Diversity of critical behavior within a universality class

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We study spatial anisotropy effects on the bulk and finite-size critical behavior of the $O(n)$ symmetric anisotropic $\varphi^4$ 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 $\epsilon = 4 - d$ 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 $\epsilon$ 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 non-monotonic 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 non-monotonic 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 $\varphi^4$ theory, on the cutoff procedure, and on subleading long-range interactions.

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)

$$f_{s,b}(t,h) = A_1|t|^{\nu_\beta\delta} W_{\pm}(A_2|h|^{-\frac{\nu_\beta}{\delta}})$$

(1.1)

with universal exponents $\nu, \beta, \delta$ 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 ($r$) dependence of bulk correlation functions [3] and to the size ($L$) dependence of quantities of confined systems [4, 3, 6] (for reviews see, e.g., [7, 8]). It is this extended hypothesis which is in 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 degree of diversity within a given $(d,n)$ universality class primarily due to spatial anisotropy in lattice systems with non-cubic symmetry, but also due to the lattice spacing $a$ in systems with cubic symmetry and due to the bare four-point coupling $u_0$ of the $\varphi^4$ 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 scal-
ing functions. All of these nonuniversal differences exist in the asymptotic critical region $|t| \ll 1$, $L \gg a$, and $r \gg a$ 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, RKKY, 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 non-cubic symmetry is the fact that there exists no unique bulk correlation-length amplitude but rather $d$ different amplitudes $\xi^{(\alpha)}_t$ in the direction $\alpha = 1, ..., d$ of the $d$ principal axes. Such systems still have a single correlation-length exponent $\nu$ 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. \(^{26}\).) Non-cubic anisotropy effects in crystals with cubic symmetry can be easily generated by applying shear forces. In earlier work on two-scale factor universality \(^{5, 8, 17, 27, 28, 29, 30}\), isotropic systems with a single bulk correlation length $\xi_t$ 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 Sect. III of the present 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

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**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 \(^{3}\).**

| classes of interactions $d \mathbf{K}(k)$ in \(^{22}\) | basic lengths, nonuniversal parameters | bulk amplitude relations | bulk correlation functions | finite-size effects |
|-----------------------------------------------|-----------------------------------|-------------------------|-------------------------|------------------|
| isotropic short range $a$ $k^2 + O(k^4)$ | correlation length $\xi_\pm$, 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 $\sum_{\alpha, \beta=1}^d A_{\alpha \beta} k_\alpha k_\beta$ | $d$ principal correlation lengths $\xi^{(\alpha)}_\pm$, up to $d(d+1)/2 + 1$ nonuniversal parameters $C_1', C_2', A_{\alpha \beta}$, four-point coupling $u_0$ | multi-parameter universality | $r/\xi^{(\alpha)}_\pm \lesssim O(1)$: universal power-law scaling form with $d(d+1)/2 + 1$ nonuniversal parameters in the scaling arguments; $r \gg \xi^{(\alpha)}_\pm$: exponential form with nonuniversal tails | $L/\xi^{(\alpha)}_\pm \lesssim O(1)$: nonuniversal power-law scaling form, restricted universality; $L \gg \xi^{(\alpha)}_\pm$: exponential form with nonuniversal tails |
| isotropic subleading long range $b$ $k^2 - b |k|^\sigma$ | correlation length $\xi_\pm$, interaction length scale $b^{1/(\sigma-2)}$, five nonuniversal parameters $C_1, C_2, b, \sigma, u_0$ | 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 $b, \sigma$ | $L/\xi_\pm \lesssim O(1)$: universal power-law scaling form; $L/\xi_\pm > O(1)$: nonuniversal power-law form depending on $b, \sigma$ |

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*a Refs. \(^{1, 8, 10, 11}\)
*b For isotropic systems, $\xi_+$ and $\xi_-$ denote the second-moment bulk correlation lengths above and below $T_c$, with a universal ratio $\xi_+/\xi_-$. For anisotropic systems, $\xi^{(\alpha)}_\pm$ are the principal bulk correlation lengths with universal ratios $\xi^{(\alpha)}_+/\xi^{(\alpha)}_- = 1, 2, ..., d$.
*c Refs. \(^{12, 13}\)
*d The reduced anisotropy matrix $\mathbf{A} = A_i/(\det \mathbf{A})^{1/d}$ has $d(d + 1)/2 - 1$ independent matrix elements $A_{\alpha \beta}$.
*e Refs. \(^{11, 14, 15, 16, 17, 18}\)
correlation functions.

For \textit{confined} systems with a characteristic length \(L\) the hypothesis of two-scale factor universality is summarized by the asymptotic (large \(h\), small \(t\), small \(L\)) scaling form for the singular part of the free energy density (divided by \(k_B T\))

\[
    f_s(t, h, L) = L^{-d} \mathcal{F}(C_1 t L^{1/\nu}, C_2 h L^{\delta_1/\nu}). \tag{1.2}
\]

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 \(1.1\). 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 \(33\) which supported the form of \(1.2\). 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 up to now for finite \(n\) in cubic geometry, except in the large-\(n\) limit \(11\). Monte Carlo (MC) simulations \(31, 85, 36\) 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 \(3, 8, 37\) 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 non-cubic 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 which 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 non-rectangular 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 Sects. IV - VI, we propose that, for anisotropic systems with the shape of a cube, \(1.2\) is to be replaced by \(40\)

\[
    f_s(t, h, L) = L^{-d} \mathcal{F}_{\text{cube}}(C_1 t L^{1/\nu}, C_2 h L^{\delta_1/\nu}; \tilde{\mathbf{A}}), \tag{1.3}
\]

with \(L' = L(\det \mathbf{A})^{-1/(2d)}\), \(h' = h(\det \mathbf{A})^{1/4}\), and with the reduced anisotropy matrix \(\mathbf{A} = \mathbf{A}/(\det \mathbf{A})^{1/4}\), \(\det \mathbf{A} > 0\). The nonuniversal constants \(C_1'\) and \(C_2'\) will be specified in Sect. VI in terms of the asymptotic amplitudes \(\xi_{bs}\) and \(\xi_{b}\) 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 \(f_s' = f_s(\mathbf{A}/(\det \mathbf{A})^{1/2})\) of the parallelepiped with the volume \(V' = V(\det \mathbf{A})^{-1/2}\) and with \(\mathbf{A}' = \mathbf{A}/(\det \mathbf{A}') = 1\) (isotropy) then attains the scaling form

\[
    f_s'(t, h', L') = L'^{-d} \mathcal{F}_{\text{iso, \tilde{A}}}(C_1' t L'^{1/\nu}, C_2' h' L'^{\delta_1/\nu}) \tag{1.4}
\]

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

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

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, \(\tilde{\mathbf{A}}\).” This index is the notation for a system with the shape of a parallelepiped whose interaction \(\delta K'(k') = k^2 + O(k^4)\) 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 \(\mathbf{A}\). These parameters appear in the calculation of \(\mathcal{F}_{\text{iso, \tilde{A}}}\) via the summation over the discrete \(k'\) vectors in the Fourier space of the parallelepiped system since the \(k'\) vectors depend explicitly on \(\mathbf{A}\), unlike the \(k\) vectors of the cubic system. Thus for the calculation of \(\mathcal{F}_{\text{iso, \tilde{A}}}\) the same nonuniversal information is required as for the calculation of \(\mathcal{F}_{\text{cube}}\).

