 12u_0'M_0'^2 \tag{4.12}$$

of the unperturbed part H_1' and to treat the term $6u_0'(\Phi'^2 - M_0'^2)\sigma_j'^2$ of H_2' as a perturbation. The treatment of the Gaussian fluctuations $\sigma_j'^2$ as a perturbation is similar in spirit to an earlier perturbation approach for Dirichlet boundary conditions [79] where part of the Gaussian fluctuations of the higher modes were included in the perturbation part of the Hamiltonian. The positivity of $r_{0L}'>0$ for all r_0 permits us to extend the theory to the region below T_c. For finite L', $M_0'^2$ and r_{0L}' interpolate smoothly between the mean-field bulk limits above and below T_c,

$$\lim_{L'\to\infty} M_0'^2 \equiv M_{\rm mf}'^2 = \begin{cases} 0 & \text{for } r_0 \geq 0, \\ -r_0/(4u_0') & \text{for } r_0 \leq 0, \end{cases} \tag{4.13}$$

$$\lim_{L'\to\infty} r_{0L}' \equiv r_{\rm mf} = \begin{cases} r_0 & \text{for } r_0 \geq 0, \\ -2r_0 & \text{for } r_0 \leq 0. \end{cases} \tag{4.14}$$

The contribution of H_1' to $L'^{-d}\overset{\circ}{\Gamma}'(\Phi'^2)$ is [compare Eq. (B4) in Appendix B]

$$-\frac{1}{L'^d}\ln\left[\prod_{\mathbf{k}'\neq\mathbf{0}}\int\frac{d\hat{\varphi}'(\mathbf{k}')}{(v')^{1/d}L'^{d/2}}\right]\exp(-H_1')$$
$$= -\frac{N-1}{2L'^d}\ln(2\pi) + \frac{1}{2L'^d}\sum_{\mathbf{k}'\neq\mathbf{0}}\ln\{[r_{0L}'+\delta\hat{K}'(\mathbf{k}')](v')^{2/d}\}. \tag{4.15}$$

The leading contributions of the perturbation term $6u_0'(\Phi'^2 - M_0'^2)\sigma_j'^2$ of H_2' to $L'^{-d}\overset{\circ}{\Gamma}'(\Phi'^2)$ read

$$6u_0'(\Phi'^2-M_0'^2)S_1(r_{0L}') - 36u_0'^2(\Phi'^2-M_0'^2)^2S_2(r_{0L}') + O[u_0'^3(\Phi'^2-M_0'^2)^3], \tag{4.16}$$

where

$$S_m(r_{0L}') = L'^{-d}\sum_{\mathbf{k}'\neq\mathbf{0}}\{[r_{0L}'+\delta\hat{K}'(\mathbf{k}')]\}^{-m}. \tag{4.17}$$

The terms $\sim u_0'\Phi'\sigma_j'^3$ and $u_0'\sigma_j'^4$ of H_2' yield higher-order contributions of $O(u_0'^2\Phi'^2,u_0')$, which will be neglected in the following. We emphasize, however, that leading finite-size effects caused by the four-point coupling u_0' are taken into account in Eq. (4.16) as it contains the coupling between the fluctuations $\Phi'^2 - M_0'^2$ of the lowest mode and those of the higher modes $\hat{\sigma}'(\mathbf{k}')$. For a discussion of the order of the neglected terms, see also Refs. [66,79].

The starting point for our perturbation expression of the bare free-energy density (2.25) is

$$f' = L'^{-d}\overset{\circ}{\Gamma}'(0) - L'^{-d}\ln\left\{\frac{L'^{d/2}}{(v')^{1/d}}\int_{-\infty}^{\infty}d\Phi'\exp[-H'^{\rm eff}]\right\}$$
$$= -\frac{N-1}{2L'^d}\ln(2\pi) + \frac{1}{2L'^d}\sum_{\mathbf{k}'\neq\mathbf{0}}\ln\{[r_{0L}'+\delta\hat{K}'(\mathbf{k}')](v')^{2/d}\}$$
$$- L'^{-d}\ln\left\{\frac{L'^{d/2}}{(v')^{1/d}}\int_{-\infty}^{\infty}d\Phi'\exp[-H'^{\rm eff}]\right\}$$
$$- 6u_0'M_0'^2S_1(r_{0L}') - 36u_0'^2M_0'^4S_2(r_{0L}'), \tag{4.18}$$

$$H'^{\rm eff} = L'^d\left(\frac{1}{2}r_0'^{\rm eff}\Phi'^2 + u_0'^{\rm eff}\Phi'^4\right), \tag{4.19}$$

$$r_0'^{\rm eff} = r_0 + 12u_0'S_1(r_{0L}') + 144u_0'^2M_0'^2S_2(r_{0L}'), \tag{4.20}$$

$$u_0'^{\rm eff} = u_0' - 36u_0'^2S_2(r_{0L}'). \tag{4.21}$$

Apart from the different form of the lattice interaction $\delta\hat{K}'(\mathbf{k}')$ and the different vectors $\mathbf{k}'$, Eq. (4.18) differs from the previous Eqs. (4.3), (4.11), and (4.12) of the isotropic field theory of Ref. [66] in two respects: (i) In Eq. (4.18), there are additive logarithmic finite-size terms proportional to $L'^{-d}\ln[(v')^{1/d}]$; in the regime (b) mentioned above, they will cancel each other, and a dependence on $\ln[(v')^{1/d}]$ will remain only in the bulk part [see Eq. (C1) in Appendix C and Eqs. (4.33)–(4.35)]. (ii) In Eq. (4.18), there are the additive logarithmic finite-size terms

$$-\frac{N-1}{2L'^d}\ln(2\pi)-\frac{1}{L'^d}\ln L'^{d/2}=-\frac{1}{2v'}\ln(2\pi)+\frac{1}{2L'^d}\ln\frac{2\pi}{L'^d},\tag{4.22}$$

where $v'=L'^d/N$. These terms are independent of t and h, therefore such terms do not affect the physical quantities considered in Ref. [66], which are *derivatives* of the free energy with respect to t and h. These terms, however, must not be omitted in the calculation of the free energy itself. While the first term on the right-hand side (r.h.s.) of Eq. (4.22) is an unimportant nonsingular *bulk* part, the second term yields a non-negligible contribution to the universal value of the finite-size scaling function $\mathcal{F}^{\rm ex}$ at T_c, which is a measurable quantity. [The second term affects the argument of the first logarithmic term of the scaling function at T_c given in Eq. (6.12) below.] Omission of this term would cause a misidentification of the finite-size scaling function of the excess free-energy density. This would yield an incorrect result in a comparison with Monte Carlo data [34–36] that measure the *total* amplitude of the L^{-d} term of the excess free energy of two- and three-dimensional spin models.

Our approach incorporates, in an approximate form, the effect of the finite-size fluctuations $\Phi'^2-M_0'^2$ of the lowest mode amplitude around its average $M_0'^2$ that are present in the central finite-size critical region. This is not taken into account in the effective Hamiltonian of [64], which contains fluctuations of Φ'^2 around zero. Setting $M_0'^2=0$ and $r'_{0L}=r_0$ in Eqs. (4.18)–(4.21) would yield the bare free-energy density corresponding to perturbation theory based on the effective Hamiltonian of [64]. This would restrict the theory to the regime $r_0\geq 0$. A foundation of Eqs. (4.18)–(4.21) can also be given on the basis of the order-parameter distribution function [67].

C. Improved perturbation expression

In its present form, the saddle-point contribution of the lowest-mode integral in Eq. (4.18) for large L' below T_c is

$$\lim_{L'\to\infty}-L'^{-d}\ln\left\{\frac{L'^{d/2}}{(v')^{1/d}}\int_{-\infty}^{\infty}d\Phi'\exp[-H'^{\rm eff}]\right\}=-\frac{(r_0'^{\rm eff})^2}{16u_0'^{\rm eff}},\tag{4.23}$$

which, after expansion of $(u_0'^{\rm eff})^{-1}$ with respect to u'_0, would produce arbitrary large powers of u'_0. On the other hand, it is clear at the outset that, because of neglecting the terms $\sim u'_0\Phi'\sigma_j'^3$ and $\sim u'_0\sigma_j'^4$ of H'_2, the neglected terms in Eq. (4.18) are bulk terms of $O(u'_0)$ corresponding to two-loop terms. Therefore, it is necessary to further improve the perturbation expression (4.18). Here our reformulation of the $\ln\int d\Phi' e^{-H'^{\rm eff}}$ term will be guided by the requirement that higher-order powers of u_0 are neglected already at the level of $H'^{\rm eff}$, *before* integrating over Φ'. For this purpose, we rewrite the logarithm of the integral over the lowest mode as

$$\ln\left\{\frac{L'^{d/2}}{(v')^{1/d}}\int_{-\infty}^{\infty}d\Phi'\exp[-H'^{\rm eff}]\right\}=\ln\int_{-\infty}^{\infty}ds\exp\left[-\frac{r_0'^{\rm eff}L'^{d/2}}{2(u_0'^{\rm eff})^{1/2}}s^2-s^4\right]+\frac{1}{2}\ln\left[\frac{L'^{d/2}}{(v')^{2/d}(u_0'^{\rm eff})^{1/2}}\right].\tag{4.24}$$

For the reason given above, it is appropriate to expand the factors $(u_0'^{\rm eff})^{-1/2}$ in both terms of Eq. (4.24) in powers of u_0 and to neglect terms of $O(u_0'^{3/2})$ corresponding to a truncation of the expansion,

$$(u_0'^{\rm eff})^{-1/2}=u_0'^{-1/2}+18u_0'^{1/2}S_2(r'_{0L})+O(u_0'^{3/2}).\tag{4.25}$$

In summary, our improved perturbation expression for the bare free-energy density reads

$$f'=-\frac{N-1}{2L'^d}\ln(2\pi)+\frac{1}{2L'^d}\sum_{\mathbf{k}'\neq\mathbf{0}}\ln\{[r'_{0L}+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\}-\frac{1}{L'^d}\ln\int_{-\infty}^{\infty}ds\exp\left(-\tfrac{1}{2}y_0'^{\rm eff}s^2-s^4\right)-\frac{1}{2L'^d}\ln\left[\frac{L'^{d/2}w_0'^{\rm eff}}{v'^{2/d}}\right]-6u'_0M_0'^2S_1(r'_{0L})-36u_0'^2M_0'^4S_2(r'_{0L})\tag{4.26}$$

with

$$y_0'^{\rm eff}=L'^{d/2}u_0'^{-1/2}\{r_0[1+18u'_0S_2(r'_{0L})]+12u'_0S_1(r'_{0L})+144u_0'^2M_0'^2S_2(r'_{0L})\},\tag{4.27}$$

$$w_0'^{\rm eff}=u_0'^{-1/2}[1+18u'_0S_2(r'_{0L})].\tag{4.28}$$

Now, because of $u'_0M_0'^2\sim O(u_0'^{1/2})$ at T_c, $y_0'^{\rm eff}$ and $w_0'^{\rm eff}$ and the last two terms in Eq. (4.26) contain terms only up to $O(u_0'^{1/2})$ at T_c. One can verify that in the bulk limit below T_c the last two terms $-6u'_0M_0'^2S_1$ and $-36u_0'^2M_0'^4S_2$ of Eq. (4.26), which are of $O(1)$, are exactly canceled by the $O(1)$ terms of the saddle-point contribution $-(y_0'^{\rm eff})^2/(16L'^d)$ of the integral term of Eq. (4.26). Thus Eq. (4.26) correctly contains the bare bulk free-energy density $f_b'^{\pm}\equiv\lim_{L'\to\infty}f'$ in one-loop order [i.e., up to $O(1)$],

$$f_b'^{+}=-\frac{\ln(2\pi)}{2v'}+\frac{1}{2}\int_{\mathbf{k}'}\ln\{[r_0+\delta\hat{K}'(\mathbf{k}')](v')^{2/d}\}+O(u'_0),\tag{4.29}$$

$$f_b'^{-}=\frac{1}{2}r_0M_{\rm mf}'^2+u'_0M_{\rm mf}'^4-\frac{\ln(2\pi)}{2v'}+\frac{1}{2}\int_{\mathbf{k}'}\ln\{[-2r_0+\delta\hat{K}'(\mathbf{k}')](v')^{2/d}\}+O(u'_0)\tag{4.30}$$

above and below T_c, respectively, where

$$\int_{\mathbf{k}'} = (\det \mathbf{A})^{1/2} \int_{\mathbf{k}} \equiv (\det \mathbf{A})^{1/2} \prod_{\alpha=1}^{d} \int_{-\pi/\tilde{a}}^{\pi/\tilde{a}} \frac{dk_\alpha}{2\pi}. \quad (4.31)$$

We shall rewrite Eq. (4.26) in terms of $r_0 - r_{0c}$, where

$$r_{0c} = -12u_0' \int_{\mathbf{k}'} \frac{1}{\delta \hat{K}'(\mathbf{k}')} = -12u_0 \int_{\mathbf{k}} \frac{1}{\delta \hat{K}(\mathbf{k})} \quad (4.32)$$

is the critical value of r_0 up to $O(u_0)$. On the level of bare perturbation theory, the application of Eq. (4.26) will be in the central finite-size regime $|r_0 - r_{0c}| \lesssim O(u_0'^{1/2} L'^{-d/2})$. On the level of the asymptotic renormalized theory, this will correspond to the finite-size regime $0 \le |t(L'/\xi_0')^{1/\nu}| \lesssim O(1)$ above, at, and below T_c, i.e., the regime (b) mentioned above. If applied to the regime $L'/\xi_-' \gg 1$ below T_c, f' also contains bulk and finite-size terms of $O(u_0')$, which would need to be complemented by two-loop calculations.

The right-hand side of Eq. (4.26) can be decomposed as

$$f'(r_0 - r_{0c}, u_0', L', K_{i,j}, v') = f'^{(1)}_{\mathrm{ns},b}(r_0 - r_{0c}, u_0', K_{i,j}, v') + \delta f'(r_0 - r_{0c}, u_0', L', K_{i,j}, v'), \quad (4.33)$$

where $f'^{(1)}_{\mathrm{ns},b}$ is a nonsingular *bulk* part up to linear order in $r_0 - r_{0c}$,

$$f'^{(1)}_{\mathrm{ns},b}(r_0 - r_{0c}, u_0', K_{i,j}, v') = -\frac{\ln(2\pi)}{2v'} + \frac{1}{2}\int_{\mathbf{k}'} \ln\{[\delta \hat{K}'(\mathbf{k}')](v')^{2/d}\} + \frac{r_0 - r_{0c}}{2}\int_{\mathbf{k}'} [\delta \hat{K}'(\mathbf{k}')]^{-1}. \quad (4.34)$$

As expected from bulk theory [80], the remaining finite-size part $\delta f'$ has a finite limit for $v' \to 0$ at fixed $r_0 - r_{0c}$ in $2 < d < 4$ dimensions. It turns out that the resulting function depends only on $\bar{\mathbf{A}}$ rather than on $\mathbf{A}$,

$$\lim_{v' \to 0} \delta f'(r_0 - r_{0c}, u_0', L', K_{i,j}, v') = \delta f'(r_0 - r_{0c}, u_0', L', \bar{\mathbf{A}}). \quad (4.35)$$

The r.h.s. of Eq. (4.35) can be further decomposed as

$$\delta f'(r_0 - r_{0c}, u_0', L', \bar{\mathbf{A}}) = f'^{(2)}_{\mathrm{ns},b}(r_0 - r_{0c}, u_0') + f_s'(r_0 - r_{0c}, u_0', L', \bar{\mathbf{A}}), \quad (4.36)$$

where $f'^{(2)}_{\mathrm{ns},b}$ is a nonsingular *bulk* part proportional to $(r_0 - r_{0c})^2$ [80]. We are interested in the asymptotic singular finite-size part f_s'. In the limit $v' \to 0$, our result for $\delta f'$ does not contain an *L-dependent nonsingular* part. The limit $v' \to 0$ is justified in the power-law regime (b) mentioned above where the v'-dependent terms of our perturbation expression (4.26) give rise only to corrections to scaling. However, although the limit (4.35) does exist in the exponential regimes (a) and (c), it is not justified to neglect the v' dependencies in the exponential arguments, as will be discussed in Sec. X.

D. Bare perturbation result

The calculation of $\delta f'$ is outlined in Appendixes B and C for the power-law regime $|r_0 - r_{0c}| \lesssim O(u_0' L'^{-d/2}), L' \gg (v')^{1/d}, |r_0 - r_{0c}|^{1/2}(v')^{1/d} \ll 1$. The result reads for $2 < d < 4$

$$\delta f'(r_0 - r_{0c}, u_0', L', \bar{\mathbf{A}}) = -A_d (r_{0L}')^{-\varepsilon/2}\left[\frac{(r_{0L}')^2}{4d} + \frac{(r_0 - r_{0c})^2}{4\varepsilon} - 18u_0'^2 M_0'^4\right] + \frac{1}{L'^d}\left\{-\ln \int_{-\infty}^{\infty} ds \exp\left[-\tfrac{1}{2} y_0'^{\mathrm{eff}}(\bar{\mathbf{A}}) s^2 - s^4\right] - \frac{1}{2}\ln\left[\frac{2\pi w_0'^{\mathrm{eff}}(\bar{\mathbf{A}})}{(L')^{\varepsilon/2}}\right] + \frac{1}{2} J_0(r_{0L}' L'^2, \bar{\mathbf{A}}) - \frac{3u_0' M_0'^2 L'^2}{2\pi^2} I_1(r_{0L}' L'^2, \bar{\mathbf{A}}) - \frac{9u_0'^2 M_0'^4 L'^4}{4\pi^4} I_2(r_{0L}' L'^2, \bar{\mathbf{A}})\right\} \quad (4.37)$$

with

$$y_0'^{\mathrm{eff}}(\bar{\mathbf{A}}) = \left(\frac{V'}{u_0'}\right)^{1/2}\left\{(r_0 - r_{0c})\left[1 + 18u_0'\left(\frac{A_d(d-2)}{2\varepsilon}(r_{0L}')^{-\varepsilon/2} + \frac{L'^\varepsilon}{16\pi^4} I_2(r_{0L}' L'^2, \bar{\mathbf{A}})\right)\right] + 12u_0'\left(-\frac{A_d}{\varepsilon}(r_{0L}')^{(d-2)/2} + \frac{(L')^{2-d}}{4\pi^2} I_1(r_{0L}' L'^2, \bar{\mathbf{A}})\right) + 144u_0'^2 M_0'^2\left(\frac{A_d(d-2)}{2\varepsilon}(r_{0L}')^{-\varepsilon/2} + \frac{L'^\varepsilon}{16\pi^4} I_2(r_{0L}' L'^2, \bar{\mathbf{A}})\right)\right\}, \quad (4.38)$$

$$w_0'^{\mathrm{eff}}(\bar{\mathbf{A}}) = u_0'^{-1/2}\left[1 + 18u_0'\left(\frac{A_d(d-2)}{2\varepsilon}(r_{0L}')^{-\varepsilon/2} + \frac{L'^\varepsilon}{16\pi^4} I_2(r_{0L}' L'^2, \bar{\mathbf{A}})\right)\right], \quad (4.39)$$

$$r_{0L}'(r_0 - r_{0c}, u_0', L') = r_0 - r_{0c} + 12u_0' M_0'^2, \quad (4.40)$$

$$M_0'^2 = (V' u_0')^{-1/2} \vartheta_2(y_0'), \quad (4.41)$$

$$y_0' = (r_0 - r_{0c})(V'/u_0')^{1/2}, \quad (4.42)$$

$$\vartheta_m(y_0') = \frac{\int_0^\infty ds\, s^m \exp\left(-\tfrac{1}{2} y_0' s^2 - s^4\right)}{\int_0^\infty ds \exp\left(-\tfrac{1}{2} y_0' s^2 - s^4\right)}, \quad (4.43)$$

$$J_0(r'_{0L}L'^2,\bar{\mathbf{A}}) = \int_0^\infty \frac{dy}{y}\left[\exp\left(-\frac{r'_{0L}L'^2 y}{4\pi^2}\right) \times\{(\pi/y)^{d/2} - K_d(y,\bar{\mathbf{A}}) + 1\} - \exp(-y)\right], \tag{4.44}$$

$$I_m(r'_{0L}L'^2,\bar{\mathbf{A}}) = \int_0^\infty dy y^{m-1}\exp[-r'_{0L}L'^2 y/(4\pi^2)] \times\{K_d(y,\bar{\mathbf{A}}) - (\pi/y)^{d/2} - 1\}, \tag{4.45}$$

$$K_d(y,\bar{\mathbf{A}}) = \sum_{\mathbf{n}} \exp(-y\mathbf{n}\cdot\bar{\mathbf{A}}\mathbf{n}) \tag{4.46}$$

with $\mathbf{n}=(n_1,n_2,\ldots,n_d), n_\alpha=0,\pm1,\ldots,\pm\infty$. The behavior of the functions J_0, I_1, and I_2 for small and large arguments $r'_{0L}L'^2$ is given in Appendix C.

The crucial information on the anisotropy is contained in the sum (4.46). By means of the Poisson identity [81] [see also Eq. (B9)], one can show that this function satisfies

$$K_d(y;\mathbf{A}) = (\det\mathbf{A})^{-1/2}\left(\frac{\pi}{y}\right)^{d/2} K_d\left(\frac{\pi^2}{y},\mathbf{A}^{-1}\right). \tag{4.47}$$

The sum (4.46) could formally be rewritten in $\mathbf{k}'$ space as $\Sigma'_{\mathbf{k}}\exp(-y'\mathbf{k}'\cdot\mathbf{k}')$ with $y'=yL'^2/(4\pi^2)$, but in practice there is no advantage to using the more complicated $\mathbf{k}'$ vectors [see the example (2.22) in Sec. II]. For this reason, the sums in the three-dimensional calculations in Sec. VIII will be performed in $\mathbf{k}$ space.

As expected, the bare perturbation result (4.37) for $\delta f'$ does not yet correctly describe the critical behavior. (i) In the bulk limit at $t\neq0$, the small-t behavior is $\delta f'_b \sim |t|^{d/2}$ rather than $\sim|t|^{d\nu}$. (ii) At $t=0$, the leading large-L' behavior is $\delta f' \sim L'^{-d^2/4}$ rather than $\sim L'^{-d}$. These defects will be removed by turning to the renormalized theory.

V. MINIMAL RENORMALIZATION AT FIXED DIMENSION

The bare perturbation form of $\delta f'$ requires additive and multiplicative renormalizations, followed by a mapping of the renormalized free energy $\delta f'_R$ from the critical to the noncritical region where perturbation theory is applicable. It is well known that, for the multiplicative renormalizations, the usual bulk Z factors are sufficient [82]. For both multiplicative and additive renormalizations, the absence of L-dependent pole terms has been checked explicitly up to $O(u_0'^2)$ for the case of periodic boundary conditions [33,79]. In particular, there is no need for an L-dependent shift of the temperature variable. We employ the minimal subtraction scheme at fixed dimension $2<d<4$ without using the ε expansion [62]. This approach has already been successfully employed in previous finite-size studies [65–70] and is applicable above, at, and below T_c with the same renormalization constants. Thus it permits us to derive a *single* finite-size scaling function of the free energy in the central finite-size critical region above, at, and below T_c.