For general \(A\) the function \(\mathcal{F}_{\text{cube}}(x, 0; \mathbf{A})\) 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 \(8, 41\)

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

for \(n = 1, 2, 3\) both in three \(12, 13\) and two \(13\) dimensions. MC simulations \(12, 43\) 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 Sects. IV - VI of this paper we derive the finite-size scaling function \(\mathcal{F}_{\text{cube}}(x, 0; \mathbf{A})\) of the singular part of the excess free energy density \(f_{\text{ex}}' = f_s - f_{s,b}\) 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 $\varphi^4$ lattice model. For the isotropic case at $T_c$, we find excellent agreement with the MC data of Mon et al. [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 [36, 37, 38]. 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 $n \rightarrow \infty$ and at $T = T_c$, the nonuniversality of the Casimir amplitude due to anisotropy was already demonstrated within the $\varphi^4$ theory in [39]. This suggests that, for given geometry and b. c., the existing theoretical [40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54] and MC [43, 46, 48, 52] 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 $\varphi^4$ 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 Sect. VIII) a three-dimensional $\varphi^4$ lattice model with the same two-dimensional anisotropy in the horizontal planes as in the two-dimensional model Ising model studied by Selke and Shchur [44]. Our theory agrees quantitatively with the non-monotonicity of the Binder cumulant as a function of the anisotropy $\text{ferromagnetic}$ next-nearest neighbor (NNN) coupling found in [44]. We also predict a non-monotonicity for small $\text{antiferromagnetic}$ couplings and the existence of a Lifshitz point at a value of this coupling. Very recent preliminary MC data by Selke [57] for the two-dimensional Ising model indeed reveal such a non-monotonicity 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 $\mathbf{A}$ approaches zero, in particular if a Lifshitz point is approached (Sect. VIII).

An important property of the scaling form (1.3) is that it depends on $\mathbf{A}$ but not on other nonuniversal parameters such as the bare four-point coupling, the lattice spacing, and the cutoff of $\varphi^4$ 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 $\overline{\mathbf{A}}$ (and the same geometry and boundary conditions). In Sect. 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 [60]).

Unlike the bulk scaling function $\tilde{W}_z(z)$, (1.4), that is valid in the entire range $-\infty \leq z \leq \infty$ of the scaling argument $z$, the finite-size scaling functions such as $F_{\text{cube}}(x, y; \overline{\mathbf{A}})$ 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 nonnegligible 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 $\bar{a}$, the inverse cutoff $\Lambda^{-1}$, the length scale $a_0^{1/\nu}$ set by the four-point coupling, and the van-der-Waals interaction-length $b^{1/(\sigma-2)}$, as discussed in Sect. X.

![FIG. 1: Asymptotic part of the $L^{-1/\nu} - t$ plane at $h = 0$ for the anisotropic $\varphi^4$ 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 $\overline{A}_{\alpha\beta}$, see (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 $L^{-35/\nu} - h'$ plane at $T = T_c$.](image-url)
we use the minimal subtraction scheme \([61]\) not within the \(\varepsilon\) 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 \([62, 64, 65, 66]\) that have been successfully used to solve several finite-size problems in the past \([67, 68, 69, 70]\). 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 normalized four-point coupling are obtained as for the standard isotropic \(\varphi^4\) 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 eliminated by transformations and that makes anisotropic confined systems distinctly different from isotropic confined systems within the same universality class.

The main result for \(f^{\bar{\varepsilon}}\) 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 \((1.3)\). We compare the result of our fixed - \(d\) perturbation approach \([62, 63, 65, 66]\) with that of the \(\varepsilon\) 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 \([64, 65]\) and lends credibility also to the quantitative features of our predictions of anisotropy effects. The \(\varepsilon\) 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 \(L' \gg \xi_\pm^I\) at fixed \(T \neq T_c\). In order to capture the exponential structure of finite-size effects for large \(L'\) we complement (in Sect. 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 \(\varphi^4\) theory, and the amplitude of subleading long-range interactions. This diversity can be traced back to a corresponding diversity of the large-distance \((r' \gg \xi_\pm^I)\) 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 Sect. 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 \([11, 14, 15, 16, 17, 50, 52]\).

![Figure 2](image-url)  
**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 \(\Phi_\pm (r'/\xi_\pm^I, 0)\) of the bulk correlation function \(G_b\). The scaling argument, however, contains the spatial variable \(r' \equiv |\mathbf{x}'|\). \([32, 64, 65, 66]\) that depends on the anisotropy matrix \((A_{\alpha \beta})\) with \((d + 1)/2\) 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 \(\xi_h' = \xi_h'^I|\mathbf{h}'|^{-\nu/(\beta d)}\).

## II. ANISOTROPIC \(\varphi^4\) LATTICE MODEL

### A. Hamiltonian with spatial anisotropy

We start from the \(O(n)\) symmetric \(\varphi^4\) lattice Hamiltonian (divided by \(k_BT\))

\[
H = v \left[ \sum_{i=1}^{N} \left( \frac{T_0}{2} \varphi_i^2 + u_0(\varphi_i^2) - h \varphi_i \right) + \sum_{i,j=1}^{N} \frac{K_{i,j}}{2}(\varphi_i - \varphi_j)^2 \right],
\]

\(r_0(T) = r_{0c} + a_0 t, t = (T - T_c)/T_c\) 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 \(\varphi_i\) vary in the continuous range \(-\infty \leq \varphi_i(\mu) \leq \infty\). The couplings \(K_{i,j} = K_{j,i} = K(\mathbf{x}_i - \mathbf{x}_j)\) and the temperature variable \(r_0(T)\) have the dimension of \(L^{-2}\) whereas the variables \(\varphi_i\) have the dimension of \(L^{(2-d)/2}\) such that \(H\) is dimensionless. The free energy per unit volume divided by \(k_BT\) is

\[
f(t, h, L) = -V^{-1} \ln Z,
\]
where $Z$ is the dimensionless partition function. The total excess free energy density is defined as

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

where $f_b(t, h) = \lim_{t \to -\infty} f(t, h, L)$ is the bulk free energy density. Following [6, 7, 8] we shall decompose $f$, for large $L$, into singular and non-singular parts

$$f(t, h, L) = f_s(t, h, L) + f_{ns}(t, L)$$

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

For periodic b.c., the Fourier representations are

$$\varphi(x_j) = V^{-1} \sum_k e^{i k x_j} \hat{\varphi}(k)$$

where the summations $\sum_k$ run over the $N$ discrete vectors $k$ of the first Brioullin zone of the reciprocal lattice. We assume finite-range interactions $K_{ij}$ with a finite value $\hat{K}(0) = N^{-1} \sum_{i,j=1}^N K_{ij}$. In terms of the Fourier components the Hamiltonian reads

$$H = V^{-1} \sum_k \left[ \frac{1}{2} \left[ r_0 + \delta \hat{K}(k) \right] \hat{\varphi}(k) \hat{\varphi}(-k) - h \hat{\varphi}(0) \right] + u_0 V^{-3} \sum_{k, p, q} \left[ \frac{\partial}{\partial k} \hat{G}(k) \hat{G}(p) \right] \left[ \hat{\varphi}(q) \hat{\varphi}(-k - p - q) \right]$$

(2.7)

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

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

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

Odd powers of $k_\alpha$ are excluded because of inversion symmetry of the Bravais lattice. (For the case of non-Bravais lattices see the discussion in section II.C of Ref. [71].) For cubic symmetry, $A$ 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 Sects. III and X we shall consider the model also in a fully isotropic form with the short-range interaction $\delta \hat{K}(k) = k^2$ including a finite cutoff $\Lambda$ and, for $n = 1$, with the subleading long-range interaction $\frac{\Lambda}{4} \sum_{\alpha, \beta}^{\text{non-Bravais}} \delta \hat{K}(k)$

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

(2.9)

with $b > 0$. The second term of the interaction is usually classified as “irrelevant” in the renormalization-group sense 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 $-b |k|^\sigma$ 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 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 Sect. X).

The expression for $A_{\alpha \beta}$ and $B_{\alpha \beta \gamma \delta}$ in terms of the microscopic couplings $K_{ij}$ is given by the second moments

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

(2.10)

and the fourth-order moments of $K_{ij}$, respectively. They have been classified and studied in the context of the bulk correlation function in Ref. [71]. The symmetric matrix $A$ depends only on the lattice structure and on the pair interactions $K_{ij}$ and is independent of the boundary conditions and the geometry of the system. Its eigenvalues $\lambda_\alpha , \alpha = 1, 2, ..., d$, and eigenvectors $e^{(\alpha)}$ are determined by the eigenvalue equation $A e^{(\alpha)} = \lambda_\alpha e^{(\alpha)}$ with $e^{(\alpha)} \cdot e^{(\beta)} = \delta_{\alpha \beta}$. In order to have an ordinary critical point of the usual $(d, n)$ universality classes we assume positive eigenvalues $\lambda_\alpha$, det $A = \prod_{\alpha=1}^d \lambda_\alpha > 0$, 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 $r_0(T_c) = r_0$.

When $q_0(t, h)$ is defined implicitly by $\lim_{t \to -\infty} q_0(t, h) = 0$ where $q_0(t, h) = -\lim_{t \to -\infty} \partial^2 f(t, h, L)/\partial q^2$ is the bulk susceptibility for $t > 0$. This implies that $r_0(T_c) = r_0(K_{ij}, v, u_0)$ depends on the lattice structure, on $v$, on $u_0$, and on all couplings $K_{ij}$.

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

$$G_0(x_i - x_j; t, h) = \lim_{V \to \infty} \left\{ \phi_i \phi_j - \phi^2 \right\}$$

(2.11)

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

$$\hat{G}_b(k; t, h) = \sum_{x} e^{-ik \cdot x} G_b(x; t, h)$$

(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 $x_i$ 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 $O(k_z k_{\parallel})$ term of $\delta \hat{K}(k)$. In real space this is equivalent to using the $\varphi^4$ continuum Hamiltonian for the vector field $\varphi(x)$

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

(2.13)

with some cutoff $\Lambda$.

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 semi-macroscopic 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 $A$, in addition to the nonuniversal parameters $r_0, u_0, h, \Lambda$. The quantities $A_{\alpha\beta}$ depend on all microscopic details (lattice structure, electronic structure, many-body interactions) which, in general, 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 $F_{\text{cube}}(0, 0; \hat{A})$, the Binder cumulant $U_{\text{cube}}(\hat{A})$, and the critical Casimir amplitude) are nonuniversal as well.

For an appropriate formulation of the bulk order-parameter correlation function (see Sect. III) and of finite-size scaling functions (see Sect. VI) it will be important to employ the reduced anisotropy matrix $\hat{A} = A/(\det A)^{1/d}$, $\hat{A} e^{(a)} = \lambda_a e^{(a)}$ with the eigenvalues $\lambda_a = \lambda_a/(\det A)^{1/d} > 0$ and with $\det \hat{A} = \prod_{a=1}^d \lambda_a = 1$. The matrix $\hat{A}$ is independent of the kind of variables $\varphi_i$ on the lattice points and independent of the number $n$ of components of $\varphi_i$. It is well defined, e.g., also for models with fixed-length spin variables $S_i$ with $|S_i| = 1$ and for Ising models with discrete spin variables $\sigma_i = \pm 1$ instead of the continuous vector variables $\varphi_i$. Thus the XY and Ising Hamiltonians $H_{XY} = -\sum_i J_{i,j} S_i \cdot S_j$ and $H_{Ising} = -\sum_i J_{i,j} \sigma_i \sigma_j$ have the same reduced anisotropy matrix $\hat{A}$ and the same reduced eigenvalues $\lambda_a$ as the $\varphi^4$ lattice Hamiltonian if these models are defined on the same lattice points $x_i$ 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 $\bar{a}$ 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 $\pm(1, 1, 1), \pm(0, 1, 1), \pm(1, 0, 1)$ directions], and a third-NN coupling $K$ only in the diagonal $\pm(1, 1, 1)$ direction (Fig. 3). The corresponding anisotropy matrix is

![FIG. 3: Lattice points $x_j$ of the primitive cell (cube) of the anisotropic simple-cubic lattice model (2.1) and (2.7) with $\bar{A} \neq 1$. Solid, dashed, and dotted lines indicate the NN couplings $K_i$, the NNN couplings $J_i$, and the third-NN coupling $K$. Obtained from (2.10) as](image)

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

(2.14)

with the diagonal elements $D_x = K_x + J_1 + J_3 + K$, $D_y = K_y + J_2 + J_1 + K$, $D_z = K_z + J_3 + J_2 + K$. 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 $K = 0$) have been performed by Schulte and Drope [42] and
by Sumour et al. The corresponding reduced anisotropy matrix (with $\mathbf{K} \neq 0$) is