The multiplicatively renormalized quantities are

$$u' = \mu^{-\varepsilon}A_d Z_{u'}^{-1}Z_{\varphi'}^2 u'_0 \tag{5.1}$$

and $r=Z_r^{-1}(r_0-r_{0c})=at$, $\varphi'_R=Z_{\varphi'}^{-1/2}\varphi'$ with an arbitrary inverse reference length μ. L' is not renormalized. Furthermore, the reduced anisotropy matrix $\bar{\mathbf{A}}$ is not renormalized either as it does not change the ultraviolet behavior at $d=4$. If our calculation is extended to a finite external field h', Eq. (2.19), the additional renormalization $h'_R=Z_{\varphi'}^{1/2}h'$ is necessary [69].

The geometric factor of bulk theory [see Eq. (3.1)],

$$A_d = \frac{\Gamma(3-d/2)}{2^{d-2}\pi^{d/2}(d-2)} = S_d\Gamma\left(1+\frac{\varepsilon}{2}\right)\Gamma\left(1-\frac{\varepsilon}{2}\right), \tag{5.2}$$

appears naturally in Eqs. (4.37)–(4.39) rather than the more commonly used factor $S_d=2^{1-d}\pi^{-d/2}[\Gamma(d/2)]^{-1}$. The perturbation results of amplitudes and scaling functions depend on the choice of the geometric factor in Eq. (5.1) [62,63,66,80,83] [see, e.g., the universal ratio Q_1 in Eq. (6.19) below; see also the comment after Eq. (5.16) below]. The advantage of the factor (5.2) is that it describes the full d dependence of single-loop integrals in $2<d<4$ dimensions such as Eq. (3.1), in contrast to the factor S_d. For this reason, we have incorporated A_d in the definition of the renormalized coupling u', Eq. (5.1). Any other choice, such as S_d instead of A_d, would introduce artificial d dependencies into the perturbation results. For the same reason, we employ A_d in the definition of the multiplicatively and additively renormalized free-energy density

$$f'_R(r,u',L',\mu,\bar{\mathbf{A}}) = \delta f'(Z_r r,\mu^\varepsilon Z_{u'}Z_{\varphi'}^{-2}A_d^{-1}u',L',\bar{\mathbf{A}}) - \frac{1}{8}\mu^{-\varepsilon}r^2 A_d A(u',\varepsilon). \tag{5.3}$$

Because of relations such as Eq. (3.1), the Z factors $Z_r(u',\varepsilon)$, $Z_{u'}(u',\varepsilon)$, and $Z_{\varphi'}(u',\varepsilon)$ depend on u' in the same way as the usual Z factors depend on u in the standard isotropic φ^4 theory. The same statement holds for the additive renormalization constant $A(u',\varepsilon)$ because of

$$\int_{\mathbf{k}}^{\infty}\ln(r_0+\mathbf{k}\cdot\mathbf{A}\mathbf{k}) = (\det\mathbf{A})^{-1/2}\int_{\mathbf{k}'}^{\infty}\ln(r_0+\mathbf{k}'\cdot\mathbf{k}') = -(\det\mathbf{A})^{-1/2}\frac{2A_d}{d\varepsilon}r_0^{d/2}. \tag{5.4}$$

Thus the renormalization constants read up to one-loop order $Z_r(u',\varepsilon)=1+12u'/\varepsilon$, $Z_{u'}(u',\varepsilon)=1+36u'/\varepsilon$, $Z_{\varphi'}(u',\varepsilon)=1$, $A(u',\varepsilon)=-2/\varepsilon$. The Z factors $Z_{u'}$ and Z_r are sufficient to renormalize y'^{eff}_0, Eq. (4.27), and w'^{eff}_0, Eq. (4.28), whereas the additive renormalization constant $A(u',\varepsilon)$ is needed to absorb the pole term $\sim -A_d(r_0-r_{0c})^2/(4\varepsilon)$ in the square brackets of Eq. (4.37). After substituting these renormalization constants, one verifies that the resulting renormalized free-energy density f'_R has a finite limit for $\varepsilon\to0$ at fixed $u'>0$.

We define the dimensionless amplitude function

$$F_R'(r/\mu^2,u',L'\mu,\bar{\mathbf{A}}) = \mu^{-d}A_d^{-1}f_R'(r,u',\mu,L',\bar{\mathbf{A}}). \quad (5.5)$$

From the μ independence of $\delta f'(r_0-r_{0c},u_0',L',\bar{\mathbf{A}})$, one can derive the renormalization-group equation (RGE) for the amplitude function,

$$(\mu\partial_\mu + r\zeta_r\partial_r + \beta_{u'}\partial_{u'} + d)F_R'(r/\mu^2,u',L'\mu,\bar{\mathbf{A}}) = -[r^2/(2\mu^4)]B(u'), \quad (5.6)$$

where the field-theoretic functions $\beta_{u'}(u',\varepsilon),\zeta_r(u')$, and $B(u')$ are defined as usual [62,63]. Equation (5.6), however, differs from the corresponding bulk RGE (119) of [80] since here we are using r rather than the bulk correlation lengths $\xi_\pm'$ as the appropriate measure of the temperature variable. Using r rather than $\xi_\pm'$ is advantageous in finite-size theories where a *single* finite-size scaling function is derived for both $r\geq 0$ and $r<0$. The functions $\zeta_r(u'),\beta_{u'}(u',1)$, and $B(u')$ as well as the fixed-point value $u'^*=u^*$ are accurately known [63,84] from Borel resummations. Integration of the RGE yields

$$F_R'\left(\frac{r}{\mu^2},u',L'\mu,\bar{\mathbf{A}}\right) = l^d\left\{F_R'\left(\frac{r(l)}{l^2\mu^2},u'(l),L'l\mu,\bar{\mathbf{A}}\right) + \frac{r(l)^2}{2l^4\mu^4}\int_1^l B[u'(l)] \times\left(\exp\int_l^{l'}\{2\zeta_r[u'(l'')]-\varepsilon\}\frac{dl''}{l''}\right)\frac{dl'}{l'}\right\}, \quad (5.7)$$

with an as yet arbitrary flow parameter l and $u'(1)\equiv u'$. The effective parameters $r(l)$ and $u'(l)$ are defined as usual [62].

Equations (4.40) and (5.7) show that in the arguments of the functions J_0,I_1,I_2 and of the pole terms $\sim\varepsilon^{-1}$ of Eqs. (4.37)–(4.39), the parameter r_{0L}' will appear in the form of the effective renormalized counterpart

$$r_L'(l) \equiv r_{0L}'(r(l),l^\varepsilon\mu^\varepsilon A_d^{-1}u'(l),L') = r(l) + 12(\mu l)^{\varepsilon/2}A_d^{-1/2}u'(l)^{1/2}(L')^{-d/2}\vartheta_2[y'(l)], \quad (5.8)$$

$$y'(l) = r(l)\mu^{-2}l^{-2}(L'\mu l)^{d/2}A_d^{1/2}u'(l)^{-1/2}. \quad (5.9)$$

Correspondingly, the effective renormalized counterparts of $y_0'^{\text{eff}}$ and of $w_0'^{\text{eff}}$ appearing in the renormalized form of the logarithmic part of $\delta f'$ are given by

$$y'^{\text{eff}}(l,\bar{\mathbf{A}}) = (l\mu L')^{d/2}A_d^{1/2}u'(l)^{-1/2} \times\left\{\frac{r(l)}{\mu^2l^2}\left[1+18u'(l)R_2\left(\frac{r_L'(l)}{\mu^2l^2},l\mu L',\bar{\mathbf{A}}\right)\right] + 12u'(l)R_1\left(\frac{r_L'(l)}{\mu^2l^2},l\mu L',\bar{\mathbf{A}}\right) + 144(l\mu L')^{-d/2}A_d^{-1/2}u'(l)^{3/2}\vartheta_2[y'(l)] \times R_2\left(\frac{r_L'(l)}{\mu^2l^2},l\mu L',\bar{\mathbf{A}}\right)\right\}, \quad (5.10)$$

$$w'^{\text{eff}}(l,\bar{\mathbf{A}}) = u'(l)^{-1/2}\left[1+18u'(l)R_2\left(\frac{r_L'(l)}{\mu^2l^2},l\mu L',\bar{\mathbf{A}}\right)\right], \quad (5.11)$$

$$R_1(q,p,\bar{\mathbf{A}}) = \varepsilon^{-1}q[1-q^{-\varepsilon/2}] + p^{\varepsilon-2}(4\pi^2A_d)^{-1}I_1(qp^2,\bar{\mathbf{A}}), \quad (5.12)$$

$$R_2(q,p,\bar{\mathbf{A}}) = -\varepsilon^{-1}[1-q^{-\varepsilon/2}] - \frac{1}{2}q^{-\varepsilon/2} + p^\varepsilon(16\pi^4A_d)^{-1}I_2(qp^2,\bar{\mathbf{A}}). \quad (5.13)$$

This suggests that the most natural choice of the flow parameter l is made by

$$r_L'(l) = \mu^2l^2. \quad (5.14)$$

It ensures the standard choice in the bulk limit both above and below T_c [62],

$$\lim_{L\to\infty}\mu^2l^2 = \begin{cases}\mu^2l_+^2 = r(l_+) & \text{for } T>T_c,\\ \mu^2l_-^2 = -2r(l_-) & \text{for } T<T_c,\end{cases} \quad (5.15)$$

and appropriately implies $\mu l\propto L'^{-1}$ for large finite L' at $T=T_c$. As a natural choice for the reference length μ^{-1}, we take $\mu^{-1}=\xi_{0+}'$, where [63]

$$\xi_{0+}' = \left[Z_r(u',\varepsilon)a_0^{-1}Q^*\exp\left(\int_{u'}^{u'^*}\frac{\zeta_r(u'^*)-\zeta_r(u'')}{\beta_{u'}(u'',\varepsilon)}du''\right)\right]^{1/2} \quad (5.16)$$

is the asymptotic amplitude of the second-moment bulk correlation length of the isotropic system above T_c, as defined in Eq. (3.6). The dimensionless amplitude $Q^*=1+O(u^{*2})=1+O(u'^{*2})$ is the fixed-point value of the amplitude function $Q(1,u',d)$ of the second-moment bulk correlation length above T_c [63]. Owing to the choice of the factor A_d, Eq. (5.2), the $O(u')$ term of $Q(1,u',d)$ and the $O(u^*)$ term of Q^* vanish [63,80,85], similar to the vanishing of the $O(u')$ contribution to the order-parameter amplitude function [63]. The same observation was recently made for the correlation-length amplitude within the ϵ expansion [51] where the same geometric factor A_d was employed (apart from a harmless factor of 2). In three dimensions, the amplitude Q^* is accurately known from Borel resummations [85].

Equations (5.8) and (5.14) determine $l=l(t,L')$ as a function of the reduced temperature t and the size L'. With this choice of l, Eqs. (5.7) and (5.5) provide a mapping of the functions F_R' and f_R' from the critical to the noncritical region.

In summary, the singular part of the contribution $\delta f'$ to the free-energy density of the isotropic system is contained in

$$f_R'(r,u',L',\mu,\bar{\mathbf{A}}) = \delta f'(Z_rr,\mu^\varepsilon Z_{u'}Z_{\varphi'}^{-2}A_d^{-1}u',L',\bar{\mathbf{A}}) - \frac{1}{8}\mu^{-\varepsilon}r^2A_dA(u',\varepsilon) = f_R'(r(l),u'(l),l\mu,L',\bar{\mathbf{A}})$$

$$+\frac{A_d r(l)^2}{2(l\mu)^\varepsilon}\int_1^l B[u'(l')] \times\left\{\times\exp\int_l^{l'}\{2\zeta_r[u'(l'')]-\varepsilon\}\frac{dl''}{l''}\right\}\frac{dl'}{l'}, \tag{5.17}$$

$$\begin{aligned} &f_R'(r(l),u'(l),l\mu,L',\bar{\mathbf{A}}) \\ &= -A_d(l\mu)^d/(4d) + 18u'(l)L'^{-d}\{\vartheta_2[y'(l)]\}^2 \\ &+\frac{1}{L'^d}\Bigg\{-\ln\int_{-\infty}^{\infty}ds\,\exp\left[-\frac{1}{2}y'^{\text{eff}}(l,\bar{\mathbf{A}})s^2-s^4\right] \\ &-\frac{1}{2}\ln\left[\frac{2\pi A_d^{1/2}w'^{\text{eff}}(l,\bar{\mathbf{A}})}{(l\mu L')^{\varepsilon/2}}\right]+\frac{1}{2}J_0(l^2\mu^2L'^2,\bar{\mathbf{A}}) \\ &-\frac{3(l\mu L')^{\varepsilon/2}u'(l)^{1/2}}{2\pi^2A_d^{1/2}}\vartheta_2[y'(l)]I_1(l^2\mu^2L'^2,\bar{\mathbf{A}}) \\ &-\frac{9(l\mu L')^{\varepsilon}u'(l)}{4\pi^4A_d}\{\vartheta_2[y'(l)]\}^2I_2(l^2\mu^2L'^2,\bar{\mathbf{A}})\Bigg\}. \end{aligned} \tag{5.18}$$

In the bulk limit, the function $f_{R,b}'^{\pm}(l_\pm\mu,u'(l_\pm))=\lim_{L\to\infty}f_R'(r(l),u'(l),l\mu,L',\bar{\mathbf{A}})$ becomes independent of $\bar{\mathbf{A}}$,

$$f'^{+}_{R,b}(l_+\mu,u'(l_+)) = -A_d(l_+\mu)^d/(4d), \tag{5.19}$$

$$f'^{-}_{R,b}(l_-\mu,u'(l_-)) = -A_d(l_-\mu)^d\left\{\frac{1}{64u'(l_-)}+\frac{1}{4d}+\frac{81}{64}u'(l_-)\right\}, \tag{5.20}$$

above and below T_c, respectively, where l_+ and l_- are determined by Eq. (5.15). The last integral term in Eq. (5.17) contains both a contribution $\propto t^2 l^{-\alpha/\nu}$ to the singular finite-size part f_s' and a contribution $\propto t^2$ to the nonsingular bulk part $f'^{(2)}_{\text{ns},b}$ of $\delta f'$ [see Eq. (4.36); compare also Eqs. (6.8) and (6.10)].

VI. FINITE-SIZE SCALING FUNCTION OF THE FREE-ENERGY DENSITY

A. Result in $2<d<4$ dimensions

In order to derive the finite-size scaling function $\mathcal{F}$, we consider in Eqs. (5.17) and (5.20) the limit of small $l\ll 1$ or $l\to 0$. In this limit, we have $u'(l)\to u'(0)\equiv u'^*=u^*$, $r(l)/(\mu^2l^2)\to Q^* t l^{-1/\nu}$,

$$y'(l)\to\tilde{y}=\tilde{x}Q^*(\mu lL')^{-\alpha/(2\nu)}A_d^{1/2}u^{*-1/2}, \tag{6.1}$$

$$\tilde{x}=t(\mu L')^{1/\nu}=t(L'/\xi'_{0+})^{1/\nu}. \tag{6.2}$$

In Eq. (6.1), we have used the hyperscaling relation

$$2-\alpha=d\nu. \tag{6.3}$$

Because of the choice (5.14), Eq. (5.8) implies $\mu lL'\to\tilde{l}=\tilde{l}(\tilde{x})$, where $\tilde{l}(\tilde{x})$ is determined implicitly by

$$\tilde{y}+12\vartheta_2(\tilde{y})=\tilde{l}^{d/2}A_d^{1/2}u^{*-1/2}, \tag{6.4}$$

$$\tilde{y}=\tilde{x}Q^*\tilde{l}^{-\alpha/(2\nu)}A_d^{1/2}u^{*-1/2}. \tag{6.5}$$

Simultaneously, these two equations determine $\tilde{y}=\tilde{y}(\tilde{x})$. Furthermore, we have

$$w'^{\text{eff}}(l,\bar{\mathbf{A}})\to W(\tilde{x},\bar{\mathbf{A}})=u^{*-1/2}[1+18u^*R_2(1,\tilde{l},\bar{\mathbf{A}})], \tag{6.6}$$

$$\begin{aligned} y'^{\text{eff}}(l,\bar{\mathbf{A}})\to Y(\tilde{x},\bar{\mathbf{A}}) &= \tilde{l}^{d/2}A_d^{1/2}u^{*-1/2}\{Q^*\tilde{x}\tilde{l}^{-1/\nu}[1 \\ &+18u^*R_2(1,\tilde{l},\bar{\mathbf{A}})]+12u^*R_1(1,\tilde{l},\bar{\mathbf{A}}) \\ &+144u^{*3/2}\tilde{l}^{-d/2}A_d^{-1/2}\vartheta_2(\tilde{y})R_2(1,\tilde{l},\bar{\mathbf{A}})\}. \end{aligned} \tag{6.7}$$

The asymptotic $(l\to 0)$ behavior of the integral in Eq. (5.17),

$$\int_1^l B[u'(l')]\left\{\exp\int_l^{l'}\{2\zeta_r[u'(l'')]-\varepsilon\}\frac{dl''}{l''}\right\}\frac{dl'}{l'} \to -\frac{\nu}{\alpha}B(u^*)+O(l^{\alpha/\nu}), \tag{6.8}$$

is known from bulk theory [80]. In Eq. (6.8), the subleading term $O(l^{\alpha/\nu})$, together with the prefactor $r(l)^2/(l\mu)^\varepsilon$ in Eq. (5.17), contributes to the regular bulk term $f'^{(2)}_{\text{ns},b}$ proportional to t^2 of Eq. (4.36).

In summary, the asymptotic form of the singular part f_s', Eq. (4.2), of the reduced free-energy density of the isotropic system at $h'=0$ is obtained from f_R', Eq. (5.17), in the limit of small l as

$$f_R'\to f_s'(t,L')=L'^{-d}\mathcal{F}(\tilde{x},\bar{\mathbf{A}}), \tag{6.9}$$

where the finite-size scaling function is given by

$$\begin{aligned} \mathcal{F}(\tilde{x},\bar{\mathbf{A}}) &= -A_d\left[\frac{\tilde{l}^d}{4d}+\frac{\nu Q^{*2}\tilde{x}^2\tilde{l}^{-\alpha/\nu}}{2\alpha}B(u^*)\right]+18u^*[\vartheta_2(\tilde{y})]^2 \\ &-\frac{1}{2}\ln\left(\frac{2\pi A_d^{1/2}W(\tilde{x},\bar{\mathbf{A}})}{\tilde{l}^{\varepsilon/2}}\right)-\ln\int_{-\infty}^{\infty}ds \\ &\times\exp\left[-\frac{1}{2}Y(\tilde{x},\bar{\mathbf{A}})s^2-s^4\right]+\frac{1}{2}J_0(\tilde{l}^2,\bar{\mathbf{A}}) \\ &-\frac{3\tilde{l}^{\varepsilon/2}u^{*1/2}}{2\pi^2A_d^{1/2}}\vartheta_2(\tilde{y})I_1(\tilde{l}^2,\bar{\mathbf{A}})-\frac{9\tilde{l}^{\varepsilon}u^*}{4\pi^4A_d}[\vartheta_2(\tilde{y})]^2I_2(\tilde{l}^2,\bar{\mathbf{A}}). \end{aligned} \tag{6.10}$$

This result is valid for $2<d<4$ in the range $L'\gg\tilde{a}$ and $0\le|\tilde{x}|\lesssim O(1)$ above, at, and below T_c (but not for the exponential regime $|\tilde{x}|\gg 1$; see Sec. X). It incorporates the correct bulk critical exponents α and ν and the complete bulk function $B(u^*)$ (not only in one-loop order). There is only one adjustable parameter that is contained in the nonuniversal bulk amplitude ξ'_{0+} of the scaling variable $\tilde{x}$, Eq. (6.2). For finite $L', f'_s(t,L')$ is an analytic function of t near $t=0$, in agreement with general analyticity requirements. From previous studies at finite external field [69,86], we infer that the extension of Eq. (6.9) to $h' \neq 0$ has the structure

$$f'_s(t,h',L') = L'^{-d}\mathcal{F}(\tilde{x},h'(L'/\xi'_c)^{\beta\delta/\nu};\bar{\mathbf{A}}), \qquad (6.11)$$

where ξ'_c is defined after Eq. (3.14). Thus the constants C'_1 and C'_2 in Eqs. (1.3) and (1.4) can be chosen most naturally as $C'_1=(\xi'_{0+})^{-1/\nu}$ and $C'_2=(\xi'_c)^{-\beta\delta/\nu}$.