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

(2.15)

which depends only on the single anisotropy parameter

$$w = \frac{J + \mathbf{K}}{K + 2J + \mathbf{K}}.$$ 

(2.16)

The eigenvalues of $\mathbf{A}$ and $\mathbf{\tilde{A}}$ are $\lambda_1 = 2a^2(K + 4J + 3\mathbf{K})$, $\lambda_2 = \lambda_3 = 2a^2(K + J)$, and $\lambda_4 = (1 - 3w^2 + 2w^3)^{-1/3}(1 + 2w)$, $\lambda_5 = \lambda_3 = (1 - 3w^2 + 2w^3)^{-1/3}(1 - w)$, respectively. The eigenvectors
eq 1 \sqrt{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, e^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, e^{(3)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \end{pmatrix}

(2.17)
defining the principal axes are not parallel to the cubic symmetry axes. The possible range of $w$ consistent with $\det(\mathbf{\tilde{A}}(w)) > 0$ is $-\frac{2}{3} < w < 1$. In the limit $K \to 0$, $J \to 0$ at fixed $K \neq 0$ corresponding to $w \to 1$ the model describes a system of variables $\varphi_i$ on decoupled one-dimensional chains with NN interactions $\mathbf{K}$. In the previous Sect. II of this model with $\mathbf{K} = 0$ the range of $w$ was restricted to $-\frac{2}{3} < w < 1$. A vanishing of $\lambda_2$ and $\lambda_3$ occurs for $J \to -K$. At some value $w = w_{\text{LIF}}$ near $-1/2$ (corresponding to $\lambda_1 = 0$) our model is predicted to have a Lifshitz point with a wave-vector instability in the direction of $e^{(1)}$, i.e., in the $(1, 1, 1)$ direction (see also Sect. VIII. E).

(ii) Model with two-dimensional anisotropy: An anisotropic NN 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 $\mathbf{K}$ vanish. This model is of interest for comparison with the MC data by Selke and Shchur for the two-dimensional anisotropic Ising model as will be discussed in Sect. VIII. For further recent studies of the anisotropic two-dimensional Ising model see also [22].

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 $J_1 = J_2 = J_3 = \mathbf{K} = 0$ provided that $\lambda_0 > 0$, $\alpha = 1, 2, 3$.

B. Rotation and rescaling: shear transformation

In order to derive an appropriate representation of the anisotropic bulk order-parameter correlation function (see Sect. III), to develop an appropriate formulation of finite-size perturbation theory (see Sect. IV), and to treat the anisotropic Hamiltonian $H$ by RG theory (see Sect. V) it is necessary to first transform $H$ such that the $O(k, k\beta)$ terms of $\delta \hat{K}(k)$ 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 $U_{\alpha\beta} = e^{(1)}_{\alpha}$, $(\mathbf{U}^{-1})_{\alpha\beta} = e^{(2)}_{\alpha}$ where $e^{(\alpha)}_{\beta}$ denote the Cartesian components of the eigenvectors $e^{(\alpha)}$. The rescaling is provided by the diagonal matrix $\lambda = \mathbf{UAU}^{-1}$ with diagonal elements $\lambda_\alpha > 0$. In $\mathbf{k}$ space the transformation is $\mathbf{k}' = \lambda^{1/2} \mathbf{U} \mathbf{k}$ such that the $O(k', k'\beta)$ term of $\delta \hat{K}$ is brought into an isotropic form with $\mathbf{A}' = 1$,

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

(2.18)

In real space the transformed lattice points are $x'_i = \lambda^{-1/2} \mathbf{U} x_i$. This transformation leaves the scalar product $\mathbf{k}' \cdot \mathbf{x}' = \mathbf{k} \cdot \mathbf{x}$ invariant. Thereby the volume of the primitive cells is changed to $V' = V \lambda^{-2/3}$. Correspondingly the total volume of the transformed system is $V' = \lambda^{-2/3} V$ with the characteristic length $L' = V^{1/4}$. Our transformation is defined such that the values of the couplings $K_{\alpha\beta}$ on the transformed lattice as well as the temperature variable $r_0(T)$ including the values of $r_{0n}, a_0$ and $t$ are invariant [see also Eq. (4.22) 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

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

(2.19)

In terms of the Fourier transform $\varphi' = \sum_{\mathbf{k}} e^{-\mathbf{i} \mathbf{k} \cdot \mathbf{x}} \varphi_j$ the transformed lattice Hamiltonian reads

$$H' = V'^{-1} \sum_{\mathbf{k}} \frac{1}{2} [r_0 + \delta \hat{K}'(\mathbf{k}')] \varphi'(\mathbf{k}') \varphi'(-\mathbf{k}')$$

$$+ u_0' V'^{-3} \sum_{\mathbf{k}'} q \mid \varphi'(\mathbf{k}') \varphi'(\mathbf{p}') \mid \varphi'(\mathbf{q}') \varphi'(-\mathbf{k}' - \mathbf{p}' - \mathbf{q}') \rangle$$

$$- h' \varphi'(0).$$

(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 $v' = (\det \mathbf{A})^{-1/2} a_0^3$ of the transformed system is shown in Fig. 3. It has the shape of a parallelepiped whose lengths and angles are determined such that the transformed second-moment matrix $\mathbf{A}' = 1$ is the unity matrix although there are still the same NN couplings $K_{\alpha\beta}$, NNN couplings $J_1$, and third-NN coupling $\mathbf{K}$ 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 Sect. V. This is not the case for the confined system. Although the $O(k'^2)$ term of $\delta \hat{K}'(\mathbf{k}')$ in (2.18) and (2.20)
looks quite simple, namely \( k' \cdot k' \) with a trivial anisotropy matrix \( A' = 1 \), the summations \( \sum_{k'} \) are nontrivial.

For concreteness consider the simplified example (i) with the matrix (2.14) and the eigenvectors (2.17). While the \( k \) vectors of the sc lattice have the simple form

\[
k = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = \frac{2\pi}{L} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}
\]

(2.21)

with the integer numbers \( m_i = 0, \pm 1, \pm 2, \ldots \), the \( k' \) vectors are considerably more complicated,

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

(2.22)

These \( k' \) vectors reflect the shape and lattice structure of the transformed system. Thus the price paid for transforming \( A \neq 1 \) to \( A' = 1 \) is to work with more complicated \( k' \) 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 \( k \) space whereas bulk integrals (with infinite cutoff) are simplified in \( k' \) space.

In real space the Hamiltonian \( H' \) reads

\[
H' = v' \left[ \sum_{i=1}^{N} \left( \frac{\tau_0}{2} \varphi_i' + u_0 \left( \varphi_i' \right)^2 - h \varphi_i' \right) + \sum_{i,j=1}^{N} \frac{K_{i,j}}{2} \left( \varphi_i' - \varphi_j' \right)^2 \right].
\]

(2.23)

By substituting the transformations defined above one easily verifies

\[
H(r_0, u_0, K_{i,j}, v, L) = H'(r_0, h, u_0, K_{i,j}, v', L'),
\]

(2.24)

The measure for the temperature distance from criticality \( r_0 - r_{0c} = a_0 t \) is the same for both \( H \) and \( H' \). Defining the free energy density \( f' \) (divided by \( k_B T \)) as

\[
f'(t, h', L') = -V'^{-1} \ln Z'(t, h', L'),
\]

(2.25)

\[
Z'(t, h', L') = \prod_{j=1}^{N} \int_{(v')^n(2d)/(24)} d^n \varphi_j' \exp (-H'),
\]

(2.26)

one obtains the exact relations

\[
Z(t, h, L) = (\det A)^{-N/(2d)} Z'(t, h', L'),
\]

(2.27)

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

(2.28)

The last term is a bulk contribution, i.e., independent of \( L \). Furthermore it is independent of \( t \), i.e., a non-singular 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

\[
f_{s,b}(t, h) = (\det A)^{-1/2} f'_{s,b}(t, h'),
\]

(2.29)

\[
f_s(t, h, L) = (\det A)^{-1/2} f'_s(t, h', L').
\]

(2.30)

The bulk correlation function of the transformed system is

\[
G_b'(x'_i - x'_j; t, h') = \lim_{V' \rightarrow \infty} \left\{ < \varphi'_i \varphi'_j >' - < \varphi' >'^2 \right\}
\]

(2.31)

where \( < \ldots >' \) denotes the average with the weight \( \sim \exp (-H') \). It is related to \( G_b \) by

\[
G_b(x; t, h) = (det A)^{-1/2} G_b'(\lambda^{-1/2} U x; t, (det A)^{1/4} h).
\]

(2.32)

The corresponding relation between the Fourier transforms is

\[
\hat{G}_b(k; t, h) = \hat{G}_b'(\lambda^{1/2} U k; t, (det A)^{1/4} h).
\]

(2.33)

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

\[
H_{field} = H'_{field} = \int_{V'} d^d x' \left[ \frac{\tau_0}{2} \varphi'(x')^2 + \frac{1}{2} \left( \nabla' \varphi' \right)^2 + u_0' (\varphi')^2 - h' \varphi' \right]
\]

(2.34)

where \( \nabla' \varphi' \equiv (\partial \varphi'/\partial x'_{i_1}, \ldots, \partial \varphi'/\partial x'_{d}) \) 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 \( \varphi^4 \) theory this is immediately seen from the relation of dimensionally regularized bulk integrals (at infinite cutoff) such as

\[
\int_\mathbf{k} \frac{1}{(r_0 + \mathbf{k} \cdot \mathbf{A})^{-1}} = \int_\mathbf{k'} \frac{1}{(r_0 + \mathbf{k'} \cdot \mathbf{k'})^{-1}} \quad = - \frac{A_d}{\varepsilon} \int_0^{(d-2)/2} u'_0, \quad (3.1)
\]

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 \( u^* \) for anisotropic and isotropic systems (see Sect. 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 \( A_d / \varepsilon \) which is finite in \( 2 < d \leq 4 \) dimensions [see (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 [8]. Its validity has been established by the RG theory only for isotropic systems at \( h = 0 \) with short-range interactions [27, 28, 29, 30]. A brief derivation was also given by Privman and Fisher [3] 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 \( \xi_\infty \). Recently it has been 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 [3] [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 \( \lambda_\alpha \) and the reduced eigenvalues \( \tilde{\lambda}_\alpha \) 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 the following subsections A and 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 \( H_{\text{field}}' \). Near \( T_c \) the bulk free energy density can be decomposed uniquely into singular and non-singular parts as \( f'_s(t,h') = f'_s,b(t,h') + f'_{\text{ns,b}}(t) \) where \( f'_{\text{ns,b}}(t) \) 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

\[
f'_s,b(t,h') = A'_1 |t|^\eta \sum x' G'_b(\mathbf{x'};t,h') |^{-\beta s} \quad (3.3)
\]

with the universal scaling function \( W_{\pm}(z) \), \( \infty \leq z \leq \infty \). This function is independent of the cutoff procedure of \( H_{\text{field}}' \). 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

\[
\xi'_s(t,h') = \left( \frac{1}{2d} \sum x' x'^2 G'_b(\mathbf{x'};t,h') \right)^{1/2} \quad (3.4)
\]

above and below \( T_c \), respectively. In [3] we have assumed sufficiently rapidly decaying correlations, i.e., general \( n \) for \( T \geq T_c \) but \( n = 1 \) for \( T < T_c \). We assume, in the asymptotic region \( |x'| \gg (v')^{1/d}, \xi'_s \gg (v')^{1/d} \) and for \( |x'|/\xi'_s \ll O(1) \) and small \( h' \), the asymptotic scaling form

\[
G'_b(\mathbf{x'};t,h') = D'_s |x'|^{-d+2-2\eta} \Phi_{\pm}(\mathbf{x'}/\xi'_s, D'_s h' |t|^{-\beta s}), \quad (3.5)
\]

\[
\xi'_s(t,h') = \xi'_{0+} |t|^{-\nu} X_{\pm}(D'_s h' |t|^{-\beta s}), \quad (3.6)
\]

with universal scaling functions \( \Phi_{\pm}(x,y) \) and \( X_{\pm}(y) \). We use the normalization \( X_{\pm}(0) = 1 \), thus \( \xi'_s(t,0) = \xi'_{0+} t^{-\nu} \) above \( T_c \). The length \( \xi'_{0+} \) will be needed as a reference length in the formulation of renormalized finite-size theory in Sect. V. The corresponding scaling form of the
Fourier transform $\hat{G}_0$ of (3.3) is

$$\hat{G}_0(k'; t, h') = D(t|k'|^{2+\eta}) \Phi_\pm (k'|\xi'_\pm, D_\infty |t|^{-\beta}) \ ,$$  

(3.7)

$$\Phi_\pm (x', y') = 2\pi (d-1)/2 \Gamma((d-1)/2)^{-1} \int_0^\infty ds s^{1-\eta} \times \int d(\cos \theta)(\sin \theta)^{d-3} e^{-is \cos \theta} \Phi_\pm (s|x', y') \ .$$  

(3.8)

The three amplitudes $D_1$, $D_2$, and $\xi'_+$ 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

$$(\xi_0')^d A_1 = Q_1(d, n) = \text{universal} \ ,$$  

(3.9)