Of particular interest is the finite-size amplitude $\mathcal{F}(0,\bar{\mathbf{A}}) \equiv \mathcal{F}_c(\bar{\mathbf{A}})$ at T_c,

$$\mathcal{F}_c(\bar{\mathbf{A}}) = \left(18 - \frac{36}{d}\right)u^*[\vartheta_2(0)]^2 - \frac{1}{2}\ln\left(\frac{2\pi A_d^{1/2}W_c(\bar{\mathbf{A}})}{\tilde{l}_c^{\varepsilon/2}}\right) - \ln\int_{-\infty}^{\infty} ds\,\exp\left[-\frac{1}{2}Y_c(\bar{\mathbf{A}})s^2 - s^4\right] + \frac{1}{2}J_0(\tilde{l}_c^2,\bar{\mathbf{A}}) - \frac{\tilde{l}_c^2}{8\pi^2}I_1(\tilde{l}_c^2,\bar{\mathbf{A}}) - \frac{\tilde{l}_c^4}{64\pi^4}I_2(\tilde{l}_c^2,\bar{\mathbf{A}}), \qquad (6.12)$$

where $\tilde{l}_c^{d/2}=12u^{*1/2}A_d^{-1/2}\vartheta_2(0)$ and

$$W_c(\bar{\mathbf{A}}) = u^{*-1/2}[1 + 18u^*R_2(1,\tilde{l}_c,\bar{\mathbf{A}})], \qquad (6.13)$$

$$Y_c(\bar{\mathbf{A}}) = 144u^*\vartheta_2(0)\{R_1(1,\tilde{l}_c,\bar{\mathbf{A}}) + R_2(1,\tilde{l}_c,\bar{\mathbf{A}})\} \qquad (6.14)$$

with $\vartheta_2(0)=\Gamma(3/4)/\Gamma(1/4)$ and

$$R_1(1,\tilde{l}_c,\bar{\mathbf{A}}) = \tilde{l}_c^{2-d}(4\pi^2A_d)^{-1}I_1(\tilde{l}_c^2,\bar{\mathbf{A}}), \qquad (6.15)$$

$$R_2(1,\tilde{l}_c,\bar{\mathbf{A}}) = -\frac{1}{2} + \tilde{l}_c^{\varepsilon}(16\pi^4A_d)^{-1}I_2(\tilde{l}_c^2,\bar{\mathbf{A}}). \qquad (6.16)$$

In the bulk (large $|\tilde{x}|$) limit, Eqs. (6.9) and (6.10) yield $\lim_{L'\to\infty}f'_s(t,L')=f'^{\pm}_{s,b}(t)$, where

$$f'^{+}_{s,b}(t) = -A_dQ^{*d\nu}\left[\frac{1}{4d} + \frac{\nu}{2\alpha}B(u^*)\right]\xi'^{-d}_{0+}t^{d\nu}, \qquad (6.17)$$

$$f'^{-}_{s,b}(t) = -A_dQ^{*d\nu}2^{d\nu}\left[\frac{1}{64u^*} + \frac{1}{4d} + \frac{81}{64}u^* + \frac{\nu}{8\alpha}B(u^*)\right]\xi'^{-d}_{0+}|t|^{d\nu} \qquad (6.18)$$

above and below T_c, respectively, with the universal bulk amplitude ratios

$$f'^{+}_{s,b}(t)\xi'^{d}_{+} \equiv Q_1 = -A_dQ^{*d\nu}\left[\frac{1}{4d} + \frac{\nu}{2\alpha}B(u^*)\right], \qquad (6.19)$$

$$\frac{f'^{-}_{s,b}(t)}{f'^{+}_{s,b}(t)} = \frac{A^-}{A^+} = 2^{d\nu}\frac{1/(64u^*) + 1/(4d) + 81u^*/64 + \nu B(u^*)/(8\alpha)}{1/(4d) + \nu B(u^*)/(2\alpha)}. \qquad (6.20)$$

[For Q_1, compare Eq. (3.12).] Here we have used the bulk identifications

$$\mu l = \begin{cases} \mu l_+ = Q^{*\nu}\xi'^{-1}_{0+}t^{\nu} & \text{for } T > T_c, \\ \mu l_- = Q^{*\nu}\xi'^{-1}_{0+}(2|t|)^{\nu} & \text{for } T < T_c, \end{cases} \qquad (6.21)$$

as implied by the choice (5.15). As noted in Sec. IV, a complete two-loop calculation would yield further bulk contributions of $O(u^*)$ in $f'^{\pm}_{s,b}$. Owing to the truncation (4.25), no terms of $O(u^{*2})$ and higher order appear in Eqs. (6.18) and (6.20), except in the exact bulk function $B(u^*)$.

In order to present the scaling function

$$\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}}) = \mathcal{F}(\tilde{x};\bar{\mathbf{A}}) - \mathcal{F}_b^{\pm}(\tilde{x}) \qquad (6.22)$$

of the excess free-energy density $f'^{\text{ex}}_s(t,L';\bar{\mathbf{A}}) = f'_s(t,L';\bar{\mathbf{A}}) - f'_{s,b}(t)$, we shall also need the $\bar{\mathbf{A}}$-independent bulk part

$$\mathcal{F}_b^{\pm}(\tilde{x}) = \begin{cases} L'^d f'^{+}_{s,b} = Q_1\tilde{x}^{d\nu} & \text{for } T > T_c, \\ L'^d f'^{-}_{s,b} = Q_1^-|\tilde{x}|^{d\nu} & \text{for } T < T_c, \end{cases} \qquad (6.23)$$

with $Q_1^-=(A^-/A^+)Q_1$ representing the large $|\tilde{x}|$ behavior of $\mathcal{F}(\tilde{x},\bar{\mathbf{A}})$. It should be noted that it is not obvious how to interpret the $d\times d$ matrix $\bar{\mathbf{A}}$ for the case of noninteger dimensions d.

In the spirit of the fixed-d minimal subtraction approach [62], we shall evaluate $\mathcal{F}(\tilde{x},\bar{\mathbf{A}})$ and $\mathcal{F}^{\text{ex}}(\tilde{x},\bar{\mathbf{A}})$ in $d=3$ dimensions without any further expansion with respect to u^*. This is in contrast to the ε expansion, which is a double expansion with respect to u^* and $\varepsilon=4-d$.

B. Epsilon expansion

Considering u^* as a smallness parameter and using the results of Appendix C, we obtain from Eq. (6.12) at fixed $2<d<4$

$$\mathcal{F}_c(\bar{\mathbf{A}}) = \frac{1}{2}\ln\left\{\frac{(12)^{4/d}[\Gamma(3/4)]^{\varepsilon/d}u^{*2/d}}{24\pi A_d^{2/d}[\Gamma(1/4)]^{\varepsilon/d}}\right\} - \ln\left[\frac{1}{2}\Gamma(1/4)\right] + \frac{1}{2}J_0(0,\bar{\mathbf{A}}) + \frac{1}{8\pi^2}\left[\frac{12\Gamma(1/4)}{A_d^{1/2}\Gamma(3/4)}\right]^{4/d}I_1(0,\bar{\mathbf{A}})u^{*2/d} + O(u^*,u^{*4/d}). \qquad (6.24)$$

Substituting $u^*=\varepsilon/36+O(\varepsilon^2)$ and expanding all d-dependent quantities with respect to $\varepsilon=4-d$ yields the ε-expansion result at T_c,

$$\mathcal{F}_c(\bar{\mathbf{A}}) = \frac{1}{4}\ln\varepsilon + f_0(\bar{\mathbf{A}}) + f_1(\bar{\mathbf{A}})\varepsilon^{1/2} + O(\varepsilon), \qquad (6.25)$$

$$f_0(\bar{\mathbf{A}}) = -\frac{1}{4}\ln 18 - \ln\left[\frac{1}{2}\Gamma(1/4)\right] + \frac{1}{2}\int_0^\infty \frac{dy}{y}\left[\left(\frac{\pi}{y}\right)^2 - K_4(y,\bar{\mathbf{A}}) + 1 - e^{-y}\right], \tag{6.26}$$

$$f_1(\bar{\mathbf{A}}) = \frac{\Gamma(1/4)}{\pi\Gamma(3/4)\sqrt{2}}\int_0^\infty dy\left[K_4(y,\bar{\mathbf{A}}) - \left(\frac{\pi}{y}\right)^2 - 1\right], \tag{6.27}$$

where now $\bar{\mathbf{A}}$ denotes a 4×4 matrix. The ε-expansion result (6.25)–(6.27) is independent of which renormalization scheme and which kind of perturbation approach is used. The same result is obtained if one starts with the effective Hamiltonian of Brézin and Zinn-Justin [64] or with the cumulant expansion of Rudnick *et al.* [32]. Because of the strict expansion with respect to u^* and ε, the exponential structure of the distribution $\sim\exp[-H'^{\text{eff}}]$ is destroyed. As expected, the ε-expansion term $\sim\ln\varepsilon$ is not well behaved for $\varepsilon\to0$ since at $d=4$ the finite lattice constant $\tilde{a}$ must not be neglected.

A nontrivial question arises if the ε-expansion result is applied to three-dimensional anisotropic systems with a matrix $\bar{\mathbf{A}}\neq\mathbf{1}$. It appears that, to some extent, it is ambiguous how the physical 3×3 matrix $\bar{\mathbf{A}}$ (which, in general, has five independent nonuniversal matrix elements) should be continued to $d=4$ in order to evaluate the coefficients $f_0(\bar{\mathbf{A}})$ and $f_1(\bar{\mathbf{A}})$. This matrix $\bar{\mathbf{A}}$ in Eq. (6.25) is necessarily a 4×4 matrix that, in general, has nine independent nonuniversal matrix elements, i.e., four additional nonuniversal parameters. It is not unique how to choose the magnitude of these four additional matrix elements. The results for $f_0(\bar{\mathbf{A}})$ and $f_1(\bar{\mathbf{A}})$ in four dimensions will significantly depend on this choice.

As a possible choice, we propose the following. In order to describe the physical system with the symmetric three-dimensional matrix

$$\bar{\mathbf{A}} = \begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix} \tag{6.28}$$

with $\det\bar{\mathbf{A}}=\mathbf{1}$, it seems reasonable to extend this matrix to the four-dimensional counterpart

$$\bar{\mathbf{A}} = \begin{pmatrix} a & b & c & 0 \\ b & d & e & 0 \\ c & e & f & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6.29}$$

This choice guarantees that no arbitrary anisotropy is introduced in the fourth dimension and that $\det\bar{\mathbf{A}}=\mathbf{1}$.

A corresponding problem would arise in an ε expansion in $d=2+\varepsilon$ dimensions. In Sec. VIII D, we shall present an example where we compare the anisotropy effects of two- and three-dimensional models. The result of this comparison supports the suggestion given above for the dimensional extension of the matrix $\bar{\mathbf{A}}$ in an ε expansion.

C. Large-*n* limit

For comparison with the case $n=1$, we also present the exact result for the finite-size scaling function $\mathcal{F}_\infty$ of the free-energy density per component $f_\infty(t,L)$ of the φ^4 lattice model (2.1) with $v=\tilde{a}^d$ and $V=L^d$ in the limit $n\to\infty$ at fixed u_0n. From Eqs. (45) and (46) of Ref. [87], we have

$$f_\infty(t,L) = \lim_{n\to\infty}\{-(nV)^{-1}\ln Z(t,0,L)\} = \hat{f}_0 - \frac{(r_0-\chi_\infty^{-1})^2}{16u_0n} + \frac{1}{2V}\sum_{\mathbf{k}}\ln\{[\chi_\infty^{-1}+\delta\hat{K}(\mathbf{k})]\tilde{a}^2\}, \tag{6.30}$$

where $Z(t,0,L)$ is defined by Eq. (2.3) and χ_∞^{-1} is determined implicitly by $\chi_\infty^{-1}=r_0+4u_0nV^{-1}\Sigma_{\mathbf{k}}[\chi_\infty^{-1}+\delta\hat{K}(\mathbf{k})]^{-1}$. The additive constant in Eq. (6.30) is $\hat{f}_0=-[\ln(2\pi)]/(2\tilde{a}^d)$. Using the results of Appendix C leads to the singular part of f_∞ in the regime $L'\gg\tilde{a}$ and $0\le|\tilde{x}|\lesssim O(1)$ at $h=0$ for $2<d<4$,

$$f_{\infty,s}(t,L;\mathbf{A}) = L^{-d}\mathcal{F}_\infty(\tilde{x};\bar{\mathbf{A}}), \tag{6.31}$$

$$\mathcal{F}_\infty(\tilde{x};\bar{\mathbf{A}}) = \frac{1}{2}\mathcal{G}_0(P^2;\bar{\mathbf{A}}) + \frac{A_d}{2(4-d)}\left[\tilde{x}P^2 - \frac{2}{d}P^d\right], \tag{6.32}$$

$$P^{d-2} = \tilde{x} - \frac{4-d}{A_d}\mathcal{G}_1(P^2;\bar{\mathbf{A}}), \tag{6.33}$$

$$\mathcal{G}_j(P^2;\bar{\mathbf{A}}) = (4\pi^2)^{-j}\int_0^\infty dy\,y^{j-1}\exp\left(-\frac{P^2y}{4\pi^2}\right)\times\left\{\left(\frac{\pi}{y}\right)^{d/2} - K_d(y,\bar{\mathbf{A}})\right\}. \tag{6.34}$$

Here $\tilde{x}=t(L'/\xi'_{0+})^{1/\nu}$ with $\nu=(d-2)^{-1}$, $L'=(\det\mathbf{A})^{-1/(2d)}L$, $\xi'_{0+}=(4u_0'nA_da_0^{-1}/\varepsilon)^\nu$, and $u_0'=(\det\mathbf{A})^{-1/2}u_0$. We note that the geometric factor A_d, Eq. (5.2), appears in Eqs. (6.31)–(6.34) in a natural way. The reason is that only diagrammatic contributions of single-loop structures contribute to the large-n limit. The function $(1/2)\mathcal{G}_0(\tilde{x};\bar{\mathbf{A}})$ with $\tilde{x}=r_0L'^2$ is the scaling function of the excess free-energy density of the Gaussian model [see Eqs. (B13)–(B17) ofAppendix B]. For $T\ge T_c$, the function $P(\tilde{x};\bar{\mathbf{A}})$ determines the finite-size scaling form of the susceptibility per component in the limit $n\to\infty$ [12],

$$\chi_\infty^+(t,L;\bar{\mathbf{A}}) = L'^{\gamma/\nu}g(\tilde{x};\bar{\mathbf{A}}),\quad \gamma/\nu=2, \tag{6.35}$$

where $g(\tilde{x};\bar{\mathbf{A}})=[P(\tilde{x};\bar{\mathbf{A}})]^{-2}$. Below we shall present the relative anisotropy effect

$$\Delta\chi_{\infty,c}^+(\bar{\mathbf{A}}) = \frac{g(0;\bar{\mathbf{A}})-g(0;\mathbf{1})}{g(0;\mathbf{1})} \tag{6.36}$$

on χ_∞^+ at T_c in three dimensions.

The result (6.31)–(6.35) is the extension of the result for the isotropic case [see Eqs. (17)–(19) of [11]] and corrects Eq. (44) of [12] where the term $-(\ln 2)/2$ should be dropped. The scaling function of the excess free-energy density above, at, and below T_c is given by

$$\mathcal{F}_\infty^{\rm ex}(\tilde{x};\bar{\mathbf{A}}) = \mathcal{F}_\infty(\tilde{x};\bar{\mathbf{A}}) - \mathcal{F}_{\infty,b}^{\pm}(\tilde{x}) \quad (6.37)$$

with the bulk part

$$\mathcal{F}_{\infty,b}^{\pm}(\tilde{x}) = \begin{cases} Y\tilde{x}^{d\nu} & \text{for } T>T_c, \\ 0 & \text{for } T<T_c, \end{cases} \quad (6.38)$$

where $Y=(d-2)A_d/[2d(4-d)]$. At T_c, the finite-size amplitude is given by

$$\mathcal{F}_\infty(0;\bar{\mathbf{A}}) = \frac{1}{2}\mathcal{G}_0(P_c^2;\bar{\mathbf{A}}) - \frac{A_d}{d(4-d)}P_c^d, \quad (6.39)$$

where $P_c(\bar{\mathbf{A}}) \equiv P(0;\bar{\mathbf{A}})$ is determined by

$$P_c^{d-2} = -\frac{4-d}{A_d}\mathcal{G}_1(P_c^2;\bar{\mathbf{A}}). \quad (6.40)$$

VII. OTHER FINITE-SIZE SCALING FUNCTIONS

The calculations of the preceding sections can be extended to other finite-size quantities. Here we consider only those quantities that have been studied in MC simulations of anisotropic Ising models [42–44]. Within our φ^4 lattice model (2.1) for $n=1$ at $h=0$ on a simple-cubic lattice with volume $V=L^d$, we shall consider the susceptibilities $\chi^+ = V\langle\Phi^2\rangle$, $\chi^- = V(\langle\Phi^2\rangle - \langle|\Phi|\rangle^2)$, and the Binder cumulant

$$U = 1 - \frac{1}{3}\langle\Phi^4\rangle/\langle\Phi^2\rangle, \quad (7.1)$$

where $\Phi = N^{-1}\Sigma_j\varphi_j$ (see, e.g., [66]). These quantities remain invariant under the transformation defined in Sec. II [13], $\chi^\pm = (\chi^\pm)', U=U'$. As a consequence we find that, in the regime (b) defined in Sec. IV A, the finite-size scaling forms of these quantities are

$$\chi^\pm(t,L;\mathbf{A}) = (\chi^\pm)'(t,L';\bar{\mathbf{A}}) = (L'/\xi'_{0+})^{\gamma/\nu}P_\chi^\pm(\tilde{x};\bar{\mathbf{A}}), \quad (7.2)$$

$$U(t,L;\mathbf{A}) = U'(t,L';\bar{\mathbf{A}}) = U(\tilde{x};\bar{\mathbf{A}}), \quad (7.3)$$

where the scaling functions $P_\chi^\pm$ and U are obtained from those of [66] by the replacements $Y \to Y(\tilde{x};\bar{\mathbf{A}})$ and $R_2 \to R_2(1,\tilde{l},\bar{\mathbf{A}})$. Note that the functions $P_\chi^\pm$ are nonuniversal even for $\bar{\mathbf{A}}=\mathbf{1}$ since they still contain nonuniversal overall amplitudes $c^\pm$ proportional to the bulk amplitudes of $\chi^\pm$ (see also [68]). Here we consider only the *relative* anisotropy effect

$$\Delta\chi_c^\pm(\bar{\mathbf{A}}) = \frac{P_\chi^\pm(0;\bar{\mathbf{A}}) - P_\chi^\pm(0;\mathbf{1})}{P_\chi^\pm(0;\mathbf{1})} \quad (7.4)$$

on the susceptibilities $\chi^\pm(0,L;\mathbf{A})$ at $T=T_c$. The analytic expressions are in $2<d<4$ dimensions,

$$P_\chi^+(0;\bar{\mathbf{A}}) = c^+[1-18u^*R_2(1,\tilde{l}_c,\bar{\mathbf{A}})]^{-1}\vartheta_2[Y_c(\bar{\mathbf{A}})], \quad (7.5)$$

$$P_\chi^-(0;\bar{\mathbf{A}}) = c^-[1-18u^*R_2(1,\tilde{l}_c,\bar{\mathbf{A}})]^{-1} \times(\vartheta_2[Y_c(\bar{\mathbf{A}})] - \{\vartheta_1[Y_c(\bar{\mathbf{A}})]\}^2), \quad (7.6)$$

where the constants $c^\pm$ are independent of $\bar{\mathbf{A}}$ and drop out of the ratio (7.4). For $Y_c(\bar{\mathbf{A}})$ and $R_2(1,\tilde{l}_c,\bar{\mathbf{A}})$, see Eqs. (6.14) and (6.16); for $\vartheta_m(Y)$, see Eq. (4.43). The anisotropy effect on the Binder cumulant $U(0;\bar{\mathbf{A}})$ at T_c will be described by the difference

$$\Delta U_c(\bar{\mathbf{A}}) = U(0;\bar{\mathbf{A}}) - U(0;\mathbf{1}), \quad (7.7)$$

where

$$U(0;\bar{\mathbf{A}}) = 1 - \frac{1}{3}\vartheta_4[Y_c(\bar{\mathbf{A}})]\{\vartheta_2[Y_c(\bar{\mathbf{A}})]\}^{-2}. \quad (7.8)$$

VIII. QUANTITATIVE RESULTS AND PREDICTIONS

For the application to three dimensions, we shall employ the same values as previously [66,75], $A_3=(4\pi)^{-1}$, $\nu=0.6335$, $u^*=0.0412$, $Q^*=0.945$, $B(u^*)=0.50$. For reasons of consistency, a slightly different value will be used for $\alpha=2-3\nu=0.0995$ in order to exactly satisfy the hyperscaling relation (6.3).

A. Universal bulk amplitude ratios

Evaluating our analytic expressions for the bulk amplitude ratios (6.19) and (6.20) in three dimensions, we obtain for *isotropic* systems [compare Eq. (3.12)]

$$f'^{+}_{s,b}\xi'^{3}_{+} = Q_1 = -0.119, \quad A^-/A^+ = 2.04. \quad (8.1)$$

This can be compared with the series expansion results for the three-dimensional Ising model by Liu and Fisher [75], who calculated the amplitude ratios $(R_\xi^+)^3 = 0.0188 \pm 0.0001$ and $A^+/A^- = 0.523 \pm 0.009$. These calculations were carried out for several different cubic (sc, bcc, fcc) lattice structures in order to test bulk universality (see also [74]). The relation between R_ξ^+ and Q_1 is $(R_\xi^+)^3 = -\alpha(1-\alpha)(2-\alpha)Q_1$. This yields the central values of the Ising model based on series expansions,

$$Q_{1|\text{Ising}} = -0.1099, \quad A^-/A^+_{|\text{Ising}} = 1.91. \quad (8.2)$$

Considering the fact that our present theory is an effective finite-size theory that is not designed to produce highly accurate bulk predictions, the results (8.1) are in acceptable agreement with Eq. (8.2). As seen from Eqs. (6.17)–(6.19), the bulk results for the free energy are sensitive to the choice of the geometrical factor in defining the renormalized coupling, Eq. (5.1). The results (8.1) demonstrate the appropriateness of the choice of A_d, Eq. (5.2).

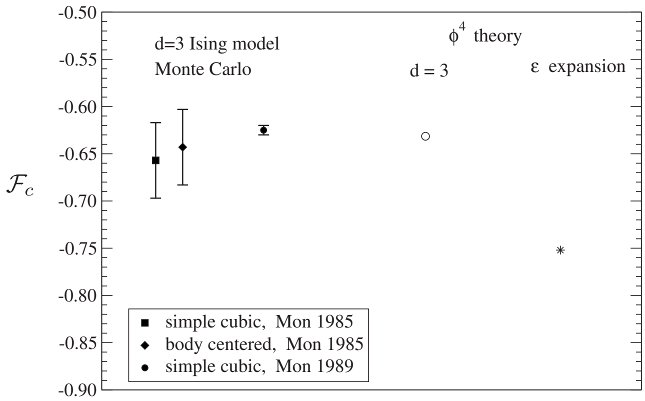

FIG. 5. Finite-size amplitude $\mathcal{F}_c(\mathbf{1})$, Eqs. (6.12) and (8.5), of the free-energy density of isotropic systems in a cubic geometry at T_c for $n=1$ in three dimensions (open circle), and at $\varepsilon=1$, Eq. (8.7) (star), of the ε expansion (6.25). MC data for the three-dimensional Ising model on sc and bcc lattices [34,35].

B. Finite-size free energy of isotropic systems

1. Test of the $d=3$ theory: Amplitude at T_c

In order to test the reliability of our finite-size theory, we first consider the isotropic case $\bar{\mathbf{A}}=\mathbf{1}$, $\xi'_{0+}=\xi_{0+}$, where accurate MC data by Mon [34–36] are available.

The first set of data was obtained for the three-dimensional Ising model with NN couplings on sc and bcc lattices. These systems have different values of T_c and different correlation-length amplitudes ξ_{0+}, but both belong to the subclass of (asymptotically) isotropic systems with $\bar{\mathbf{A}}=\mathbf{1}$. Within the error bars, the MC results for the finite-size amplitude $\mathcal{F}_c(\mathbf{1})$ of the free-energy density at T_c [34],

$$\mathcal{F}_c(\mathbf{1})^{\mathrm{MC}} = \begin{cases} -0.657 \pm 0.03 & \text{(sc lattice)} \\ -0.643 \pm 0.04 & \text{(bcc lattice)}, \end{cases} \tag{8.3}$$

are consistent with the universality hypothesis. Subsequently, the more accurate MC result at T_c was obtained [35],

$$\mathcal{F}_c(\mathbf{1})^{\mathrm{MC}} = -0.625 \pm 0.005 \quad \text{(sc lattice)}, \tag{8.4}$$

which is also consistent with Eq. (8.3).