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

(3.10)

$$D_1'(A_2')^{-2}A_1' = P_3(d, n) = \text{universal} \ .$$  

(3.11)

In Ref. [7] 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. (3.12) and (3.13) below. For the sake of clarity we present the explicit expressions for $Q_1$ and $P_3$ in terms of universal scaling functions in Appendix A. An equivalent formulation of Eq. (3.3) is

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

(3.12)

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

Furthermore, the following amplitude ratios

$$(\Gamma'_c/\Gamma'_\xi)(\xi'_0/\xi'_b)^{2-\eta} = Q_2(d, n) = \text{universal} \ ,$$  

(3.13)

$$\bar{D}'_\infty (\xi'_0)^{2-\eta}/\Gamma'_\xi = Q_3(d, n) = \text{universal} \ ,$$  

(3.14)

have been proposed [74] to be universal. The constants $\Gamma'_\xi$, $\Gamma'_c$ and $\xi'_c$ are defined as follows: $\xi'_c(t, 0) = 0$, $\Gamma'_\xi = \Gamma'_c$, and $\xi'_c(h') = \xi'_c(h')^{-(2-\eta)/\beta(3)}$. The length $\xi'_c$ with the amplitude $\xi'_c$ is a natural reference length of finite-size theory at $t = 0$, $h' \neq 0$ [see (6.11) below]. $\bar{D}'_\infty$ is the asymptotic (small $k'$) amplitude of $\hat{G}_0(k'; 0, 0) \approx \bar{D}'_\infty |k'|^{-2+\eta}$. Alternatively, Eq. (3.14) can be formulated as $D'_\infty (\xi'_b)^{2-\eta}/\Gamma'_\xi = Q_3(d, n)$, or, equivalently,

$$\lim_{|x'| \to -\infty} \left\{ G_0(x'; 0, 0) (|x'|/\xi'_0)^{d-2-\eta} \right\} (\xi'_0)^d / \Gamma'_\xi = Q_3(d, n) = (D'_\infty / \bar{D}'_\infty) Q_3(d, n) = \text{universal} \ .$$  

(3.15)

where $D'_\infty$ is the asymptotic (large-$x'$) amplitude of $G'_0(x'; 0, 0) \approx D'_\infty |x'|^{-d-2+\eta}$. The derivation of Eqs. (3.3) - (3.15) is sketched in App. A. Again, all of the constants on the left-hand sides of (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

$$\xi'_0 - \xi'_0 = X_0(0) = \text{universal} \ .$$  

(3.16)

Previously the bulk relations (3.9) - (3.10) were expected to be universal for all systems within a given universality class [5]. Consistency with the universality of (3.13) and (3.14) was found 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 $A = c_0 1$ or $A = 1$ and with an isotropic scattering intensity [73]. 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 Subsect. B below, Eqs. (3.9) and (3.12) - (3.15) must be reformulated for anisotropic systems with noncubic anisotropy at $O(k_\sigma k_d)$ whereas (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, 10, 11, 16] that the universal scaling form (3.5) - (3.6) is not valid in the regime $r' \equiv |x'| > \xi'_+ > T_c$. The same can be shown for $n = 1$ in the regime $r' > \xi'_+ > T_c$. Note that this regime is part of the asymptotic critical regime $r' > \bar{\lambda}$ and $\xi'_+ > \bar{\lambda}$ corresponding to the shaded area in the $r'^{-1}$ - $\xi'_\pm$ 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 $\varphi^4$ lattice model with short-range interactions, the exponential decay above $T_c$ depends explicitly on the lattice spacing $\bar{\lambda}$ via the exponential correlation length $\xi'_\pm$ [11, 76] in Sect. X. We shall show that it also depends on the bare four-point coupling $u_0$. (ii) For the $\varphi^4$ continuum theory with a smooth cutoff $\Lambda$, the exponential decay depends explicitly on $\Lambda$ via $\xi'_\pm(\Lambda)$ [9, 10] (see also Sect. X). (iii) For the $\varphi^4$ continuum theory with a sharp cutoff $\Lambda$, a nonuniversal oscillatory power-law decay dominates the exponential decay [11, 77]. (iv) In the presence of subleading long-range interactions of the type (2.9), the power law $\sim b|\varphi'|^{-d-\sigma}$ 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 $|\varphi'|/\xi'_+ > 1$ at $h = 0$ is [16]

$$G'_0(x'; t, 0) = \frac{D'_\infty}{|x'|^{d-2}} \left[ \Phi_+ (|x'|/\xi'_+) + \frac{b}{|x'|^{d-2}} D(|x'|/\xi'_+) \right] \ .$$  

(3.17)
sality are violated in the regime $|\mathbf{x}'| \gg \xi_+^d$ (shaded area in Fig. 2) because, in addition to the reference length $\xi_+^d$, the nonuniversal lengths $\bar{a}$, $u_0^{-1/\nu}$, $\Lambda^{-1}$, 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 (2.19), (2.29) and (3.3), the asymptotic scaling form of $f_{s,b}$ is given by (1.1) with the nonuniversal amplitudes

$$A_1 = A_1'(\det A)^{-1/2}, \quad A_2 = A_2'(\det A)^{1/4}.$$  \hspace{1cm} (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 $\hat{A}$ and $\tilde{\hat{A}}$ with diagonal elements $\lambda_0$ and $\bar{\lambda}_0$. Using (2.32), (2.33), (3.3) and (3.4) we write $G_b$ and $\tilde{G}_b$ as

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

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

with the nonuniversal amplitudes

$$D_1 = D_1'(\det A)^{-(2+n)/(2d)}, \hspace{1cm} D_2 = D_2'(\det A)^{1/4}.$$  \hspace{1cm} (3.21)

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

$$r' \equiv |\mathbf{x}'| = |\hat{\lambda}^{-1/2} U \mathbf{x}|,$$ \hspace{1cm} (3.23)

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

While the simple transformations (3.18) and (3.22) follow immediately from the transformations of $h, \varphi, t$, 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:

$$A_2/D_2 = P_2(d, n) = universal.$$  \hspace{1cm} (3.24)

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

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

$$\chi_b'(t, h') = -\partial^2 f_b'(t, h')/\partial h'^2 = v' \sum_x G_b'(\mathbf{x}'; t, h')$$

$$= \chi_b(t, h) = -\partial^2 f_b(t, h)/\partial h^2 = v \sum_x G_b(\mathbf{x}; t, h)(3.26)$$