In three dimensions, the numerical values of the quantities $\tilde{l}_c, J_0, I_1$, and I_2 in our analytical result (6.12) are $\tilde{l}_c=2.042$, $J_0(\tilde{l}_c^2,\mathbf{1})=1.6430$, $I_1(\tilde{l}_c^2,\mathbf{1})=-4.1581$, and $I_2(\tilde{l}_c^2,\mathbf{1})=-15.4032$. This yields the theoretical prediction for the finite-size amplitude,

$$\mathcal{F}_c(\mathbf{1})_{d=3} = -0.6315, \tag{8.5}$$

in excellent agreement with the MC results (8.3) and (8.4) (Fig. 5).

2. Epsilon expansion at T_c

For comparison, we also evaluate the result of the ε expansion (6.25). For isotropic systems ($\bar{\mathbf{A}}=\mathbf{1}$), the coefficients in Eq. (6.25) are well defined. The numerical values are

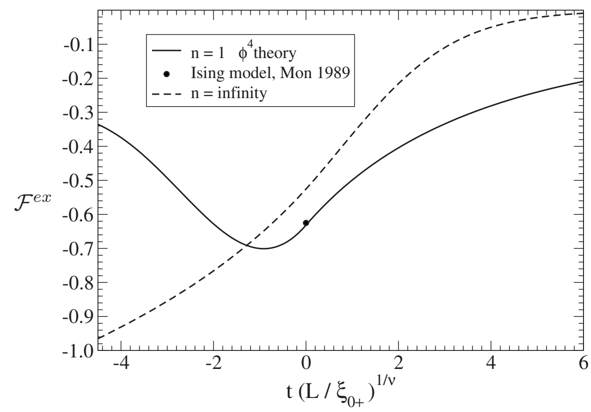

FIG. 6. Scaling functions $\mathcal{F}^{\mathrm{ex}}(\tilde{x};\mathbf{1})$, Eqs. (6.22), (6.10), and (6.23) for $n=1$ (solid line), and $\mathcal{F}^{\mathrm{ex}}_\infty(\tilde{x};\mathbf{1})$, Eqs. (6.37), (6.32), and (6.38) for $n=\infty$ (dashed line), for the excess free-energy density of isotropic systems in three dimensions as a function of the scaling variable $\tilde{x}=t(L/\xi_{0+})^{1/\nu}$. MC result (full circle) for the Ising model on a sc lattice [35].

$$f_0(\mathbf{1}) = -0.3302, \quad f_1(\mathbf{1}) = -0.4218, \tag{8.6}$$

where $\mathbf{1}$ denotes the 4×4 unity matrix. For $\varepsilon=1$, the terms up to $O(\varepsilon^{1/2})$ of Eq. (6.25) yield

$$\mathcal{F}_c(\mathbf{1})_{\varepsilon=1} = -0.7520, \tag{8.7}$$

which is in less good agreement with the MC results (8.3) and (8.4) (Fig. 5).

3. Finite-size scaling function

In three dimensions, the numerical evaluation of the scaling function $\mathcal{F}^{\mathrm{ex}}(\tilde{x},\mathbf{1})_{d=3}$ as given in Eqs. (6.22), (6.10), and (6.23) yields the curve shown in Fig. 6 in the range $-4.5 \leq \tilde{x} \leq 6$ (solid curve). This range corresponds to the central finite-size regime (b) mentioned in Sec. IV A. A minimum with

$$\mathcal{F}^{\mathrm{ex}}(\tilde{x}_{\min};\mathbf{1})_{d=3} = -0.701, \quad \tilde{x}_{\min} = -0.910 \tag{8.8}$$

exists slightly below T_c. For the subclass of isotropic systems within the $(d=3,n=1)$ universality class, both the position $\tilde{x}_{\min}$ and the value $\mathcal{F}^{\mathrm{ex}}(\tilde{x}_{\min};\mathbf{1})_{d=3}$ are predicted to be universal numbers. This can be tested by MC simulations for families of three-dimensional Ising models with $\bar{\mathbf{A}}=\mathbf{1}$ (e.g., on sc, fcc, or bcc lattices with isotropic interactions) in a cube with periodic boundary conditions. The nonuniversal differences of these models are predicted to be absorbable entirely in different values of ξ'_{0+}. In *two* dimensions, such tests of universality for the critical Binder cumulant of isotropic systems at T_c have been performed very recently by Selke [59].

Our analytical result for $\mathcal{F}^{\mathrm{ex}}(\tilde{x};\mathbf{1})_{d=3}$ is not applicable far outside the range of $\tilde{x}$ shown in Fig. 6. In the limits $\tilde{x} \to \pm\infty$, this result does not correctly describe the exponential decay to zero in the regimes (a) and (c) mentioned in Sec. IV A, as expected.

For comparison, we also present the exact result for the scaling function $\mathcal{F}^{\mathrm{ex}}_\infty(\tilde{x};\mathbf{1})$ in the large-n limit in three dimensions. For $\bar{\mathbf{A}}=\mathbf{1}$ and $d=3$, the numerical solutions of Eqs.

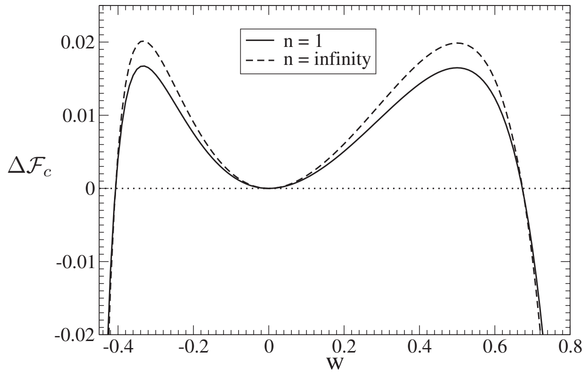

FIG. 7. Differences $\Delta\mathcal{F}_c[\bar{\mathbf{A}}(w)]$, Eq. (8.10), and $\Delta\mathcal{F}_{c,\infty}[\bar{\mathbf{A}}(w)]$, Eq. (8.11), of the finite-size amplitudes (6.12) and (6.39) of the free-energy density of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}(w)$, Eq. (2.15), in a cubic geometry at T_c for $n=1$ (solid line) and $n=\infty$ (dashed line) in three dimensions as a function of the anisotropy parameter w, Eq. (2.16).

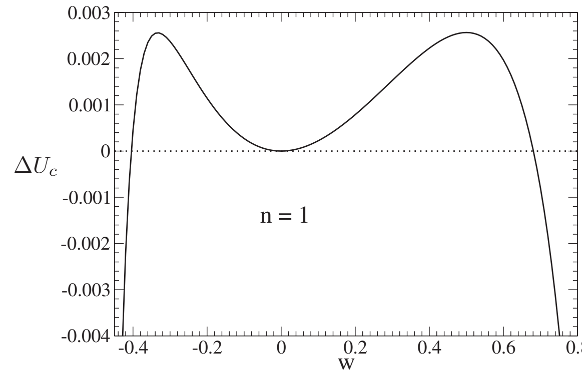

FIG. 8. Difference $\Delta U_c[\bar{\mathbf{A}}(w)]$, Eq. (7.7), of the Binder cumulant (7.8) of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}(w)$, Eq. (2.15), in a cubic geometry at T_c for $n=1, d=3$ as a function of the anisotropy parameter w, Eq. (2.16).

(6.40) and (6.39) at $T=T_c$ are $P_c(\mathbf{1})=1.946$ and

$$\mathcal{F}_\infty^{\text{ex}}(0;\mathbf{1}) = \mathcal{F}_\infty(0;\mathbf{1}) = -0.526. \tag{8.9}$$

In Fig. 6, the scaling function $\mathcal{F}_\infty^{\text{ex}}(\tilde{x};\mathbf{1})$, Eq. (6.32), is shown in three dimensions (dashed curve). Unlike the case $n=1$, $\mathcal{F}_\infty^{\text{ex}}(\tilde{x};\mathbf{1})$ does not have a minimum at finite $\tilde{x}$ below T_c but has a slow monotonic decrease toward a finite negative constant $\mathcal{F}_\infty^{\text{ex}}(-\infty;\mathbf{1})=-3.18$. Above T_c, it decays exponentially to zero (but not with the correct exponential form, see Sec. X.).

C. Three-dimensional anisotropy

In the following, we present quantitative predictions for the nonuniversal effect of a noncubic anisotropy on the finite-size scaling functions in three dimensions. We illustrate the three-dimensional anisotropy effects for the example of $\mathbf{A}$ and $\bar{\mathbf{A}}$ given in Eqs. (2.14) and (2.15) of Sec. II. In this example, $\bar{\mathbf{A}}(w)$ depends only on the single anisotropy parameter w, Eq. (2.16), $-\frac{1}{2}<w<1$. The crucial anisotropy function is given by Eq. (4.46), which enters the functions J_0, I_1, and I_2 defined in Eqs. (4.44) and (4.45).

First we consider the anisotropy effect on the finite-size amplitude of the free-energy density for $n=1$ and $n=\infty$ at $T=T_c$ as described by the differences

$$\Delta\mathcal{F}_c[\bar{\mathbf{A}}(w)] = \mathcal{F}(0;\bar{\mathbf{A}}(w)) - \mathcal{F}(0;\mathbf{1}), \tag{8.10}$$

$$\Delta\mathcal{F}_{c,\infty}[\bar{\mathbf{A}}(w)] = \mathcal{F}_\infty(0;\bar{\mathbf{A}}(w)) - \mathcal{F}_\infty(0;\mathbf{1}), \tag{8.11}$$

where $\mathcal{F}(0;\bar{\mathbf{A}})$ and $\mathcal{F}_\infty(0;\bar{\mathbf{A}})$ are given by Eqs. (6.12) and (6.39). This is shown in Fig. 7 in the range $-0.45<w<0.80$. The anisotropy effect is well pronounced for both positive and negative values of w, with a non-negligible n dependence. For both $n=1$ and $n=\infty$, two maxima of almost equal heights exist at $w_{\max}=-0.333$ and 0.500, with $\Delta\mathcal{F}_{c,\max}=0.0167$ and 0.0165, respectively, for $n=1$. (The slight difference of the two heights is presumably not a consequence of the approximations made for $n=1$; such a difference exists also for the exact result for $n=\infty$, where $\Delta\mathcal{F}_{c,\infty,\max}=0.0202$ and 0.0199 at $w_{\max}=-0.333$ and 0.500, respectively.) At $w=-0.45$ and 0.80, we predict the larger negative values $\Delta\mathcal{F}_c=-0.069$ and -0.079, respectively (not shown in Fig. 7).

The corresponding anisotropy effect on the Binder cumulant for $n=1$ at T_c is shown in Fig. 8 as described by the difference $\Delta U_c[\bar{\mathbf{A}}(w)]$, Eq. (7.7) [88]. Figures 7 and 8 imply that the *relative* anisotropy effect on the free energy $\Delta\mathcal{F}_c[\bar{\mathbf{A}}(w)]/\mathcal{F}_c(\mathbf{1})$ for $n=1$ is considerably larger than that on the Binder cumulant. For the free energy, it is predicted to be of $O(2.5\%)$ at the maxima, which may be detectable in future MC simulations of the three-dimensional Ising model. By contrast, the corresponding relative effect on the Binder cumulant $\Delta U_c[\bar{\mathbf{A}}(w)]/U(0;\mathbf{1})$ for $n=1$ is predicted to be only of $O(0.6\%)$ at the maxima. It becomes quite large, however, in the regime $w<-0.45$, as shown in Fig. 1 of [12], and in the regime $w>0.8$. Previous MC simulations[42] of the anisotropic three-dimensional Ising model in the range $-0.48\le w\le 0$ are in disagreement with our results for the Binder cumulant (see also [43]).

In Fig. 9, we also show the predicted relative anisotropy effect on the susceptibilities χ^+ and χ^- for $n=1$ and on χ_∞^+ for $n=\infty$ at T_c in the same range of w. While this effect is of $O(1\%)$ near the maxima of the susceptibilities χ^+ and χ_∞^+, the corresponding effect on the susceptibility χ^- is only of $O(0.1\%)$. Previous MC simulations [42,43] on χ^- did not resolve this small anisotropy effect.

Our prediction of the anisotropy effect on the finite-size scaling function $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}}(w))$ for $n=1$ near the minimum below T_c is shown in Fig. 10 for several w. While the position of the minimum $\tilde{x}_{\min}$ depends only weakly on the anisotropy, the value $\mathcal{F}^{\text{ex}}(\tilde{x}_{\min};\mathbf{1})$ is significantly changed relative to the isotropic case (dotted curve in Fig. 10). This effect is well outside the error bars of the MC data by Mon for the isotropic case [34,35] and may be detectable in future MC simulations.

D. Two-dimensional anisotropy

Highly precise numerical information on the nonuniversal anisotropy effect on the critical Binder cumulant U of the

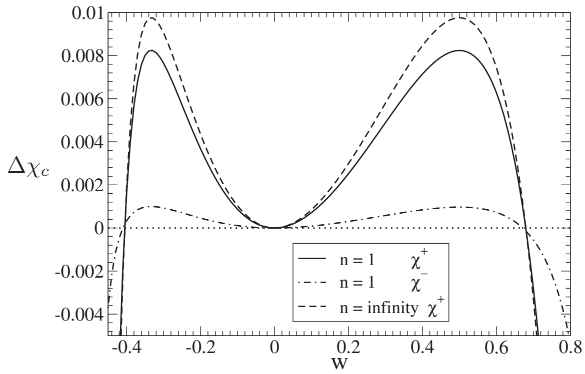

FIG. 9. Relative anisotropy effect on the susceptibilities χ^+ and χ^- for $n=1$, Eq. (7.2), and χ^+_∞ for $n=\infty$, Eq. (6.35), at T_c of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}(w)$, Eq. (2.15), in three dimensions in a cubic geometry as a function of the anisotropy parameter w, Eq. (2.16), as described by $\Delta\chi^\pm_c[\bar{\mathbf{A}}(w)]$, Eq. (7.4) (solid and dot-dashed lines) and $\Delta\chi^+_{\infty,c}[\bar{\mathbf{A}}(w)]$, Eq. (6.36) (dashed line).

two-dimensional Ising model has been provided recently by MC simulations of Selke and Shchur [44]. They considered finite square lattices with isotropic ferromagnetic NN couplings $K_x=K_y\equiv K>0$ and an anisotropic NNN coupling J only in the $\pm(1,1)$ directions but not in the $\pm(-1,1)$ directions [Fig. 11(a)]. They found a nonmonotonic dependence of U on the ratio J/K (as shown in Fig. 4 of Ref. [44]).

The anisotropy matrix of the corresponding two-dimensional φ^4 lattice model is [13]

$$\mathbf{A}_2 = 2\tilde{a}^2\begin{pmatrix} K+J & J \\ J & K+J \end{pmatrix} \tag{8.12}$$

with the reduced anisotropy matrix

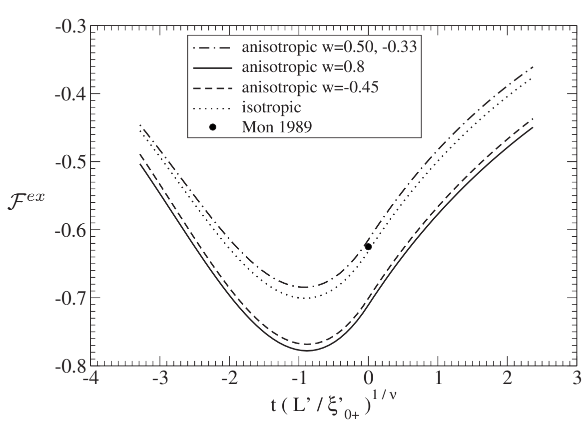

FIG. 10. Scaling function $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}}(w))$, Eqs. (6.22), (6.10), and (6.23), of the excess free-energy density of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}(w)$, Eq. (2.15), for $n=1$ in a cubic geometry in three dimensions as a function of the scaling variable $\tilde{x}=t(L'/\xi'_{0+})^{1/\nu}$ for several values of the anisotropy parameter w, Eq. (2.16): $w=0.50,-0.33$ (dot-dashed line), $w=0.80$ (solid line), $w=-0.45$ (dashed line), and $w=0$ (dotted line). MC result (full circle) for the three-dimensional Ising model on a sc lattice [35].

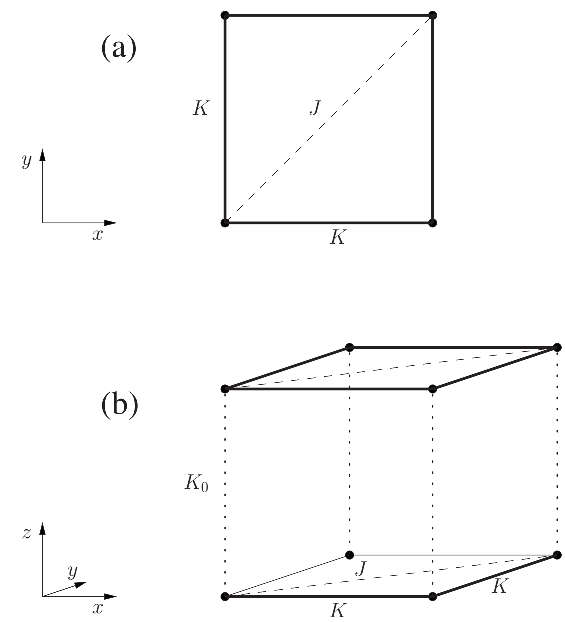

FIG. 11. Lattice points of the primitive cell of (a) a square lattice, (b) a simple-cubic lattice, with isotropic NN couplings $K_x=K_y=K$ (solid lines), with an anisotropic NNN coupling J in the x-y planes (dashed lines), and a NN coupling K_0 in the z direction (dotted lines). The corresponding anisotropy matrices $\mathbf{A}_2,\bar{\mathbf{A}}_2$ and $\mathbf{A}_3,\bar{\mathbf{A}}_3$ are given by Eqs. (8.12) and (8.13) and Eqs. (8.15) and (8.17), respectively.

$$\bar{\mathbf{A}}_2(s) = \mathbf{A}_2/(\det \mathbf{A}_2)^{1/2} = (1-s^2)^{-1/2}\begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix} \tag{8.13}$$

and with the single anisotropy parameter

$$s = \frac{J}{K+J} = (1+K/J)^{-1}. \tag{8.14}$$

By universality it is expected [13] that (in some range of $\bar{\mathbf{A}}_2$ near $\mathbf{1}$ and for sufficiently large L) the two-dimensional φ^4 model has the same anisotropy effects at T_c as the two-dimensional Ising model if both models have the same reduced anisotropy matrix $\bar{\mathbf{A}}_2$. Unfortunately, at present, it is not known how to perform quantitative finite-size calculations for the φ^4 model in *two* dimensions.

It is possible, however, to incorporate a two-dimensional anisotropy of the type shown in Fig. 11(a) in a three-dimensional φ^4 (or Ising) model on a simple-cubic lattice with isotropic NN couplings $K_x=K_y=K>0$, with an anisotropic NNN coupling $J_1\equiv J\neq 0$ in the x-y planes, and with an additional NN coupling $K_0>0$ in the z direction [Fig. 11(b)]. The corresponding anisotropy matrix is

$$\mathbf{A}_3 = 2\tilde{a}^2\begin{pmatrix} K+J & J & 0 \\ J & K+J & 0 \\ 0 & 0 & K_0 \end{pmatrix}. \tag{8.15}$$

The eigenvalues and eigenvectors are $\lambda_1=2\tilde{a}^2(K+2J)$, $\lambda_2=2\tilde{a}^2K$, $\lambda_3=2\tilde{a}^2K_0$,

$$\mathbf{e}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad \mathbf{e}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\end{pmatrix}, \quad \mathbf{e}^{(3)} = \begin{pmatrix}0\\0\\1\end{pmatrix}. \tag{8.16}$$

The eigenvalues are positive in the range $-\frac{1}{2} < J/K < \infty$, $K > 0$, $K_0 > 0$. In the limit $J/K \to \infty$ and $J/K_0 \to \infty$ (or $K \to 0_+$ and $K_0 \to 0_+$ at finite $J > 0$), the model represents a system of variables φ_i on decoupled one-dimensional chains with ferromagnetic NN interactions.

In its present form, the matrix $\mathbf{A}_3$, Eq. (8.15), contains both a two-dimensional anisotropy due to J and an additional anisotropy due to the coupling K_0. Although $\mathbf{A}_3$ contains $\mathbf{A}_2$ as a decoupled 2×2 submatrix, it is not expected that, for general fixed K_0, this three-dimensional model exhibits the same type of anisotropy effect (as a function of the ratio J/K) as the two-dimensional model with the matrix (8.12). The reason is that it is not $\mathbf{A}_3$ itself but rather the *reduced* anisotropy matrix $\bar{\mathbf{A}}_3 = \mathbf{A}_3/(\det \mathbf{A}_3)^{1/3}$ that governs the anisotropy effect according to the results of the preceding sections. This matrix is given by

$$\bar{\mathbf{A}}_3 = [\overline{K_0}(1-s^2)]^{-1/3}\begin{pmatrix}1 & s & 0\\ s & 1 & 0\\ 0 & 0 & \overline{K_0}\end{pmatrix}, \tag{8.17}$$

$$\overline{K_0} = \frac{K_0}{(K+J)} = \frac{K_0}{K}(1-s). \tag{8.18}$$

We see that the J dependence of $\bar{\mathbf{A}}_3$ differs qualitatively from that of $\bar{\mathbf{A}}_2$ because of the additional s dependence of $\overline{K_0}$ at given $K_0/K > 0$. What is needed is a kind of *isotropic extension* of the two-dimensional matrix (8.13) to three dimensions parallel to the proposed four-dimensional extension (6.29) of the three-dimensional matrix $\bar{\mathbf{A}}$, Eq. (6.28). This is achieved by the choice $\overline{K_0} = 1$ or $K_0 = K + J$. Then the reduced anisotropy matrix becomes

$$\bar{\mathbf{A}}_3(s) = (1-s^2)^{-1/3}\begin{pmatrix}1 & s & 0\\ s & 1 & 0\\ 0 & 0 & 1\end{pmatrix} \tag{8.19}$$

with the same anisotropy parameter s as in Eqs. (8.13) and (8.14). [Naively one might have expected that the choice of the additional NN coupling should have been $K_0 = K$ instead of $K_0 = K + J$. But in this case the third diagonal element of $\bar{\mathbf{A}}_3$ would become $(\bar{A}_3)_{zz} = (1-s^2)^{-1/3}(1-s)^{2/3}$ rather than $(1-s^2)^{-1/3}$, which would produce a qualitatively different anisotropy effect that is not an even function of s.]

We have evaluated numerically the expressions (7.8), (4.43), and (6.14) in three dimensions for the Binder cumulant $U(0;\bar{\mathbf{A}}_3(s))$ at T_c using the matrix $\bar{\mathbf{A}}_3(s)$, Eq. (8.19). The result is shown in Fig. 12 in the range $-0.8 < s < 0.8$. The range $0 \le s \le 0.8$ corresponds to the range $0 \le J/K \le 4.0$ studied by Selke and Shchur [44]. The anisotropy effect shows up as a nonmonotonic dependence on s. It is an even function of the anisotropy parameter s and exhibits two

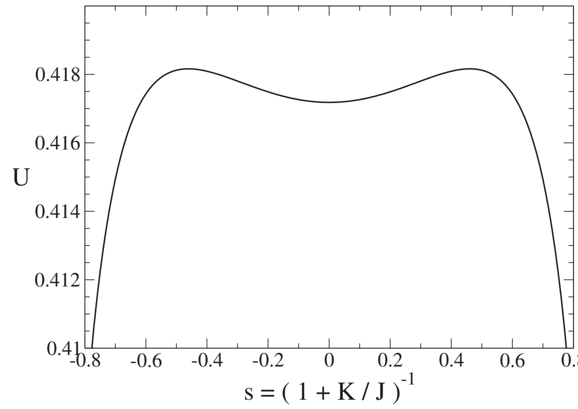

FIG. 12. Binder cumulant $U(0;\bar{\mathbf{A}}_3(s))$, Eqs. (7.8), (4.43), and (6.14), for anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}_3(s)$, Eq. (8.19), in a cubic geometry at T_c for $n=1$ in three dimensions as a function of the anisotropy parameter s, Eq. (8.14).

maxima of equal height at $s_{max} = \pm 0.461$ corresponding to $J/K = 0.855$ and -0.316. This symmetry is a consequence of the symmetry property $K_3(y, \bar{\mathbf{A}}_3(s)) = K_3(y, \bar{\mathbf{A}}_3(-s))$ of the function (4.46). The symmetry is hidden if U is plotted as a function of J/K, in which case the curve is asymmetrically distorted (see our Fig. 13 and Fig. 4 of [44]). Our theoretical value $U(0;\mathbf{1}) = U(0;\bar{\mathbf{A}}_3(0)) = 0.417$ for the isotropic three-dimensional φ^4 theory [66] differs somewhat from the MC result [89] 0.465 of the three-dimensional Ising model on a sc lattice and is, of course, far from the MC result 0.6107 [39] of the *two-dimensional* Ising model on a square lattice. The magnitude of the anisotropy effect, however, turns out to be rather insensitive to the precise value of $U(0;\mathbf{1})$ of the isotropic system.

To exhibit clearly the *deviations* from isotropy and for the purpose of a comparison with the MC data [44] for the anisotropic two-dimensional Ising model, we have plotted in Fig. 13 our theoretical result for the *difference* $\Delta U_c[\bar{\mathbf{A}}_3(s)]$, Eq. (7.7), as a function of J/K together with the correspond-

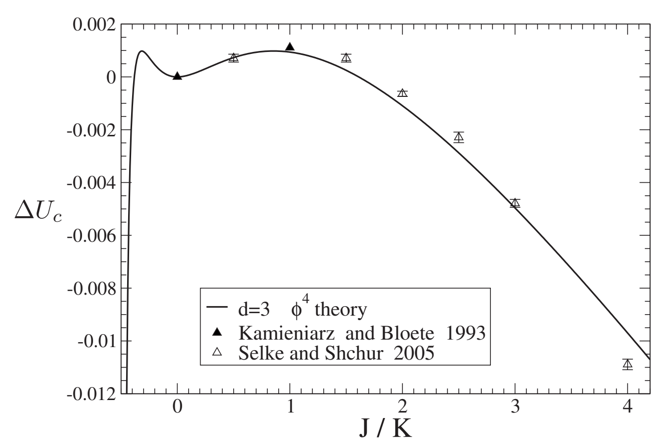

FIG. 13. Difference $\Delta U_c[\bar{\mathbf{A}}_3(s)]$, Eq. (7.7), of the Binder cumulant $U(0;\bar{\mathbf{A}}_3(s))$ shown in Fig. 12 but plotted as a function of J/K, together with the corresponding difference of the MC data of Fig. 4 of [44] for the two-dimensional Ising model.

ing difference of the MC data of Fig. 4 by Selke and Shchur [44]. The theoretical maximal value is $\Delta U_{c,\max}=0.0010$ at $J/K=0.855$ and -0.316. The isotropic value, i.e., $\Delta U_c=0$, is found at $s=0$ and at $s=\pm 0.6169$ corresponding to $J/K=1.611$ and -0.3815. We see that for positive J/K there is remarkable agreement between the MC data in two dimensions and the anisotropic φ^4 theory in three dimensions, thus confirming our expectation regarding the similarity of the anisotropy effect in the two- and three-dimensional models. It should be noted, of course, that no *exact* agreement can be expected. Only the anisotropic *two-dimensional* φ^4 theory (with $n=1$) is expected to yield exactly the same anisotropy effects (in the asymptotic critical region) as the two-dimensional Ising model.

The nonmonotonicity for small *negative* values of J/K and the maximum at $J/K=-0.316$ predicted by our theory was not detected in the preliminary MC simulations by Selke and Shchur [44], who found a *monotonic decrease* of U when taking a weak antiferromagnetic coupling J [90]. It would be interesting to perform more detailed MC simulations for the anisotropic two-dimensional Ising model in the regime of negative J/K.

Very recently, such MC simulations were started by Selke [57] in order to test our prediction for the Binder cumulant in the regime of negative values of J/K. The *positive* value of his MC result [57], $\Delta U_c^{\mathrm{MC}}=0.00056\pm 0.00015$ for $J/K=-0.25$, indeed confirms the predicted *increase* of ΔU_c for small negative J/K according to Fig. 13. More quantitively, there is indeed reasonable agreement with our theoretical result $\Delta U_c=0.00073$ at $J/K=-0.25$ (as shown in Fig. 13) corresponding to $s=-\frac{1}{3}$. It remains to be seen whether the predicted symmetry with regard to s is also confirmed by MC simulations.

We also apply our general result (6.12) for the finite-size amplitude of the free-energy density at T_c to the case of the two-dimensional anisotropy determined by the matrix (8.19). The anisotropy effect as described by the difference $\Delta\mathcal{F}_c[\bar{\mathbf{A}}_3(s)]$ is shown in Fig. 14 for $n=1$ (solid curve). The curve is an even function of s and has two maxima of equal height at $s_{\max}=\pm 0.450$ corresponding to $J/K=0.818$ and -0.310. The theoretical maximal value is $\Delta\mathcal{F}_{c,\max}=0.0060$ for $n=1$. The corresponding effect for $n=\infty$ (dashed curve) as computed from the exact result (6.39) is slightly more pronounced than for $n=1$. Nevertheless, the anisotropy effect for $n=1$ may be detectable by MC calculations for both the three-dimensional and two-dimensional anisotropic Ising models. The two-dimensional model is of course a better candidate, as noted by Selke and Shchur [44], because the value of T_c is known analytically as a function of J/K. Although the solid curve in Fig. 14 is calculated on the basis of the φ^4 theory in *three* dimensions with the reduced anisotropy matrix (8.19), we predict that this curve should be close to the difference $\Delta\mathcal{F}_c[\bar{\mathbf{A}}_2(s)]$ of the free-energy density of the *two-dimensional* Ising model with the reduced anisotropy matrix (8.13). It would be interesting to test this prediction by MC simulations.

For comparison with Fig. 10, we have also computed the nonuniversal anisotropy effect on the finite-size scaling function of $\mathcal{F}^{\mathrm{ex}}$ for the reduced anisotropy matrix (8.19) near the

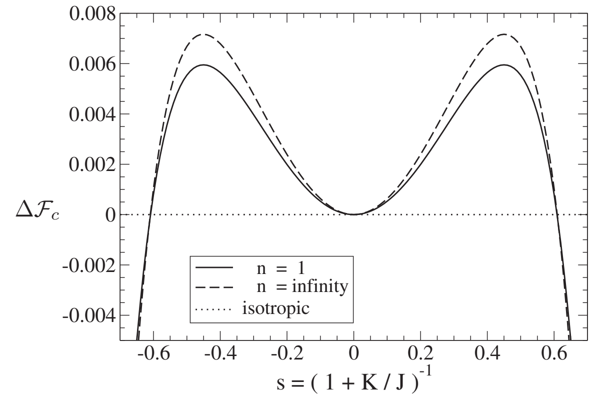

FIG. 14. Differences $\Delta\mathcal{F}_c[\bar{\mathbf{A}}_3(s)]$, Eq. (8.10), and $\Delta\mathcal{F}_{c,\infty}[\bar{\mathbf{A}}_3(s)]$, Eq. (8.11), of the finite-size amplitudes (6.12) and (6.39) of the free-energy density of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}_3(s)$, Eq. (8.19), in a cubic geometry at T_c for $n=1$ (solid line) and $n=\infty$ (dashed line) in three dimensions as a function of the anisotropy parameter s, Eq. (8.14).

minimum below T_c as shown in Fig. 15 for several values of s. Again this effect for $s=\pm 0.80$ is well outside the error bars of the MC data by Mon [34,35] for the isotropic case and may be detectable in future MC simulations.

E. Limit $|s|\to 1$ and Lifshitz point

In Secs. VIII C and VIII D, we assumed the positivity of all eigenvalues $\lambda_\alpha, \alpha=1,2,3$. They vanish in the limits $w\to 1, w\to -1/2$, and $s\to\pm 1$ in which cases our results for ΔU_c and $\Delta\mathcal{F}_c$ are not applicable: they become singular as indicated by the curves in Figs. 7–9 and 12–14. In the following, we confine ourselves to a brief discussion of the limit $s\to\pm 1$ of the model shown in Fig. 11. (A similar dis-

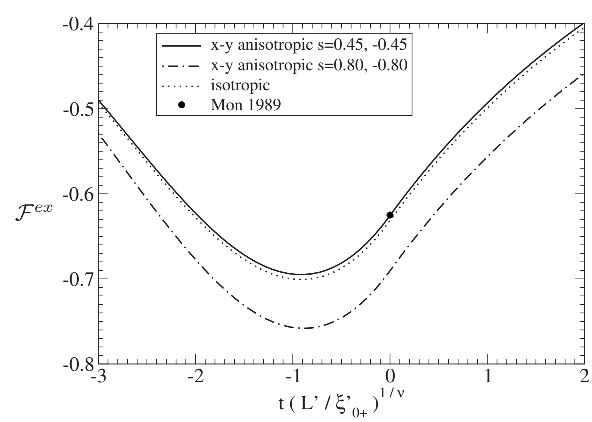

FIG. 15. Scaling function $\mathcal{F}^{\mathrm{ex}}(\tilde{x};\bar{\mathbf{A}}_3(s))$, Eqs. (6.22), (6.10), and (6.23), of the excess free-energy density of anisotropic systems with the reduced anisotropy matrix $\bar{\mathbf{A}}_3(s)$, Eq. (8.19), for $n=1$ in a cubic geometry in three dimensions as a function of the scaling variable $\tilde{x}=t(L'/\xi'_{0+})^{1/\nu}$ for several values of the anisotropy parameter s, Eq. (8.14): $s=0.45,-0.45$ (solid line), $s=0.80,-0.80$ (dot-dashed line), and $s=0$ (dotted line). MC result (full circle) for the three-dimensional Ising model on a sc lattice [35].

cussion could be given for the model shown in Fig. 3 in the limits $w \to 1, w \to -1/2$.)

(i) According to Eq. (8.14), the limit $s \to 1$ can be performed as $K \to 0_+$ at fixed $J>0$ and $K_0>0$ (keeping $\lambda_1>0$ and $\lambda_3>0$ positive while $\lambda_2 \to 0_+$). In this limit, our model is reduced to decoupled *two-dimensional* lattices, which have ferromagnetic NN couplings J and K_0 in the $\pm(1,1,0)$ directions and in the $\pm(0,0,1)$ directions, respectively. Such a model has a ferromagnetic critical point of the $(d=2,n=1)$ universality class. Therefore, it is expected at the outset that the results of our φ^4 theory at fixed $d=3$ must break down for $s \to 1$.

(ii) To discuss the limit $s \to -1$, we first perform a rotation in wave-vector space, $\mathbf{q}=\mathbf{U}_3\mathbf{k}$, by means of the orthogonal matrix determined by the eigenvectors (8.16),

$$\mathbf{U}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}. \tag{8.20}$$

Correspondingly, the inverse propagator $r_0+\delta\hat{K}(\mathbf{k})$ of the Hamiltonian (2.7) is transformed to $r_0+\delta\widetilde{K}(\mathbf{q})$, where $\delta\widetilde{K}(\mathbf{q}) \equiv \delta\hat{K}(\mathbf{U}_3^{-1}\mathbf{q})$ with the interaction part

$$\delta\widetilde{K}(\mathbf{q}) = \sum_{\alpha=1}^{3} \lambda_\alpha q_\alpha^2 + \sum_{\alpha,\beta,\gamma,\delta}^{d} \widetilde{B}_{\alpha\beta\gamma\delta} q_\alpha q_\beta q_\gamma q_\delta + O(q^6), \tag{8.21}$$

where λ_α is given after Eq. (8.15).

On the level of Landau theory, a Lifshitz point exists at $\lambda_1=0$ corresponding to $s=-1$ or $J/K=-\frac{1}{2}$ with a wave-vector instability in the $(1,1,0)$ direction. It is expected, however, that, due to fluctuations, the Lifshitz point occurs at a shifted value $\lambda_1=\lambda_{1\mathrm{LP}}$ that depends on nonuniversal details of the model. [Similarly, r_{0c} depends on all details of the interaction; see Eq. (4.32).] This corresponds to a shifted coupling ratio $(J/K)_{\mathrm{LP}}=-1/2+\lambda_{1\mathrm{LP}}/(2\tilde{a}^2)$, presumably with $\lambda_{1\mathrm{LP}}<0$. To describe the critical behavior near the Lifshitz point would require us to introduce a renormalized shifted eigenvalue according to $\lambda_R=Z_\lambda(\lambda_1-\lambda_{1\mathrm{LP}})$ [91]. It would be interesting to locate this Lifshitz point by MC simulations and to detect the nonuniversal change of finite-size effects [critical Binder cumulant and free energy at $T_c(J/K)$] upon approaching this point along the "λ line" $T=T_c(J/K)$ as $J/K \to (J/K)_{\mathrm{LP}}$. This change can be compared with our predictions shown in the curves of Figs. 12–14 for negative J/K and negative s.

IX. HYPOTHESIS OF RESTRICTED UNIVERSALITY

The results for the finite-size scaling functions (6.10)–(6.16), (6.22), (6.32), (7.3), and (7.8) depend on the nonuniversal anisotropy matrix $\bar{\mathbf{A}}$ but are independent of the bare coupling u_0, of the lattice spacing $\tilde{a}$, of the cutoff of φ^4 field theory, and of the fourth-order moments $B_{\alpha\beta\gamma\delta}$, etc. We anticipate that the finite-size scaling functions would also remain independent of higher-order couplings, such as those of φ^6 terms and of higher-order gradient terms, etc., if they were included in the Hamiltonian. A special matrix $\bar{\mathbf{A}}$ with given matrix elements $\bar{A}_{\alpha\beta}$ can be obtained from various different lattice structures with a large variety of different couplings, both in $O(n)$ symmetric φ^4 lattice models and in $O(n)$ symmetric fixed-length spin models. We expect that $\mathcal{F}(\tilde{x},\bar{\mathbf{A}})$ and $U(\tilde{x},\bar{\mathbf{A}})$ are the same for all those systems whose geometry and boundary conditions are the same and whose reduced anisotropy matrix $\bar{\mathbf{A}}$ is the same. We consider this feature as a kind of *restricted universality within a* (d,n) *universality class*. A nontrivial aspect of this feature is that it is governed by the *bare* anisotropy matrix $\bar{\mathbf{A}}$ containing the *unrenormalized microscopic* couplings. Our approximate results do not yet provide a rigorous proof for the validity of this hypothesis. It would be interesting to test this hypothesis by MC simulations for microscopic spin models with such anisotropy matrices.

For concreteness, consider the three-dimensional anisotropic model (i) of Sec. II A with the three couplings K, J, and $\bar{K}$ as described by the matrix

$$\mathbf{A} = 2\tilde{a}^2\begin{pmatrix} D & J+\bar{K} & J+\bar{K} \\ J+\bar{K} & D & J+\bar{K} \\ J+\bar{K} & J+\bar{K} & D \end{pmatrix}, \tag{9.1}$$

with $D=K+2J+\bar{K}$ and with the reduced matrix $\bar{\mathbf{A}}$, Eq. (2.15). For a given fixed value of the anisotropy parameter w, Eq. (2.16), a family of anisotropic spin models with different couplings K,J, and $\bar{K}$ are predicted to have the same finite-size scaling functions if the third-NN coupling $\bar{K}$ is chosen as

$$\bar{K} = \frac{1}{1-w}[wK-(1-2w)J] \tag{9.2}$$

in the range where $\lambda_\alpha>0$. Equation (9.2) represents a surface in the space of the three couplings K,J, and $\bar{K}$. At $\bar{K}=0$, this surface becomes a "λ line,"

$$J = \frac{w}{1-2w}K, \tag{9.3}$$

along which, at a given fixed value of w, $-\frac{1}{2}<w<\frac{1}{2}$, all finite-size scaling functions of models with the anisotropy matrix (9.1) are predicted to remain unchanged when changing K and J simultaneously according to Eq. (9.3) (in the range $K+J>0, K+4J>0$).

A nontrivial test of our hypothesis applied to *two* dimensions can be performed for the following example. Consider a triangular-lattice model with a shape of a rhombus and with three NN couplings K_1, K_2, K_3, and a NNN coupling J only in the $\pm(3/2,\sqrt{3}/2)$ directions (Fig. 16). The anisotropy matrix of this system with lattice constant $\tilde{a}=1$ is

$$\mathbf{A} = \frac{1}{2}\begin{pmatrix} 4K_1+K_2+K_3+9J & \sqrt{3}(K_2-K_3+3J) \\ \sqrt{3}(K_2-K_3+3J) & 3(K_2+K_3+J) \end{pmatrix}. \tag{9.4}$$

In the absence of the NNN coupling J, isotropy is possible only for the symmetric case $K_1=K_2=K_3$. In this case, the critical Binder cumulant for the $(n=1,d=2)$ universality

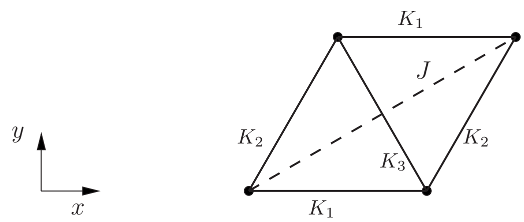

FIG. 16. Lattice points of a triangular lattice with the shape of a rhombus. The solid lines indicate the anisotropic NN couplings K_1, K_2, K_3, the dashed line indicates the anisotropic NNN coupling J. The anisotropy matrix $\mathbf{A}$ is given by Eq. (9.4).

class for periodic boundary conditions is known to very high accuracy [39]: $U=0.611\,827\,7\pm 0.000\,000\,1$. Apart from this case, the system can become isotropic even for $K_3\neq K \equiv K_1=K_2$ if the NNN coupling J is chosen as

$$J=\frac{1}{3}(K_3-K) \tag{9.5}$$

according to Eq. (9.4), in which case

$$\mathbf{A}=\frac{1}{2}\begin{pmatrix} 2K+4K_3 & 0 \\ 0 & 2K+4K_3 \end{pmatrix} \tag{9.6}$$

and $\bar{\mathbf{A}}=\mathbf{1}$. Then, on the basis of our hypothesis of restricted universality, the critical Binder cumulant for $K_3\neq K, J\neq 0$ is predicted to have exactly the same value as found by Kamieniarz and Blöte [39] for $J=0$, $K_3=K$. A corresponding prediction should hold also for other boundary conditions (e.g., free boundary conditions).

X. FINITE-SIZE EFFECTS OUTSIDE THE CENTRAL FINITE-SIZE REGIME

The result $\mathcal{F}^{\rm ex}(\tilde{x};\bar{\mathbf{A}})$, Eqs. (6.22) and (6.10), needs to be complemented outside the central finite-size regime where this result does not have the correct exponential structure for large $|\tilde{x}|$. This is the regime below the dashed lines in Fig. 1. It turns out that it is necessary to further distinguish between a scaling and a nonscaling regime (the latter is the shaded region in Fig. 1). Both regimes belong to the asymptotic critical region. In these regimes, ordinary perturbation theory is appropriate. Here we perform the corresponding analysis above and below T_c at the one-loop level. In order to distinguish the perturbation results of this section from those of the preceding sections, we explicitly include the indices + and − in the notation of $\mathcal{F}^{\rm ex,+}$, f'^{+}, $\mathcal{F}^{\rm ex,-}$, and f'^{-}.