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 App. A). The physical significance of (3.24) is that, at criticality, the bulk correlation function and its Fourier transform, if expressed in term of $\hat{\lambda}$,

$$\tilde{G}_b(\mathbf{k}; 0, 0) = D_1 \tilde{\Phi}_\pm(0, 0)|\tilde{\lambda}^{1/2} U \mathbf{k}|^{-2+\eta},$$ \hspace{1cm} (3.27)

$$\tilde{G}_b(\mathbf{k}; 0, 0) = D_1 \tilde{\Phi}_\pm(0, 0)|\tilde{\lambda}^{1/2} U \mathbf{k}|^{-2+\eta},$$ \hspace{1cm} (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 $\tilde{G}_b$ at criticality are governed by the $d$ reduced nonuniversal eigenvalues $\bar{\lambda}_0$ (with $d-1$ independent parameters). In addition, the 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 $e^{(\alpha)}$ of the principal axes relative to the symmetry axes of the system. Thus $1 + (d-1)/2 = d(d+1)/2$ nonuniversal parameters are needed at $T = T_c$ and $h = 0$, and $d(d+1)/2$ 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 $e^{(\alpha)}$ of the principal axis $\alpha$ the spatial dependence of $G_b$ is, for $|\tilde{\mathbf{x}}^{(\alpha)}|/\xi_+^d \lesssim O(1)$,

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

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

$$\xi_+^{(\alpha)}(t, h) = \lambda_0^{\alpha d/2} \xi_+^{(\alpha)}(t, (\det A)^{1/4} h)$$

$$= \xi_+^{(\alpha)} |t|^{-\nu} \xi_+^{(\alpha)}(D_2 h |t|^{-\beta \delta}).$$ \hspace{1cm} (3.30)

Thus along the different principal axes (see Fig. 1 (b) of Ref. 13) there exist $d$ different principal correlation lengths $\xi_+^{(\alpha)}(t, h)$ which constitute $d$ different nonuniversal reference lengths with $d$ nonuniversal amplitudes $\xi_+^{(\alpha)} = \lambda_0^{1/2} \xi_+^{(\alpha)}$. Their ratios

$$\xi_0^{(\alpha)}/\lambda_0^{(\beta)} = (\lambda_\alpha/\lambda_\beta)^{1/2}.$$ \hspace{1cm} (3.31)
are also nonuniversal. Below $T_c$ at $h = 0$ we have $\xi^{-}(\alpha) = \xi^{-}(\alpha)[t^{-\nu}$ with the universal ratio for each $\alpha$

$$\xi^{-}(\alpha)/\xi^{+(\alpha)} = X_{-}(0) = \text{universal} \quad (3.32)$$

but for $\alpha \neq \beta$ the ratios $\xi^{-}(\alpha)/\xi^{+(\beta)} = (\lambda_{\alpha}/\lambda_{\beta})^{1/2}$ and $\xi^{-}(\alpha)/\xi^{+(\beta)} = (\lambda_{\alpha}/\lambda_{\beta})^{1/2}X_{-}(0)$ are nonuniversal. For all of $A_{1}' = A_{1}\prod_{\delta=1}^{d} = \lambda_{\alpha}^{1/2}$, Eqs. (3.9) and (3.12) imply

$$A_{1}\prod_{\delta=1}^{d} \xi^{+(\alpha)} = \lim_{t \to \infty} \left[f_{s,b}(t,0) \prod_{\delta=1}^{d} \xi^{+(\alpha)}(t,0)\right]^{d} = Q_{1}(d,n) = \text{universal} \quad (3.33)$$

The susceptibility $\chi_{e}(t, h)$ with $\chi_{e}(t, h) = \Gamma_{+} t^{-\gamma}$ above $T_c$ and $\chi_{b}(0, h) = \Gamma_{0} t^{-\gamma/\beta_{0}}$ have the amplitudes $\xi^{+} = \Gamma_{+}$ and $\Gamma_{c} = \Gamma_{c}(\det A)^{-\gamma/(4\beta)}$. Here we have used (2.19) and (3.29). From Eq. (3.30) we have $\xi^{+(\alpha)}(0, h) = \xi^{+(\alpha)}[h^{-\nu/(4\beta)}]$ with

$$\xi^{+(\alpha)} = \lambda_{\alpha}^{1/2}(\det A)^{-\gamma/(4\beta)} \xi^{+} \quad (3.34)$$

Eq. (3.33) then implies for each $\alpha = 1, \ldots, d$

$$\left(\Gamma_{+}/\Gamma_{c}\right) \left(\xi^{+(\alpha)}/\xi^{+(\beta)}\right)^{2-\eta} = Q_{2}(d,n) = \text{universal} \quad (3.35)$$

and from Eqs. (3.1) and (3.2) we obtain for each $\beta$

$$\lim_{|\xi^{+(\beta)}| \to \infty} \left\{G_{b}(\xi^{+(\beta)}; 0, 0) \left[\frac{\xi^{+(\beta)}}{\xi^{+(\beta)}}\right]^{d-2+\eta} \prod_{\alpha=1}^{d} \xi^{+(\alpha)} \right\}^{d} = \bar{Q}_{3}(d,n) = \text{universal} \quad (3.36)$$

$Q_{1}, Q_{2}$ and $\bar{Q}_{3} = (D_{\infty}/D_{\infty}) Q_{3}$ 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 $R_{\xi}$ and $R_{f}$ 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 [78] such as $R_{s}, R_{d}, R_{m}$, and $R_{t}$ 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. (4.43), and of the universality of the scaling function $W_{\xi}(z)$ that 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 $A_+^{\prime}$ and $\Gamma_+^{\prime}$ of the bulk specific heat $C_{b}^{\prime} = \partial^{2} f_{s,b}^{\prime}/\partial h^{2} = (A_{+}^{\prime}/\alpha)|t|^{-\alpha}$ and of the bulk susceptibility $\chi_{+}^{\prime} = -\partial^{2} f_{s,b}^{\prime}/\partial t^{2} = \Gamma_{+}^{\prime}|t|^{-\gamma}$. The isotropic system above and below $T_{c}$ at $h' = 0$, respectively, and, correspondingly, $C_{b}^{\prime} = \partial^{2} f_{s,b}^{\prime}/\partial h^{2} = (A_{+}^{\prime}/\alpha)|t|^{-\alpha}$, $\chi_{b} = -\partial^{2} f_{s,b}^{\prime}/\partial t^{2} = \Gamma_{+}^{\prime}|t|^{-\gamma}$ of the anisotropic system. (For $\chi_{b}^{\prime} = \chi_{b}$ below $T_{c}$ we consider, for simplicity, only $n = 1$.) Their amplitude ratios are given by $A_{+}^{\prime}/A_{+}^{\prime} = A_{++}^{\prime} = W_{+}(0)/W_{-}(0)$ and by

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

Thus the nonuniversal parameters $A_{\alpha\beta}$ drop out completely. Corresponding statements hold for the amplitude combinations denoted by $R_{X_{+}}$, $R_{C_{+}}$, $R_{A_{+}}$ 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 (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 $\langle \phi(\mathbf{x})^{2} \rangle^{2} >$. 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 [78] and to boundary critical phenomena [79, 80].