A. Scaling regime

The starting point of ordinary perturbation theory for the bare free-energy density (2.25) for $n=1$ at $h'=0$ is in one-loop order [i.e., up to $O(1)$] (see Appendix B)

$$f'^{+}=f_0'(r_0,L',K_{i,j},v')+O(u_0'), \tag{10.1}$$

$$f'^{-}=\frac{1}{2}r_0 M_{\rm mf}'^{2}+u_0' M_{\rm mf}'^{4}+f_0'(-2r_0,L',K_{i,j},v')+O(u_0') \tag{10.2}$$

above and below T_c, respectively, where $M_{\rm mf}'^{2}$ is given by Eq. (4.13) and

$$f_0'(r_0,L',K_{i,j},v')=-\frac{\ln(2\pi)}{2v'}+\frac{1}{2L'^{d}}\sum_{\mathbf{k}'}\ln\{[r_0+\delta\hat{K}'(\mathbf{k}')]\times(v')^{2/d}\}. \tag{10.3}$$

Because of the $\mathbf{k}'=\mathbf{0}$ term, the sum exists only for $r_0>0$. Rewriting these expressions in terms of r_0-r_{0c} with r_{0c} given by Eq. (4.32) yields up to $O(1)$

$$f'^{+}=f_0'(r_0-r_{0c},L',K_{i,j},v'), \tag{10.4}$$

$$f'^{-}=-\frac{1}{64u_0'}[-2(r_0-r_{0c})]^2+\frac{3}{2}(r_0-r_{0c})\int_{\mathbf{k}'}\frac{1}{\delta\hat{K}'(\mathbf{k}')}+f_0'(-2(r_0-r_{0c}),L',K_{i,j},v'). \tag{10.5}$$

We define the finite-size parts $\delta f'^{\pm}$ of $f'^{\pm}$ in the same way as $\delta f'$ in Eqs. (4.33) and (4.34). Calculating the sum in the continuum limit $v'\to 0$ at fixed $|r_0-r_{0c}|\neq 0$ (see Appendices B and C), one obtains for $2<d<4$

$$\delta f'^{+}(r_0-r_{0c},u_0',L',\bar{\mathbf{A}})=-\frac{A_d}{d\varepsilon}(r_0-r_{0c})^{d/2}+\frac{1}{2L'^{d}}\mathcal{G}_0((r_0-r_{0c})L'^{2};\bar{\mathbf{A}})+O(u_0'), \tag{10.6}$$

$$\delta f'^{-}(r_0-r_{0c},u_0',L',\bar{\mathbf{A}})=-\frac{1}{64u_0'}[-2(r_0-r_{0c})]^2-\frac{A_d}{d\varepsilon}[-2(r_0-r_{0c})]^{d/2}+\frac{1}{2L'^{d}}\mathcal{G}_0(-2(r_0-r_{0c})L'^{2};\bar{\mathbf{A}})+O(u_0'), \tag{10.7}$$

where $\mathcal{G}_0$ is given by Eq. (6.34). Equations (10.6) and (10.7) correspond to Eq. (4.37). The renormalized counterparts $f_R'^{\pm}$ of $\delta f'^{\pm}$ are defined in the same way as f_R' in Eqs. (5.3) and (5.17). The explicit form of the functions $f_R'^{\pm}$ depends on the choice of the flow parameter. For the application to the regime $|\tilde{x}|\gg 1$, we make the bulk choice $\mu^2 l_+^2=r(l_+)$ for $T>T_c$ and $\mu^2 l_-^2=-2r(l_-)$ for $T<T_c$, with $\mu^{-1}=\xi_{0+}'$, Eq. (5.16) (the same choice will be made for the calculations in Sec. X B). Then the functions $f_R'^{\pm}$ are given by

$$f_R'^{+}(r(l_+),u'(l_+),l_+\mu,L',\bar{\mathbf{A}})=-A_d(l_+\mu)^{d}/(4d)+\frac{1}{2L'^{d}}\mathcal{G}_0(l_+^2\mu^2 L'^{2};\bar{\mathbf{A}})+O[u'(l_+)], \tag{10.8}$$

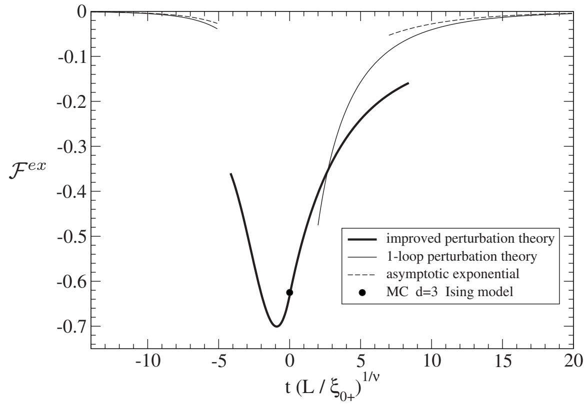

FIG. 17. Scaling functions $\mathcal{F}^{\text{ex}}(\tilde{x};\mathbf{1})$, Eqs. (6.22), (6.10), and (6.23), for $d=3$ (thick solid line); $\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}(\tilde{x};\mathbf{1})$, Eq. (10.10), for $d=3$ (thin solid lines); and Eq. (10.13) (dashed lines) for the excess free-energy density of isotropic systems as a function of the scaling variable $\tilde{x}=t(L/\xi_{0+})^{1/\nu}$. MC result (full circle) for the Ising model on a sc lattice [35]. No scaling function exists in the large - $|\tilde{x}|$ regions above and below T_c, which are sensitive to all nonuniversal details of the model according to $\mathcal{F}^{\text{ex},\pm}(L/\xi_\pm;\mathbf{1};\tilde{a}/\xi_\pm)$, Eq. (10.15), with Eq. (10.25).

$$f_R'^{-}(r(l_-),u'(l_-),l_-\mu,L',\bar{\mathbf{A}}) = -A_d(l_-\mu)^d\left\{\frac{1}{64u'(l_-)}+\frac{1}{4d}\right\}+\frac{1}{2L'^d}\mathcal{G}_0(l_-^2\mu^2L'^2;\bar{\mathbf{A}}) + O[u'(l_-)]. \quad (10.9)$$

For $l_\pm \to 0$, this leads to the finite-size scaling function of the excess free-energy density in one-loop order in the limit of zero lattice spacing,

$$\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}(\tilde{x};\bar{\mathbf{A}}) = \frac{1}{2}\mathcal{G}_0(L'^2/\xi_\pm'^2;\bar{\mathbf{A}}) + O(u^*), \quad (10.10)$$

where $\xi_+'=\xi_{0+}'t^{-\nu}$ and

$$\xi_-' = \xi_{0-}'|t|^{-\nu}, \quad \xi_{0-}'/\xi_{0+}' = 2^{-\nu} + O(u^*) \quad (10.11)$$

are the bulk second-moment correlation lengths above and below T_c, respectively [for ξ_{0+}', see Eq. (5.16)]. Here we have confined ourselves to the simplest form of perturbation theory for the regime $|\tilde{x}|\gg 1, \tilde{x}=t(L'/\xi_{0+}')^{1/\nu}$. As a shortcoming of this approach, $\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}$ diverges for $\tilde{x}\to 0$ at fixed finite L', which originates from the $\mathbf{k}'=\mathbf{0}$ term of Eq. (10.3). (This divergence could formally be suppressed by an L'-dependent choice of $l_\pm$, but this would not avoid a structurally incorrect nonanalytic t dependence at $t=0$ for finite L'.)

$\mathcal{F}^{\text{ex},+}_{1\text{-loop}}(\tilde{x};\bar{\mathbf{A}})$ serves the purpose of complementing $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}})$, Eqs. (6.22) and (6.10), in the large- $\tilde{x}$ regime. This is illustrated by the thin solid line in Fig. 17 for the example of three-dimensional *isotropic* systems (and for systems with cubic symmetry) with $\bar{\mathbf{A}}=\mathbf{1}$, $L'=L$, $\xi_{0+}'=\xi_{0+}$, $\xi_{0-}'=\xi_{0-}$. The curves match reasonably well above T_c. [No perfect matching can be expected because of the missing $O(u^*)$ terms in Eq. (10.10) and because $\mathcal{F}^{\text{ex}}(\tilde{x};\mathbf{1})$is not applicable to the region $\tilde{x}\gg 1$ where it has an *algebraic* approach to a *finite* limit $\mathcal{F}^{\text{ex}}(\infty;\mathbf{1})=-2u^*=-0.082$ for $\tilde{x}\to\infty$.]

By contrast, $\mathcal{F}^{\text{ex},-}_{1\text{-loop}}(\tilde{x};\bar{\mathbf{A}})$ and $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}})$ do not match well below T_c for two reasons: (i) The two-loop terms of $O(u^*)$ in Eq. (10.10) are non-negligible, (ii) our approximate result $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}})$ as represented by Eqs. (6.22), (6.10), and (6.23) is not applicable to the region $\tilde{x}<-5$. [In this region, this result for $\mathcal{F}^{\text{ex}}(\tilde{x};\mathbf{1})$ has an unphysical maximum $\mathcal{F}^{\text{ex}}(\tilde{x}_{\text{max}};\mathbf{1})=-0.303$ at $\tilde{x}_{\text{max}}=-5.61$ and has an algebraic approach to a finite limit $\mathcal{F}^{\text{ex}}(-\infty;\mathbf{1})=-0.49$ for $\tilde{x}\to-\infty$.] Thus substantial further work is needed for a satisfactory description of the region well below T_c.

Nevertheless, $\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}$ has the advantage of displaying the expected *exponential* large $|\tilde{x}|$ behavior. The leading large-$\tilde{x}$ behavior of $\mathcal{G}_0$ for the isotropic case is (see Appendix B)

$$\mathcal{G}_0(\tilde{x}^{2\nu};\mathbf{1}) = -2d\left(\frac{\tilde{x}^\nu}{2\pi}\right)^{(d-1)/2}\exp(-\tilde{x}^\nu) + O[\exp(-2\tilde{x}^\nu)]. \quad (10.12)$$

For $d=3$, Eqs. (10.12) and (10.10) yield for $|\tilde{x}|^\nu \gg 1$

$$\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}(\tilde{x};\mathbf{1}) = -\frac{3}{2\pi}(L/\xi_\pm)\exp(-L/\xi_\pm) + O(u^*), \quad (10.13)$$

as shown by the dashed lines in Fig. 17 (with $L/\xi_+=\tilde{x}^\nu$, $L/\xi_-=2^\nu|\tilde{x}|^\nu$).

In the case of noncubic anisotropy, all curves in Fig. 17 including the thin solid lines and dashed lines are, of course, affected by the anisotropy matrix $\bar{\mathbf{A}}\neq 1$ in a way similar to that shown in Figs. 10 and 15. It would be straightforward to illustrate this effect by complementing Fig. 17 accordingly by means of curves representing $\mathcal{F}^{\text{ex}}(\tilde{x};\bar{\mathbf{A}}_3(s))$ and $\mathcal{F}^{\text{ex},\pm}_{1\text{-loop}}(\tilde{x};\bar{\mathbf{A}}_3(s))$, with $\bar{\mathbf{A}}_3(s)$ given by Eq. (8.19), for several examples of s. In this case, the scaling argument (horizontal axis of Fig. 17) needs to be replaced by $t(L'/\xi_{0+}')^{1/\nu}$.

B. Nonscaling regime

1. Anisotropic φ^4 lattice model with finite lattice constant

So far we have taken the continuum limit, which is well justified in the range shown in Figs. 10, 15, and 17 provided that $\xi_\pm'/\tilde{a}\gg 1$ is sufficiently large. In earlier work [9], it was pointed out for the example of the susceptibility that the finite lattice constant $\tilde{a}$ becomes non-negligible in the limit of large $L/\tilde{a}$ at fixed $T\neq T_c$ in the regime where the finite-size scaling function has an exponential form. Here we discuss this issue further in the context of the excess free energy of the model (2.1) with $V=L^d$ and cubic anisotropy, i.e., on a simple-cubic lattice with lattice constant $\tilde{a}$ and only NN couplings K. In this case, we have $\mathbf{A}=2\tilde{a}^2K\mathbf{1}$, $\bar{\mathbf{A}}=\mathbf{1}$, $L=(2\tilde{a}^2K)^{1/2}L', \tilde{a}=(2\tilde{a}^2K)^{1/2}\tilde{a}'$, and there exist well-defined bulk second-moment correlation lengths $\xi_\pm=(2\tilde{a}^2K)^{1/2}\xi_\pm'$ above and below T_c (for $n=1$). As shown in Appendix B, the excess free-energy density in one-loop order attains the following form in the limit of large $L/\tilde{a}=L'/\tilde{a}'$ at fixed arbitrary $\tilde{a}/\xi_\pm=\tilde{a}'/\xi_\pm'>0$:

$$f^{\text{ex},\pm}(t,L) \underset{L/\tilde{a}\gg 1}{\longrightarrow} L^{-d}\mathcal{F}^{\text{ex},\pm}(L/\xi_\pm;\mathbf{1};\tilde{a}/\xi_\pm), \quad (10.14)$$

$$\mathcal{F}^{\mathrm{ex},\pm}(L/\xi_\pm;\mathbf{1};\tilde{a}/\xi_\pm) = -d\left[1+\left(\frac{\tilde{a}}{2\xi_\pm}\right)^2\right]^{d-1}\left(\frac{L}{2\pi\xi_\pm}\right)^{(d-1)/2} \times\exp\left\{-\frac{L}{\xi_\pm}\left[\frac{2\xi_\pm}{\tilde{a}}\,\mathrm{arsinh}\left(\frac{\tilde{a}}{2\xi_\pm}\right)\right]\right\}. \quad (10.15)$$

This result applies to the shaded region of Fig. 1. The exponential part of Eq. (10.15) can be rewritten as $\exp(-L/\xi_{\mathbf{e}\pm})$ with the *exponential correlation lengths*

$$\xi_{\mathbf{e}\pm} = \frac{\tilde{a}}{2}\left[\mathrm{arsinh}\left(\frac{\tilde{a}}{2\xi_\pm}\right)\right]^{-1} \quad (10.16)$$

above and below T_c, respectively. As a nontrivial relation between bulk properties and finite-size effects [10], the lengths $\xi_{\mathbf{e}\pm}$ describe the exponential part of the *bulk* order-parameter correlation function [92] in the large-distance limit in the direction of one of the cubic axes at arbitrary fixed $T\neq T_c$ above and below T_c (for $n=1$), respectively. This relation is exact in the large-n limit above T_c [10].

It has been shown [9] that, because of the exponential structure of the finite-size part of the susceptibility, the $\tilde{a}$ dependence of $\xi_{\mathbf{e}\pm}$ cannot be neglected even for small $\tilde{a}/\xi_\pm \ll 1$ if $L/\xi_\pm > [24\ln 2](\xi_\pm/\tilde{a})^2$ is sufficiently large (see Fig. 1 of Ref. [9]). The same argument now applies to the $\tilde{a}$ dependence of the exponential part of $\mathcal{F}^{\mathrm{ex},\pm}(L/\xi_\pm;\mathbf{1};\tilde{a}/\xi_\pm)$, Eq. (10.15). This implies that finite-size scaling and universality are violated in the large-$|\tilde{x}|$ tails of $\mathcal{F}^{\mathrm{ex},\pm}$ at any $\tilde{a}/\xi_\pm > 0$ even arbitrarily close to T_c because ultimately, for $|x|\to\infty$ (i.e., for large L at fixed $|t|\neq 0$), the tails of $\mathcal{F}^{\mathrm{ex},\pm}$ become explicitly dependent on $\tilde{a}$. (Below we shall show that the tails depend also on the bare four-point coupling u_0.) Thus no finite-scaling form (1.2), (1.3), or (1.4) with a single scaling argument $\propto tL^{1/\nu}$ and with a single nonuniversal amplitude C_1 can be defined in this large-$|\tilde{x}|$ region [93]. Higher-loop contributions cannot remedy this violation. It is obvious that an even larger variety of different nonscaling effects exists in the exponential finite-size region of systems with *noncubic* anisotropies ($\bar{\mathbf{A}}\neq\mathbf{1}$).

2. Isotropic φ^4 field theory

The diversity of nonuniversal nonscaling effects in the region $L/\xi_\pm \gg 1$ discussed above exists not only in anisotropic lattice models but also in fully isotropic systems. We demonstrate this point for the isotropic φ^4 field theory based on the standard Hamiltonian

$$H_{\mathrm{field}} = \int_V d^dx\left[\frac{r_0}{2}\varphi^2 + \frac{1}{2}(\nabla\varphi)^2 + u_0\varphi^4\right] \quad (10.17)$$

in a cube with $V=L^d$ and periodic b.c. and with some cutoff Λ in $\mathbf{k}$ space. Keeping the cutoff finite may be a valuable tool for testing universality, as has been convincingly demonstrated by Nicoll and Albright [94] in the context of *bulk* universality [8]. In a similar spirit, this was done in [9,11] with regard to *finite-size* universality in the large-n limit at and above T_c. We shall show that $\mathcal{F}^{\mathrm{ex},\pm}$ depends on the *bare* coupling u_0 and on the cutoff procedure for large L above and below T_c of the $n=1$ universality classes. For the case of a sharp cutoff, we shall also correct a previous misinterpretation [11,95] of the *singular* part of the excess free-energy density at T_c.

Since $f^{\mathrm{ex},\pm}$ has a finite limit for $\Lambda\to\infty$, first we calculate $f^{\mathrm{ex},\pm}$ at infinite cutoff $\Lambda=\infty$ within the minimal renormalization scheme at fixed dimension $2<d<4$ [62,63,80]. In one-loop order, we obtain

$$f^{\mathrm{ex},\pm}_{\Lambda=\infty}(t,L) = L^{-d}\mathcal{F}^{\mathrm{ex},\pm}_{\Lambda=\infty}(L/\xi_\pm), \quad (10.18)$$

where for large $L/\xi_\pm$

$$\mathcal{F}^{\mathrm{ex},\pm}_{\Lambda=\infty}(L/\xi_\pm) = -d\left(\frac{L}{2\pi\xi_\pm}\right)^{(d-1)/2}\exp\left\{-\frac{L}{\xi_\pm}\right\} \quad (10.19)$$

with the bulk second-moment correlation lengths

$$\xi_\pm(t;u) = \xi_{0\pm}(u)|t|^{-\nu}\{1+C_\pm(t,u)\}. \quad (10.20)$$

(There is no difference between exponential and second-moment correlation lengths at infinite cutoff at the one-loop level.) The function $C_\pm(t,u)$ represents the Wegner series

$$C_\pm(t,u) = \sum_{m=1}^{\infty} a_\pm^{(m)}(u)|t|^{\Delta m} \quad (10.21)$$

with the universal Wegner exponent $\Delta=\omega\nu$, $\omega=\partial\beta_u(u,\varepsilon)/\partial u|_{u=u*}$, and the Wegner amplitudes $a_\pm^{(m)}(u)$ depending in the nonuniversal renormalized coupling u. The latter is defined by

$$u = A_d Z_u(u,\varepsilon)^{-1}Z_\varphi(u,\varepsilon)^2 u_0\xi_{0+}^{\varepsilon} \quad (10.22)$$

(with the choice $\mu=\xi_{0+}^{-1}$), where $Z_u(u,\varepsilon)$ and $Z_\varphi(u,\varepsilon)$ are the standard Z factors [84]. Equation (10.22) determines u as an implicit function of $u_0\xi_{0+}^{\varepsilon}$. Although $C_\pm$ is a negligible additive correction in Eq. (10.20) for sufficiently small $|t|$, this is not the case in the exponential part of Eq. (10.19), which, for small $C_\pm$, can be rewritten as

$$\exp\left\{-\frac{L}{\xi_\pm}\right\} = A(L,t,u)\exp\left\{-\frac{L}{\xi_{0\pm}|t|^{-\nu}}\right\}, \quad (10.23)$$

$$A(L,t,u) = \exp\left\{C_\pm(t,u)\frac{L}{\xi_{0\pm}|t|^{-\nu}} + O(C_\pm^2)\right\}, \quad (10.24)$$

with the nonuniversal nonscaling prefactor $A(L,t,u)$ that cannot simply be replaced by 1 for small $|t|$. Even for arbitrarily small $|t|\neq 0$, the prefactor becomes non-negligible if L is sufficiently large, $L \gg |C_\pm|^{-1}\xi_{0\pm}|t|^{-\nu}$. Thus the tails of the large L dependence of $\mathcal{F}^{\mathrm{ex},\pm}_{\Lambda=\infty}$ become nonuniversal and have a nonscaling L dependence through the prefactor $A(L,t,u)$. This applies to the shaded area of the asymptotic critical region above and below T_c shown in Fig. 1. The same argument applies to the preceding subsection: it is necessary to keep the complete nonasymptotic form of the second-moment bulk correlation lengths at finite $\tilde{a}$,

$$\xi_\pm(t;u_0\tilde{a}^\varepsilon) = \xi_{0\pm}|t|^{-\nu}\{1 + C_\pm(t,u_0\tilde{a}^\varepsilon)\}, \qquad (10.25)$$

in Eqs. (10.15) and (10.16) and to include all correction terms in $C_\pm(t,u_0\tilde{a}^\varepsilon)$ [93].

The reasoning described above must also be extended to the case in which a smooth cutoff Λ in **k** space is taken into account. This can be done by including an isotropic (Pauli-Villars type) term $\frac{1}{2}(\nabla^2\varphi)^2/\Lambda^2$ in the Hamiltonian (10.17) [9,96]. In this case, the structure of $\mathcal{F}^{\text{ex},\pm}$ still remains exponential $\propto\exp[-L/\xi_{\mathbf{e}\pm}(\Lambda)]$ for large $L/\xi_\pm$ but the exponential correlation lengths

$$\xi_{\mathbf{e}\pm}(\Lambda) = \xi_\pm\left[1 - \tfrac{1}{2}\Lambda^{-2}\xi_\pm^{-2} + O(\Lambda^{-4}\xi_\pm^{-4})\right] \qquad (10.26)$$

become cutoff-dependent. This causes a cutoff-dependent prefactor $A(L,t,u,\Lambda)$ in Eq. (10.23).

As pointed out in [10], there exists a close relation between the L dependence of finite-size effects and the **x** dependence of the bulk order-parameter correlation function G_b discussed in Sec. III. In retrospect, the arguments presented above apply also to the exponential part of $G_b \propto|\mathbf{x}|^{-d+2}\exp(-|\mathbf{x}|/\xi_{\mathbf{e}\pm})$ even if it is isotropic because here the same correlation lengths $\xi_{\mathbf{e}\pm}$ appear as in the large L decay of the finite-size quantities. No scaling functions $\Phi_\pm$, Eqs. (3.5), (3.6), and (3.19), can be defined in the exponential large-distance regime $|\mathbf{x}|/\xi_\pm \gg 1$ (shaded region in Fig. 2). Thus the exponential tails of $G_b(\mathbf{x};t)$ of the φ^4 theory have a nonscaling form that depends on u_0 and the (smooth) cutoff even for arbitrarily small $t\neq 0$, $h=0$ and $t=0$, $h\neq 0$. In addition, for anisotropic systems, it depends on the anisotropy matrix **A** and the higher-order tensors **B**, etc.

Although the nonscaling effect on the *relative* quantity $\mathcal{F}^{\text{ex},\pm}/\mathcal{F}_b^\pm$ becomes arbitrarily large for sufficiently large $L/\xi_\pm$, this happens in a region where the magnitude of $\mathcal{F}^{\text{ex},\pm}$ itself is exponentially small. Thus, from a purely quantitative point of view, this is only a very small effect for systems with short-range interactions and periodic boundary conditions.

This is in contrast to the corresponding nonscaling finite-size effects in the presence of (effective) long-range correlations caused by a *sharp* momentum cutoff $-\Lambda\le k_\alpha<\Lambda$ used in [9,11]. Such a cutoff has often been used in the formulation and application of the RG theory based on the φ^4 Hamiltonian (10.17) (see, e.g., [94,97,98]). As far as thermodynamic bulk properties are concerned, this is well justified as the sharp cutoff does not affect the critical exponents and the thermodynamic bulk scaling functions. Thus the φ^4 model (10.17) with a sharp cutoff is a legitimate model of statistical mechanics that belongs to the same (d,n) universality class as systems with short-range interactions or with subleading long-range interactions. This implies the validity of thermodynamic two-scale factor universality in the presence of a sharp cutoff. Chen and the present author [9,11] have raised the question of whether this remains true also for confined systems. It was found, for the susceptibility and for the excess free energy in the large-n limit above T_c, that a sharp cutoff is not compatible with an exponential size dependence and violates finite-size scaling in the large-L regime above T_c. This behavior was traced back to the well known [11,97] artifact that the sharp cutoff in **k** space causes long-range correlations in real space, as can be demonstrated in the bulk order-parameter correlation function $G_b(\mathbf{x};t;\Lambda)$ [11,99] whose algebraically decaying nonscaling part dominates the exponentially decaying scaling part. By means of a RG one-loop calculation for $n=1$, we find that this property holds both above and below T_c for sufficiently large L.

In contrast to [11], however, we do not obtain a violation of finite-size scaling in the central finite-size region including $T=T_c$. Our present analysis is based on an appropriate decomposition of the excess free energy into singular and nonsingular parts in the sense of Eq. (2.5), whereas in [11] no L-dependent *nonsingular* part was defined. We find that, in the presence of a sharp cutoff Λ and for large $L\Lambda$, Eq. (10.18) with Eq. (10.19) is to be replaced by

$$f_\Lambda^{\text{ex},\pm}(t,L) = f_{\Lambda,s}^{\text{ex},\pm}(t,L) + f_{\Lambda,\text{ns}}^{\text{ex}}(L), \qquad (10.27)$$

with the singular part

$$f_{\Lambda,s}^{\text{ex},\pm}(t,L) = L^{-2}\Lambda^{d-2}\tilde{\Phi}_d(\xi_\pm^{-1}\Lambda^{-1}) + f_{\Lambda=\infty}^{\text{ex},\pm}(t,L), \qquad (10.28)$$

$$\tilde{\Phi}_d(z) = \int_0^\infty dy[e^{-(1+z^2)y} - e^{-y}]E_d(y), \qquad (10.29)$$

$$E_d(y) = \frac{d}{6(2\pi)^{d-2}}\left[\int_{-1}^{1} dq e^{-q^2y}\right]^{d-1}, \qquad (10.30)$$

and the L-dependent nonsingular part

$$f_{\Lambda,\text{ns}}^{\text{ex}}(L) = L^{-2}\Lambda^{d-2}\int_0^\infty dy e^{-y}E_d(y). \qquad (10.31)$$

Although our one-loop result (10.27)–(10.31) for the *total* excess free-energy density $f_\Lambda^{\text{ex},\pm}(t,L)$ is equivalent to Eqs. (8) and (16) of [11], there is a crucial difference with regard to the singular part. In contrast to the nonvanishing function $\Phi_{d,d'}(z)$ of [11], our function $\tilde{\Phi}_d(z)$ vanishes at criticality, $\tilde{\Phi}_d(0)=0$. The temperature-independent part (10.31) $\propto L^{-2}$ should not be attributed to the singular part as was done in [11]. Our definition of the nonsingular part $f_{\Lambda,\text{ns}}^{\text{ex}}(L)\propto L^{-2}$ is parallel to the standard analysis of bulk systems with a specific heat $C_\pm=A_\pm|t|^{-\alpha}+C_B$ with a negative critical exponent α whose finite value C_B at the finite cusp must *not* be included in the singular scaling part $\sim|t|^{-\alpha}$but rather in the nonsingular "background" contribution of the specific heat. The nonuniversal power-law term $\propto L^{-2}\Lambda^{d-2}$ in Eq. (10.28) dominates in the shaded region of Fig. 1 compared to the scaling part $f_{\Lambda=\infty}^{\text{ex},\pm}\propto L^{-d}$ but vanishes at $T=T_c$ and is subleading in the central finite-size regime. Thus the *leading* finite-size contributions in the φ^4 model with a sharp cutoff are in agreement with universal finite-size scaling *in the central finite-size regime* if the singular part of the free energy is identified correctly. Consequently, the leading singular part of the Casimir force (in film geometry) at bulk T_c [11] remains universal within the subclass of isotropic systems even in the presence of a sharp cutoff, but an additional regular part $\propto L^{-2}$ exists that is nonuniversal and is dominant compared to the singular part $\propto L^{-d}$. This unusual behavior is due to the long-range correlations caused by the sharp cutoff [100], as noted already in [11], which is of course a mathematical artifact and not generic for systems with purely short-range interactions. As pointed out by Dantchev *et al.* [95], the sharp cutoff implies an unphysical discontinuity of the slope of the interaction $\delta\hat{K}(\mathbf{k})=k^2$ at the boundary of theBrillouin zone, which is the mathematical origin of the L^{-2} terms. For the reasons given above, however, we disagree with the opinion expressed in [95] that the concept of finite-size scaling as developed for systems with short-range interactions does not apply to the φ^4 model (10.17) with a sharp cutoff. The authors of [95] did not perform an analysis based on a decomposition of the type (2.5) and (10.27). Our analysis shows that, in spite of the mathematical artifact of $\hat{K}(\mathbf{k})$ at the Brillouin-zone boundary, the concept of finite-size scaling is well applicable to the central finite-size regime including $T=T_c$ and that a violation of finite-size scaling occurs only in the large-L regime at $T\neq T_c$ (shaded region in Fig. 1), as in the other cases discussed above in the presence of a lattice cutoff or a smooth cutoff.

Finally, we discuss the case of an additional subleading long-range interaction of the van der Waals type as defined in Eqs. (2.7) and (2.9). It was pointed out by Dantchev and Rudnick [15] that it affects the finite-size susceptibility in the regime $L/\xi_+ \gg 1$, similar to the effect caused by a sharp cutoff [9]. The effect of this interaction on the excess free energy f_s^{ex} and on the critical Casimir force in the case of film geometry was first studied by Chen and the present author [11,18]. The asymptotic structure for $L/\xi_+ \gg 1$ in one-loop order above T_c at $h=0$ is [11]

$$f_s^{\mathrm{ex}}(t,L) = L^{-d}[\mathcal{F}^{\mathrm{ex}}(L/\xi_+) + bL^{2-\sigma}\Psi(L/\xi_+)], \quad (10.32)$$

which is similar to Eq. (3.17). We have verified that, for $n=1$, the same structure is valid also for cubic geometry with periodic b.c. above and below T_c where the function Ψ_{cube} has an algebraic large-L behavior $\sim(L/\xi_\pm)^{-2}$. The latter dominates the exponentially decaying scaling part $\mathcal{F}^{\mathrm{ex},\pm} \sim \exp(-L/\xi_{\mathbf{e}\pm})$ in the shaded region of Fig. 1. This implies that, in this region, *two* nonuniversal length scales $b^{1/(\sigma-2)}$ and $\xi_\pm$ at $h=0$ govern the *leading* singular part of the excess free-energy density

$$f_s^{\mathrm{ex},\pm}(t,L) \sim L^{-d}\left[\frac{b^{1/(\sigma-2)}}{L}\right]^{\sigma-2}\left[\frac{\xi_\pm}{L}\right]^2, \quad (10.33)$$

even arbitrarily close to criticality. In addition, there is the nonuniversal u_0-dependent exponential tail of $\mathcal{F}^{\mathrm{ex},\pm}$. In Eq. (10.33), both the amplitude $\sim b$ and the power $-d-\sigma$ of the L dependence are nonuniversal. Thus the universal scaling form (1.2), with only *one* length scale $C_1^{-\nu}$ at $h=0$, is not valid in the entire range of its scaling arguments for isotropic systems with van der Waals type interactions, although such systems are members of the same $(d, n=1)$ universality class as, e.g., Ising models with short-range interactions. The structure of Eqs. (10.32) and (10.33) and the corresponding structure for the critical Casimir force in film geometry has been confirmed in [50,52,95].

ACKNOWLEDGMENTS

I thank W. Selke for informing me about his new MC data prior to publication. I also thank B. Kastening and W. Selke for useful discussions. Support by DLR under Grant No. 50WM0443 is gratefully acknowledged.

APPENDIX A: UNIVERSAL BULK AMPLITUDE RELATIONS

In this appendix, we present explicit expressions for the universal constants Q_i, $\tilde{Q}_3$, and P_i, Eqs. (3.9)–(3.15), in terms of universal scaling functions. Near T_c, the sum rule (3.26) yields

$$\chi_b'(t,h') = -A_1'|t|^{d\nu}\partial^2 W_\pm(A_2'h'|t|^{-\beta\delta})/\partial h'^2$$
$$= D_1'\xi_\pm'(t,h')^{2-\eta}\tilde{\Phi}_\pm(D_2'h'|t|^{-\beta\delta}) \quad (A1)$$

with the universal function

$$\tilde{\Phi}_\pm(y) = 2\pi^{d/2}\Gamma(d/2)^{-1}\int_0^\infty ds\, s^{1-\eta}\Phi_\pm(s,y). \quad (A2)$$

At $t>0$, $h'=0$, Eq. (A1) yields $\chi_b'(t,0)=\Gamma_+'|t|^{-\gamma}$ with

$$\Gamma_+' = -A_1'A_2'^2W_2 = D_1'(\xi_{0+}')^{2-\eta}\tilde{\Phi}_+(0), \quad (A3)$$

where $W_2=\lim_{y\to 0}\partial^2 W_+(y)/\partial y^2$. At $t=0$, $h'\neq 0$ we have from Eq. (3.6) $\xi_\pm'(0,h')\equiv\xi_h'=\xi_c'|h'|^{-\nu/(\beta\delta)}$ with

$$\xi_c' = \xi_{0+}'(D_2')^{-\nu/(\beta\delta)}\hat{X}, \quad (A4)$$

thus Eq. (A1) yields $\chi_b'(0,h')=\Gamma_c'|h'|^{-\gamma/(\beta\delta)}$ with

$$\Gamma_c' = -A_1'A_2'^{1+1/\delta}\hat{W} = D_1'[\xi_{0+}'D_2'^{-\nu/(\beta\delta)}\hat{X}]^{2-\eta}\tilde{\Phi}(\infty), \quad (A5)$$

where $\tilde{\Phi}(\infty)\equiv\tilde{\Phi}_\pm(\infty)$ and

$$\hat{W} = \lim_{y\to\infty}\{|y|^{\gamma/(\beta\delta)}\partial^2 W_\pm(y)/\partial y^2\}, \quad (A6)$$

$$\hat{X} = \lim_{y\to\infty}\{|y|^{\nu/(\beta\delta)}X_\pm(y)\}. \quad (A7)$$

Equations (A3) and (A5) yield

$$\Gamma_+'/\Gamma_c' = A_2'^{1-1/\delta}W_2\hat{W}^{-1} = D_2'^{1-1/\delta}\tilde{\Phi}_+(0)[\hat{X}^{2-\eta}\tilde{\Phi}(\infty)]^{-1}, \quad (A8)$$

thus we obtain the universal ratio

$$P_2 = \frac{A_2'}{D_2'} = \left[\frac{\hat{W}\tilde{\Phi}_+(0)}{W_2\hat{X}^{2-\eta}\tilde{\Phi}(\infty)}\right]^{\delta/(\delta-1)}. \quad (A9)$$

Equations (A4) and (A8) yield a universal ratio Q_2 different from P_2,

$$Q_2 = \frac{\Gamma_+'}{\Gamma_c'}\left(\frac{\xi_c'}{\xi_{0+}'}\right)^{2-\eta} = \frac{\tilde{\Phi}_+(0)}{\tilde{\Phi}(\infty)}, \quad (A10)$$

where we have used $1-1/\delta=\gamma/(\beta\delta)$ and $(2-\eta)\nu=\gamma$.

Following Privman and Fisher [5], we assume that the *unsubtracted* bulk correlation function $\tilde{G}'_b(\mathbf{x}'_i-\mathbf{x}'_j;t,h') = \lim_{V'\to\infty}\langle\varphi'(\mathbf{x}'_i)\varphi'(\mathbf{x}'_j)\rangle'$ has the asymptotic scaling form

$$\tilde{G}'_b(\mathbf{x}';t,h') = D'_1|\mathbf{x}'|^{-d+2-\eta}Z_\pm(|\mathbf{x}'|/\xi',D'_2h'|t|^{-\beta\delta}) \tag{A11}$$

with the same constants D'_1 and D'_2 as in Eq. (3.5) and with a universal scaling function $Z_\pm(x,y)$. From Eqs. (A11), (2.31), and (3.3), we obtain the square of the bulk order parameter below T_c,

$$[m'_b(t)]^2 = \lim_{h'\to 0}\lim_{|\mathbf{x}'|\to\infty}\tilde{G}'_b(\mathbf{x}';t,h') = D'_1(\xi'_{0-})^{-d+2-\eta}|t|^{\nu(d-2+\eta)}\hat{Z}$$
$$= \lim_{h'\to 0}[\partial f'_b(t,h')/\partial h']^2 = (A'_1A'_2)^2|t|^{2\beta}W_1 \tag{A12}$$

with $\hat{Z}=\lim_{y\to 0}\lim_{x\to\infty}\{x^{-d+2-\eta}Z_-(x,y)\}$ and $W_1 = \lim_{y\to 0}\partial W_-(y)/\partial y$. In order to derive Q_1 and P_3, we use Eqs. (A3) and (A12) and obtain

$$D'_1 = -A'_1A'^2_2(\xi'_{0+})^{-2+\eta}W_2/\tilde{\Phi}_+(0) = (A'_1A'_2)^2(\xi'_{0-})^{d-2+\eta}W_1/\hat{Z}. \tag{A13}$$

Together with Eq. (3.16), this yields the universal quantities

$$Q_1 = A'_1(\xi'_{0+})^d = -\hat{Z}W_2[X_-(0)]^{-d+2-\eta}/[W_1\tilde{\Phi}_+(0)] \tag{A14}$$

and

$$P_3 = D'_1A'^{-1-\gamma/(d\nu)}_1(A'_2)^{-2} = -Q_1^{-\gamma/(d\nu)}W_2/\tilde{\Phi}_+(0). \tag{A15}$$

Finally we consider the universal ratio (3.14). The amplitude $\hat{D}'_\infty$ is given by $\hat{D}'_\infty = D'_1\Phi_\pm(0,0)\hat{C}$ with the universal constant [13,101]

$$\hat{C} = \frac{\hat{D}'_\infty}{D'_\infty} = \frac{\hat{\Phi}_\pm(0,0)}{\Phi_\pm(0,0)} = \frac{(4\pi)^{d/2}\Gamma\left(\frac{2-\eta}{2}\right)}{2^{d-2+\eta}\Gamma\left(\frac{d-2+\eta}{2}\right)}. \tag{A16}$$

Together with Eq. (A3), this yields a universal ratio Q_3 different from P_3,

$$Q_3 = \hat{D}'_\infty(\xi'_{0+})^{2-\eta}/\Gamma'_+ = \Phi_\pm(0,0)\hat{C}/\tilde{\Phi}_+(0). \tag{A17}$$

The universal constant $\tilde{Q}_3$ in Eq. (3.15) is

$$\tilde{Q}_3 = \Phi_\pm(0,0)/\tilde{\Phi}_+(0). \tag{A18}$$

APPENDIX B: GAUSSIAN MODEL WITH LATTICE ANISOTROPY

In order to derive the Gaussian part of Eq. (4.26) and the results of Sec. X, we consider the Hamiltonian (2.1) and (2.7) for $r_0=a_0t>0$, $u_0=0$, and $h=0$ with N scalar variables φ_j on a simple-cubic lattice with lattice constant $\tilde{a}$ in a cubic volume $V=L^d=N\tilde{a}^d$ with periodic boundary conditions. This Hamiltonian will be denoted by H^G. The Jacobian of the linear transformation $\varphi_j\to\hat{\varphi}(\mathbf{k})$ is $|\partial\varphi_j/\partial\hat{\varphi}(\mathbf{k})| = (\tilde{a}L)^{-dN/2}$. The dimensionless partition function is

$$Z^G = \left[\prod_{j=1}^N\int_{-\infty}^{\infty}\frac{d\varphi_j}{\tilde{a}^{1-d/2}}\right]\exp(-H^G)$$
$$= \left[\prod_{\mathbf{k}}\frac{1}{\tilde{a}L^{d/2}}\int d\hat{\varphi}(\mathbf{k})\right]$$
$$\times\exp(-H^G) = \prod_{\mathbf{k}}\left(\frac{2\pi}{[r_0+\delta\hat{K}(\mathbf{k})]\tilde{a}^2}\right)^{1/2}. \tag{B1}$$

For the transformed system, one obtains

$$Z'^G = \left[\prod_{\mathbf{k}'}\frac{1}{v'^{1/d}L'^{d/2}}\int d\hat{\varphi}'(\mathbf{k}')\right]\exp(-H'^G)$$
$$= \prod_{\mathbf{k}'}\left(\frac{2\pi}{[r_0+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}}\right)^{1/2} \tag{B2}$$

with $v'=(\det\mathbf{A})^{-1/2}\tilde{a}^d$. Equations (B1) and (B2) define the integration measure $\int d\hat{\varphi}(\mathbf{k})$ and $\int d\hat{\varphi}'(\mathbf{k}')$. The Gaussian free-energy densities divided by k_BT are

$$f^G = -\frac{\ln(2\pi)}{2\tilde{a}^d} + \frac{1}{2L^d}\sum_{\mathbf{k}}\ln\{[r_0+\delta\hat{K}(\mathbf{k})]\tilde{a}^2\}, \tag{B3}$$

$$f'^G = -\frac{\ln(2\pi)}{2v'} + \frac{1}{2L'^d}\sum_{\mathbf{k}'}\ln\{[r_0+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\}. \tag{B4}$$

The correctness of the additive constant of f^G can be checked by performing the integrations of Z^G in real space for $K_{i,j} = 0$, $\delta\hat{K}(\mathbf{k})=0$,

$$\prod_{j=1}^N\int_{-\infty}^{\infty}\frac{d\varphi_j}{\tilde{a}^{1-d/2}}\exp\left[-\tilde{a}^d\sum_{j=1}^N\frac{r_0}{2}\varphi_j^2\right] = \left(\frac{2\pi}{r_0\tilde{a}^2}\right)^{N/2}. \tag{B5}$$

This is valid also for free boundary conditions. The additive constant of f^G was not correct in previous work [102,103]. In order to calculate Eq. (B3), we consider

$$\Delta(r_0,L,K_{i,j},\tilde{a}) = L^{-d}\sum_{\mathbf{k}}\ln\{[r_0+\delta\hat{K}(\mathbf{k})]\tilde{a}^2\}$$
$$-\int_{\mathbf{k}}\ln\{[r_0+\delta\hat{K}(\mathbf{k})]\tilde{a}^2\}, \tag{B6}$$

where the sum $\Sigma_{\mathbf{k}}$ and the integral $\int_{\mathbf{k}}$ have finite cutoffs $\pm\pi/\tilde{a}$ for each k_α [see Eq. (4.31)]. Using the integral representation

$$\ln w = \int_0^\infty dy\, y^{-1}[\exp(-y)-\exp(-wy)] \tag{B7}$$

and interchanging the integration $\int dy$ with $\Sigma_{\mathbf{k}}$ and $\int_{\mathbf{k}}$ we obtain, because of $L^{-d}\Sigma_{\mathbf{k}}1=\int_{\mathbf{k}}1$,

$$\Delta(r_0,L,K_{i,j},\tilde{a}) = \int_0^\infty dy\, y^{-1} e^{-r_0\tilde{a}^2 y}\left[\int_{\mathbf{k}} \exp\{-\,\delta\hat{K}(\mathbf{k})\tilde{a}^2 y\} - L^{-d}\sum_{\mathbf{k}} \exp\{-\,\delta\hat{K}(\mathbf{k})\tilde{a}^2 y\}\right]. \tag{B8}$$

Since $\delta\hat{K}(\mathbf{k})$ is a periodic function of each component k_α of $\mathbf{k}$, the sum in Eq. (B8) satisfies the Poisson identity [10,81]

$$L^{-d}\sum_{\mathbf{k}} \exp\{-\,\delta\hat{K}(\mathbf{k})\tilde{a}^2 y\} = \sum_{\mathbf{n}} \int_{\mathbf{k}} \exp\{-\,\delta\hat{K}(\mathbf{k})\tilde{a}^2 y + i\mathbf{k}\cdot\mathbf{n}L\}, \tag{B9}$$

where $\mathbf{n}=(n_1,n_2,\ldots,n_d)$ and $\mathbf{k}\cdot\mathbf{n}=\Sigma_{\alpha=1}^d k_\alpha n_\alpha$. The sum $\Sigma_{\mathbf{n}}$ runs over all integers $n_\alpha, \alpha=1,2,\ldots,d$ in the range $-\infty \le n_\alpha \le \infty$. This leads to the exact representation

$$\Delta(r_0,L,K_{i,j},\tilde{a}) = -\int_0^\infty dy\, y^{-1} e^{-r_0\tilde{a}^2 y} \times \sum_{\mathbf{n}\neq\mathbf{0}} \int_{\mathbf{k}} \exp\{-\,\delta\hat{K}(\mathbf{k})\tilde{a}^2 y + i\mathbf{k}\cdot\mathbf{n}L\}. \tag{B10}$$

Note that here the integral $\int_{\mathbf{k}}$ still has finite lattice cutoffs $\pm\pi/\tilde{a}$. We shall evaluate $\Delta(r_0,L,K_{i,j},\tilde{a})$ for large $L/\tilde{a} \gg 1$ and distinguish two regimes: (i) $Lr_0^{1/2} \lesssim O(1)$, $r_0^{1/2}\tilde{a} \ll 1$ and (ii) $Lr_0^{1/2} \gg 1$ for arbitrary fixed $r_0^{1/2}\tilde{a} > 0$.

In the regime (i), the large-$\mathbf{k}$ dependence of $\delta\hat{K}(\mathbf{k})$ does not matter. Therefore, we may replace $\delta\hat{K}(\mathbf{k})$ by its small-$\mathbf{k}$ form $\mathbf{k}\cdot\mathbf{A}\mathbf{k}$ and let the integration limits of $\int_{\mathbf{k}}$ go to ∞. Furthermore, it is useful to substitute the integration variable $z = 4\pi^2\tilde{a}^2 y/L^2$. Then we obtain

$$\Delta(r_0,L,K_{i,j},\tilde{a}) \to \Delta(r_0,L;\mathbf{A}) = -\int_0^\infty dz\, z^{-1} e^{-r_0 L^2 z/(4\pi^2)} \times \sum_{\mathbf{n}\neq\mathbf{0}} \int_{\mathbf{k}}^\infty \exp[-\,\mathbf{k}\cdot\mathbf{A}\mathbf{k}L^2 z/(4\pi^2) + i\mathbf{k}\cdot\mathbf{n}L]. \tag{B11}$$

The Gaussian integral over $\mathbf{k}$ yields

$$\int_{\mathbf{k}}^\infty \exp[-\,\mathbf{k}\cdot\mathbf{A}\mathbf{k}L^2 z/(4\pi^2) + i\mathbf{k}\cdot\mathbf{n}L] = (\det\mathbf{A})^{-1/2}\left(\frac{\pi}{L^2 z}\right)^{d/2} \exp(-\,\mathbf{n}\cdot\mathbf{A}^{-1}\mathbf{n}\pi^2/z). \tag{B12}$$

Equations (B11) and (B12) lead to

$$\Delta(r_0,L;\mathbf{A}) = L^{-d}\mathcal{G}_0(r_0 L'^2, \bar{\mathbf{A}}), \tag{B13}$$

where $\mathcal{G}_0$ and $K_d(y,\bar{\mathbf{A}})$ are given by Eqs. (6.34) and (4.46). Thus, in the regime (i), we derive from Eqs. (B3), (B6), (B8), and (B13)

$$f^G = f_b^G + \frac{1}{2}L^{-d}\mathcal{G}_0(r_0 L'^2;\bar{\mathbf{A}}), \tag{B14}$$

where the bulk part f_b^G is obtained from Eq. (B3) by the replacement $L^{-d}\Sigma_{\mathbf{k}} \to \int_{\mathbf{k}}$. We note that within the *anisotropic* Gaussian model there exists no unique correlation length. This exists only for the transformed system with the (asymptotically isotropic) Hamiltonian H'^G [Eqs. (2.20) and (2.23) for $u_0'=0$, $h'=0$] for which the corresponding result reads

$$f'^G = f_b'^G + \frac{1}{2}L'^{-d}\mathcal{G}_0(r_0 L'^2;\bar{\mathbf{A}}), \tag{B15}$$

with the bulk part f'^G given in Eq. (4.29) for $u_0'=0$. Now the parameter r_0 is related to the second-moment bulk correlation length of H'^G [see (3.4)],

$$\xi_+'^G = r_0^{-1/2} = \xi_{0+}'^G t^{-1/2}, \quad \xi_{0+}'^G = a_0^{-1/2}. \tag{B16}$$

This leads to the identification of the scaling function of the Gaussian excess free-energy density in the regime (i),

$$\mathcal{F}^{G,\mathrm{ex}}(\tilde{x};\bar{\mathbf{A}}) = (1/2)\mathcal{G}_0(\tilde{x};\bar{\mathbf{A}}) \tag{B17}$$

with $\tilde{x} = t(L'/\xi_{0+}'^G)^{1/\nu}$, $\nu=\frac{1}{2}$.

In the regime (ii), $\Delta(r_0,L,K_{i,j},\tilde{a})$ will attain an exponential L dependence and the complete $\mathbf{k}$ dependence of $\delta\hat{K}(\mathbf{k})$ does matter. For simplicity, we consider only nearest-neighbor couplings $K_{i,j}=K$ on a sc lattice, $\delta\hat{K}(\mathbf{k}) = 4K\Sigma_{\alpha=1}^d[1-\cos(\tilde{a}k_\alpha)]$, with the second-moment bulk correlation length of the Gaussian model

$$\xi_+^G = \tilde{a}\left(\frac{2K}{r_0}\right)^{1/2} = \xi_{0+}^G t^{-1/2}, \quad \xi_{0+}^G = \tilde{a}\left(\frac{2K}{a_0}\right)^{1/2}. \tag{B18}$$

At the level of the Gaussian model, there exist no Wegner corrections to Eq. (B18). Using Eq. (B7), we obtain, similar to Appendix A of [99], the exact representation for Eq. (B6),

$$\Delta(r_0,L,K,\tilde{a}) = \tilde{a}^{-d}\int_0^\infty dy y^{-1} e^{-\tilde{r}_0 y}\{[S(\infty,y)]^d - [S(L/\tilde{a},y)]^d\}, \tag{B19}$$

$$S(L/\tilde{a},y) = S(\infty,y) + 2e^{-2y}\sum_{m=1}^\infty I_{mL/\tilde{a}}(2y), \tag{B20}$$

with $S(\infty,y)=e^{-2y}I_0(2y)$ and $\tilde{r}_0 \equiv r_0/(2K) = (\tilde{a}/\xi_+^G)^2$, where

$$I_M(2y) = (2\pi)^{-1}\int_{-\pi}^{\pi} d\theta \cos(M\theta) e^{2y\cos\theta} \tag{B21}$$

are the modified Bessel functions with integer M [see (9.6.19) of [104]]. In the limit of large $L/\tilde{a}$ for fixed $\tilde{r}_0 > 0$, only the range of $y \sim O(L/\tilde{a})$ is relevant and only the $m=1$ term of Eq. (B20) suffices to obtain the leading exponential behavior. Thus we substitute $2y = zL/\tilde{a}$ in Eq. (B19) and use the asymptotic formulas for large $L/\tilde{a}$ [see (9.7.7) and (9.7.1) of [104] and Appendix A of [10]],

$$I_{L/\tilde{a}}(zL/\tilde{a}) \sim (2\pi Lq/\tilde{a})^{-1/2}\exp\left\{\frac{L}{\tilde{a}}\left[q+\ln\left(\frac{z}{1+q}\right)\right]\right\}, \quad \text{(B22)}$$

$$I_0(zL/\tilde{a}) \sim e^{zL/\tilde{a}}(2\pi zL/\tilde{a})^{-1/2}, \quad \text{(B23)}$$

where $q=(1+z^2)^{1/2}$. The maximum of the resulting exponential part of the integrand of Eq. (B19) is at $z=\bar{z}$, where $\bar{z}=[\tilde{r}_0(1+\tilde{r}_0/4)]^{-1/2}$. Expanding around $z=\bar{z}$ and performing the integration over z yields for large $L/\tilde{a}$ at arbitrary fixed $\tilde{r}_0>0$

$$\Delta(r_0,L,K,\tilde{a}) = -\frac{2d}{L^d}\left(\frac{L/\tilde{a}}{2\pi\bar{z}}\right)^{(d-1)/2} e^{-L/\xi_{\mathbf{e}}^G} \quad \text{(B24)}$$

with the exponential correlation length

$$\xi_{\mathbf{e}}^G = \frac{\tilde{a}}{2}\left[\text{arsinh}\left(\frac{\tilde{a}}{2\xi_+^G}\right)\right]^{-1}. \quad \text{(B25)}$$

No universal finite-size scaling function of the Gaussian model can be defined in the region $L/\xi_+^G \gg 1$ because of the explicit $\tilde{a}$ dependence of Eqs. (B24) and (B25).

Within a RG treatment of the φ^4 lattice model, the Gaussian results can be considered as the bare one-loop contribution. By means of such a RG treatment at finite lattice constant $\tilde{a}$ parallel to Sec. II and Appendix A of [9], the results derived above acquire the correct critical exponents of the $n=1$ universality class including corrections to scaling. This leads to the one-loop results (10.14)–(10.16), which are valid for arbitrary $\tilde{a}/\xi_\pm>0$.

For field theory with $\delta\hat{K}(\mathbf{k})=k^2$ and a sharp cutoff $-\Lambda \le k_\alpha < \Lambda$, the Gaussian excess free-energy density is given by $(1/2)\Delta_\Lambda$, where Δ_Λ is given by Eq. (B6) with $\tilde{a}$ replaced by Λ^{-1}. From Eq. (A31) of Appendix A of [87] and a RG treatment at finite Λ, we obtain Eqs. (10.27)–(10.31).

APPENDIX C: SUMS OVER HIGHER MODES

Using Eq. (B6) and the integral representation (B7) with $w=rL'^2/(4\pi^2)$, we obtain from Eqs. (B13) and (6.34)

$$\frac{1}{2L'^d}\sum_{\mathbf{k}'\neq 0}\ln\{[r+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\} = \frac{1}{2}\int_{\mathbf{k}'}\ln\{[r+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\} + \frac{1}{2L'^d}\ln\left(\frac{L'^2}{v'^{2/d}4\pi^2}\right) + \frac{1}{2L'^d}J_0(rL'^2,\bar{\mathbf{A}}), \quad \text{(C1)}$$

$$J_0(rL'^2,\bar{\mathbf{A}}) = \int_0^\infty \frac{dy}{y}\left[\exp\left(-\frac{rL'^2y}{4\pi^2}\right)\{(\pi/y)^{d/2}-K_d(y,\bar{\mathbf{A}})+1\} - \exp(-y)\right]. \quad \text{(C2)}$$

The v'-dependent finite-size part in Eq. (C1) comes from the absence of the $\mathbf{k}'=\mathbf{0}$ term and is exactly cancelled by the corresponding logarithmic term in Eq. (4.26). For $d>0$, the function $J_0(rL'^2,\mathbf{A})$ is finite for all $0\le rL'^2<\infty$ and diverges for large rL'^2 as $J_0(rL'^2,\mathbf{A})\sim -\ln[rL'^2/(4\pi^2)]$. By means of differentiation with respect to r, we obtain

$$S_m(r) = L'^{-d}\sum_{\mathbf{k}'\neq\mathbf{0}}[r+\delta\hat{K}'(\mathbf{k}')]^{-m} = \int_{\mathbf{k}'}[r+\delta\hat{K}'(\mathbf{k}')]^{-m} + \frac{(L')^{2m-d}}{(2\pi)^{2m}}I_m(rL'^2,\bar{\mathbf{A}}), \quad \text{(C3)}$$

$$I_m(rL'^2,\bar{\mathbf{A}}) = \int_0^\infty dy\, y^{m-1}\exp[-rL'^2y/(4\pi^2)] \times\{K_d(y,\bar{\mathbf{A}})-(\pi/y)^{d/2}-1\}. \quad \text{(C4)}$$

For $2<d<4$, the behavior of these functions for $r\to 0$ is $I_1(r,\bar{\mathbf{A}})\to I_1(0,\bar{\mathbf{A}})=\text{finite}$, $r^2I_2(r,\bar{\mathbf{A}})\sim O(r^{d/2})$,

$$J_0(r,\bar{\mathbf{A}}) - \frac{r}{4\pi^2}I_1(r,\bar{\mathbf{A}}) - \frac{r^2}{32\pi^4}I_2(r,\bar{\mathbf{A}}) = J_0(0,\bar{\mathbf{A}}) + O(r^{d/2}). \quad \text{(C5)}$$

For $d>0$, the behavior for $r\to\infty$ is $rI_1(r,\bar{\mathbf{A}})\to -4\pi^2$, $r^2I_2(r,\bar{\mathbf{A}})\to -16\pi^4$. For $2<d<4$ and $r>0$, the bulk integral in Eq. (C1) is

$$\int_{\mathbf{k}'}\ln\{[r+\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\} = \int_{\mathbf{k}'}\ln\{[\delta\hat{K}'(\mathbf{k}')]v'^{2/d}\} + r\int_{\mathbf{k}'}[\delta\hat{K}'(\mathbf{k}')]^{-1} - 2A_d r^{d/2}/(d\varepsilon), \quad \text{(C6)}$$

apart from nonasymptotic corrections that depend on $rv'^{2/d}$ and vanish for $r\to 0$ at fixed finite $\tilde{v}'$. The bulk integrals in Eq. (C3) follow by differentiation with respect to r.

[1] M. E. Fisher, Rev. Mod. Phys. **46**, 597 (1974).
[2] E. Vicari, e-print arXiv:0709.1014.
[3] D. Stauffer, M. Ferer, and M. Wortis, Phys. Rev. Lett. **29**, 345 (1972).
[4] M. E. Fisher, in *Critical Phenomena*, Proceedings of the 1970 International School of Physics "Enrico Fermi," Course 51, edited by M. S. Green (Academic, New York, 1971), p. 1.
[5] V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).
[6] V. Privman, Phys. Rev. B **38**, 9261 (1988).
[7] V. Privman, in *Finite Size Scaling and Numerical Simulation of*

Statistical Systems, edited by V. Privman (World Scientific, Singapore, 1990), p. 1.
[8] V. Privman, A. Aharony, and P. C. Hohenberg, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1991), Vol. 14, p. 1.
[9] X. S. Chen and V. Dohm, Eur. Phys. J. B **10**, 687 (2000).
[10] X. S. Chen and V. Dohm, Eur. Phys. J. B **15**, 283 (2000).
[11] X. S. Chen and V. Dohm, Phys. Rev. E **66**, 016102 (2002).
[12] X. S. Chen and V. Dohm, Phys. Rev. E **70**, 056136 (2004).
[13] V. Dohm, J. Phys. A **39**, L259 (2006).
[14] B. Widom, J. Chem. Phys. **41**, 74 (1964); R. F. Kayser and H. J. Raveché, Phys. Rev. A **29**, 1013 (1984).
[15] D. Dantchev and J. Rudnick, Eur. Phys. J. B **21**, 251 (2001).
[16] D. Dantchev, Eur. Phys. J. B **23**, 211 (2001).
[17] H. Chamati and D. M. Dantchev, Eur. Phys. J. B **26**, 89 (2002).
[18] X. S. Chen and V. Dohm, Physica B **329-333**, 202 (2003).
[19] F. Wegner, Phys. Rev. B **5**, 4529 (1972).
[20] T. Schneider, in *The Physics of Conventional and Unconventional Superconductors*, edited by K. H. Bennemann and J. B. Ketterson (Springer-Verlag, Berlin, in press).
[21] A. D. Bruce and R. A. Cowley, *Structural Phase Transitions* (Taylor & Francis Ltd., London, 1981).
[22] E. K. H. Salje, *Phase Transitions in Ferroelastic and Coelastic Crystals* (Cambridge University Press, Cambridge, MA, 1990); Phys. Rep. **215**, 49 (1992).
[23] L. L. Liu, Phys. Rev. Lett. **31**, 459 (1973); D. Belitz, T. R. Kirkpatrick, and A. Rosch, Phys. Rev. B **73**, 054431 (2006); M. Bode, M. Heide, K. von Bergmann, P. Ferriani, S. Heinze, G. Bihlmayer, A. Kubetzka, O. Pietzsch, S. Blügel, and R. Wiesendanger, Nature **447**, 190 (2007).
[24] H. G. Katzgraber, M. Körner, and A. P. Young, Phys. Rev. B **73**, 224432 (2006).
[25] A. Drewitz, R. Leidl, Th. W. Burkhardt, and H. W. Diehl, Phys. Rev. Lett. **78**, 1090 (1997); D. B. Abraham and P. J. Upton, *ibid.* **85**, 2541 (2000).
[26] N. S. Tonchev, Phys. Rev. E **75**, 031110 (2007), and references therein.
[27] F. Wegner, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6, p. 7.
[28] A. Aharony, Phys. Rev. B **9**, 2107 (1974).
[29] P. R. Gerber, J. Phys. A **8**, 67 (1975).
[30] P. C. Hohenberg, A. Aharony, B. I. Halperin, and E. D. Siggia, Phys. Rev. B **13**, 2986 (1976).
[31] S. Singh and R. K. Pathria, Phys. Rev. B **31**, 4483 (1985).
[32] J. Rudnick, H. Guo, and D. Jasnow, J. Stat. Phys. **41**, 353 (1985).
[33] H. Guo and D. Jasnow, Phys. Rev. B **35**, 1846 (1987); **39**, 753(E) (1989).
[34] K. K. Mon, Phys. Rev. Lett. **54**, 2671 (1985).
[35] K. K. Mon, Phys. Rev. B **39**, 467 (1989).
[36] K. K. Mon, in *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990), p. 261.
[37] A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6, p. 357.
[38] J. L. Cardy, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1987), Vol. 11, p. 55.
[39] G. Kamieniarz and H. W. J. Blöte, J. Phys. A **26**, 201 (1993).
[40] A corresponding scaling form $\xi_{\parallel}(t,h,L) = LX_{\text{cylinder}}(C_1' t L'^{1/\nu}, C_2' h' L'^{\beta\delta/\nu}; \bar{\mathbf{A}})$ should be valid for the correlation length in an anisotropic system with the shape of an $L^{d-1}\times\infty$ cylinder considered in [5].
[41] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[42] M. Schulte and C. Drope, Int. J. Mod. Phys. C **16**, 1217 (2005).
[43] M. A. Sumour, D. Stauffer, M. M. Shabat, and A. H. El-Astal, Physica A **368**, 96 (2006).
[44] W. Selke and L. N. Shchur, J. Phys. A **38**, L739 (2005).
[45] D. Dantchev and M. Krech, Phys. Rev. E **69**, 046119 (2004).
[46] O. Vasilyev, A. Gambassi, A. Maciolek, and S. Dietrich, Europhys. Lett. **80**, 60009 (2007).
[47] M. Krech and S. Dietrich, Phys. Rev. A **46**, 1886 (1992); **46**, 1922 (1992); M. Krech, *The Casimir Effect in Critical Systems* (World Scientific, Singapore, 1994).
[48] M. Krech, Phys. Rev. E **56**, 1642 (1997).
[49] R. Zandi, J. Rudnick, and M. Kardar, Phys. Rev. Lett. **93**, 155302 (2004).
[50] D. Dantchev, H. W. Diehl, and D. Grüneberg, Phys. Rev. E **73**, 016131 (2006).
[51] H. W. Diehl, D. Grüneberg, and M. A. Shpot, Europhys. Lett. **75**, 241 (2006); D. Grüneberg and H. W. Diehl, Phys. Rev. B **77**, 115409 (2008).
[52] D. Dantchev, F. Schlesener, and S. Dietrich, Phys. Rev. E **76**, 011121 (2007).
[53] R. Zandi, A. Shackell, J. Rudnick, M. Kardar, and L. P. Chayes, Phys. Rev. E **76**, 030601(R) (2007).
[54] Z. Borjan and P. J. Upton, e-print arXiv:0804.2340.
[55] A. Hucht, Phys. Rev. Lett. **99**, 185301 (2007).
[56] G. A. Williams, Phys. Rev. Lett. **92**, 197003 (2004).
[57] W. Selke (private communication).
[58] W. Selke, Eur. Phys. J. B **51**, 223 (2006).
[59] W. Selke, J. Stat. Mech.: Theory Exp. 2007, P04008.
[60] E. Brézin, J. C. Le Guillou, J. Zinn-Justin, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1976), Vol. 6, p. 125; G. Parisi, J. Stat. Phys. **23**, 49 (1980).
[61] G. 't Hooft and M. Veltman, Nucl. Phys. B **44**, 189 (1972); G. 't Hooft, *ibid.* **61**, 455 (1973).
[62] V. Dohm, Z. Phys. B: Condens. Matter **60**, 61 (1985); **61**, 193 (1985).
[63] R. Schloms and V. Dohm, Nucl. Phys. B **328**, 639 (1989); R. Schloms and V. Dohm, Phys. Rev. B **42**, 6142 (1990).
[64] E. Brézin and J. Zinn-Justin, Nucl. Phys. B **257**, 867 (1985).
[65] A. Esser, V. Dohm, M. Hermes, and J. S. Wang, Z. Phys. B: Condens. Matter **97**, 205 (1995).
[66] A. Esser, V. Dohm, and X. S. Chen, Physica A **222**, 355 (1995).
[67] X. S. Chen, V. Dohm, and N. Schultka, Phys. Rev. Lett. **77**, 3641 (1996).
[68] X. S. Chen, V. Dohm, and Talapov, Physica A **232**, 375 (1996).
[69] X. S. Chen and V. Dohm, Physica A **235**, 555 (1997); Int. J. Mod. Phys. B **12**, 1277 (1998).
[70] X. S. Chen, V. Dohm, and D. Stauffer, Eur. Phys. J. B **14**, 699 (2000); X. S. Chen, V. Dohm, and A. Esser, J. Phys. I **5**, 205 (1995); W. Koch, V. Dohm, and D. Stauffer, Phys. Rev. Lett.

77, 1789 (1996); W. Koch and V. Dohm, Phys. Rev. E **58**, R1179 (1998).
[71] M. Campostrini, A. Pelisetto, P. Rossi, and E. Vicari, Phys. Rev. E **57**, 184 (1998).
[72] H. J. W. Zandvliet, Europhys. Lett. **73**, 747 (2006); A. Nußbaumer, E. Bittner, and W. Janke, *ibid.* **78**, 16004 (2007); R. Schumann and S. Kobe, Physica A **386**, 187 (2007).
[73] A. D. Bruce, J. Phys. C **7**, 2089 (1974).
[74] H. B. Tarko and M. E. Fisher, Phys. Rev. B **11**, 1217 (1975).
[75] A. J. Liu and M. E. Fisher, Physica A **156**, 35 (1989).
[76] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
[77] H. W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1986), Vol. 10, p. 76; Int. J. Mod. Phys. B **11**, 3503 (1997).
[78] S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1988), Vol. 12, p. 1.
[79] V. Dohm, Z. Phys. B: Condens. Matter **75**, 109 (1989).
[80] M. Strösser and V. Dohm, Phys. Rev. E **67**, 056115 (2003); **70**, 069902(E) (2004).
[81] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).
[82] E. Brézin, J. Phys. (Paris) **43**, 15 (1982).
[83] H. Kleinert and B. Van den Bossche, Phys. Rev. E **63**, 056113 (2001).
[84] S. A. Larin, M. Mönnigmann, M. Strösser, and V. Dohm, Phys. Rev. B **58**, 3394 (1998).
[85] H. J. Krause, R. Schloms, and V. Dohm, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[86] X. S. Chen and V. Dohm, Physica B **284**, 45 (2000).
[87] X. S. Chen and V. Dohm, Eur. Phys. J. B **5**, 529 (1998).
[88] The curve in our Fig. 8 for $w<0$ is the same as that in Fig. 1 of [12]. In (55) of [12], $\tilde{l}^2$ and $\tilde{l}^4$ should read $\tilde{l}^{-2}$ and $\tilde{l}^{-4}$, respectively.
[89] H. W. J. Blöte, E. Luijten, and J. R. Heringa, J. Phys. A **28**, 6289 (1995).
[90] We have been informed by W. Selke that the preliminary simulations of [44] for $J<0$ were performed at $J/K=-0.5$ and -0.75.
[91] H. W. Diehl and M. Shpot, Phys. Rev. B **62**, 12338 (2000).
[92] M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967).
[93] The interpretation in [10] that finite-size scaling is restored if the variable $L/\xi_{\mathrm{e}\pm}$ is employed instead of $L/\xi_{\pm}$ is not correct. The reason is that $\xi_{\mathrm{e}\pm}$ must be represented in its complete nonuniversal nonasymptotic form, i.e., as a non-power-law function of t with the nonuniversal parameters $\xi_{0\pm}$ and $u_0\tilde{a}^{\varepsilon}$ and different powers $|t|^{\nu}$ and $|t|^{\Delta m}$ according to Eqs. (10.16), (10.20), and (10.25). This violates the simple structure of the universal power-law scaling form (1.2). Furthermore, two different arguments $L/\xi_{\mathrm{e}+}$ and $L/\xi_{\mathrm{e}-}$ would be needed above and below T_c whose ratio $\xi_{\mathrm{e}+}/\xi_{\mathrm{e}-}$ is nonuniversal because the nonasymptotic corrections must not be neglected in the exponential arguments.
[94] J. F. Nicoll and P. C. Albright, Phys. Rev. B **34**, 1991 (1986).
[95] D. Dantchev, M. Krech, and S. Dietrich, Phys. Rev. E **67**, 066120 (2003).
[96] G. Parisi, *Statistical Field Theory* (Addison-Wesley, Reading, MA, 1992).
[97] K. G. Wilson and J. Kogut, Phys. Lett., C **12**, 75 (1974).
[98] See, e.g., D. J. Amit, *Field Theory, the Renormalization Group, and Critical Phenomena* (McGraw-Hill, New York, 1978); J. J. Binney, N. J. Dowrick, A. J. Fisher, and M. E. J. Newman, *The Theory of Critical Phenomena* (Clarendon, Oxford, 1992).
[99] X. S. Chen and V. Dohm, Phys. Rev. E **67**, 056127 (2003).
[100] Similar anomalies exist in the φ^4 theory with a sharp cutoff above the upper critical dimension $d=4$ as found in X. S. Chen and V. Dohm, Phys. Rev. E **63**, 016113 (2000), and references therein.
[101] B. Kastening and V. Dohm (unpublished).
[102] In Eq. (52) of Ref. [99], the term $[\ln \pi+(\tilde{L}/\tilde{a})^{1-d}\ln 2]$ should be replaced by $\ln(2\pi)$. I thank B. Kastening for pointing out this correction to me.
[103] In Eq. (14) of Ref. [11], the term $\ln \pi$ should read $\ln(2\pi)$.
[104] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).