In conclusion, all critical exponents and bulk scaling functions $W_{\pm}(z), \Phi_{\pm}(x', y')$ with $|x'| \lesssim O(1)$, and $\Phi_{\pm}(y')$ 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 $\Phi_{\pm}(x', y')$ would be 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 $|\bar{X}|^{-1/2} U_{X}$ - $d-2+\eta$ [see (2.27)]. 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 (3.10), (3.11), (3.24), (3.25), (3.29), (3.37), and those of Ref. [8] mentioned above]. The other relations [such as (3.4), (3.5), (3.6)] 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 multi-parameter 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 subsection A above.

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 $f_s(t, L') - f_s(t, L)$ where $f_s(t, L)$ is the singular bulk part: (a) the exponential $L'$ dependence $\sim \exp(-L'/\xi_{e+}^t)$ for large $L'/\xi_{e+}^t \gg 1$ at fixed temperature $T > T_c$ with $\xi_{e+}^t$ being the exponential bulk correlation length above $T_c$, (b) the power-law behavior $\sim L'^{-d}$ for large $L'$ at fixed $L'/\xi_{e-}^t$ such that $L'/\xi_{e-}^t \ll 1$, above, at and below $T_c$, where $\xi_{e-}^t$ is the second-moment bulk correlation length (3.3) (c) the exponential $L'$ dependence $\sim \exp(-L'/\xi_{e-}^t)$ for large $L'/\xi_{e-}^t \gg 1$ at fixed temperature $T < T_c$ with $\xi_{e-}^t$ being the exponential bulk correlation length below $T_c$. For a description of the cases (a) and (c), ordinary perturbation theory with respect to $u_0$ of the isotropic $\varphi^4$ theory is sufficient. For the case (b), a separation of the lowest mode and a perturbation treatment of the higher modes is necessary.

For anisotropic systems, the distinction between the regimes (a), (b) and (c) remains relevant except that there exist no single correlation lengths $\xi_{e+}, \xi_{e-}$, and $\xi_{e-}$. In this and the subsequent sections we treat the case (b) on the lattice Hamiltonian (2.1) for $n = 1, h = 0$ and defer the cases (a) and (c) to Section X. The 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 run over $N$ discrete vectors $k \equiv (k_1, k_2, \ldots, k_d)$ with Cartesian components $k_\alpha = 2\pi n_\alpha/L, n_\alpha = 0, \pm 1, \pm 2, \ldots, \alpha = 1, 2, \ldots, d$ 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 $A$. We shall show that, for small $|t|$ and large $L$ in the regime (b), $f_s$ has the scaling form

$$f_s(t, L; A) = L^{-d} dF(t((L'/\xi_0^t)^{-1/\nu}; \tilde{A})$$

(4.1)

where the scaling argument is expressed in terms of the transformed length $L' = (\det A)^{-1/2} L$, rather than in terms of $L$, and where $\xi_0^t$ is the asymptotic amplitude of the bulk correlation length defined in (3.3) on the basis of the transformed Hamiltonian $H'$. Because of (2.20), $\mathcal{F}$ is identical with the finite-size scaling function of the free energy density of the transformed system

$$f_s(t, L'; \tilde{A}) = L'^{-d} dF(t((L'/\xi_0^t)^{-1/\nu}; \tilde{A})$$

(4.2)

The advantage of the transformed system is that its bulk renormalizations (see Sect. V) are well known from the standard isotropic $\varphi^4$ 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 $H'$, (2.20) and (2.23), with $\nu' = (\det A)^{-1/2} \tilde{a}^d$.

B. Perturbation approach

It is necessary to reformulate in detail 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 $\varphi'_j = \Phi' + \sigma'_j$, $\Phi' = L'^{-d} \varphi'(0) = N^{-1} \sum_j \varphi'_j$, $\sigma'_j = L'^{-d} \sum_{k' \neq 0} e^{i k' \cdot \hat{x}_j} \varphi'(k')$, (4.3) (4.4)

where $L'^{d}$ is the finite-size scaling function of the free energy density of the transformed system $f'_s(t, L'; \tilde{A})$ (4.2)

The partition function of the anisotropic system (2.1) for $n = 1$ at fixed temperature $T > T_c$ is expressed in terms of the partition function $H'_0, \tilde{A}$, and the partition function $Z', (2.20)$, are decomposed as $H' = H'_0 + \tilde{H}'(\Phi', \sigma')$,

$$H'_0(r_0, u_0, L', \Phi'^2) = L'^d \left[ \frac{1}{2} \tilde{r}_0 \Phi'^2 + u_0 \Phi'^4 \right]$$

(4.5)

$$\tilde{H}'(\Phi', \sigma') = v \left\{ \sum_{j=1}^N \left[ \left( \frac{v_0}{2} + 6u_0 \Phi'^2 \right) \sigma'^2 + 4u_0 \Phi'^4 \sigma'^3 + u_0 \sigma'^4 \right] \right\}$$

(4.6)

$$Z' = \frac{L'^{d/2}}{(\nu'')^{-d}} \int d\Phi' \exp \left\{ - \left[ H'_0 + \tilde{H}'(\Phi'^2) \right] \right\}$$

(4.7)

$$\tilde{\Gamma}'(\Phi'^2) = - \ln \prod_{k' \neq 0} (\nu'')^{-d/2} \int d\tilde{x}'(k')$$

(4.8)
The crucial point is to incorporate the lowest-mode approximation of \( \Phi' \) into a smooth interpolation between the mean-field bulk limits of the Gaussian fluctuations \( \Phi \) not explicitly defined in Eq. (2.11) of [66]. The quantity \( \int \Gamma''(\Phi'^2) \) can be interpreted as a constraint free energy, with the constraint being that the zero-mode amplitude \( \Phi' \) is fixed. The quantity \( \exp[-\Gamma''(\Phi'^2)] \) 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 \( \varepsilon \) expansion approach of [32] and [64], we shall not expand the exponential form \( \exp[-\Gamma''(\Phi'^2)] \) but only \( \Gamma''(\Phi'^2) \). The advantage of our approach has been demonstrated for the specific heat below \( T_c \) in Refs. [66, 68].

Following [65] and [66] we decompose \( \tilde{H}(\Phi', \sigma') = H'_1 + H'_2 \) into an unperturbed Gaussian part

\[
H'_1 = v' \left( \sum_{j=1}^N \frac{R_{ij}^j}{2} \sigma_j^2 + \sum_{i,j=1}^N \frac{K_{ij}}{2} (\sigma'_i - \sigma'_j)^2 \right)
\]

and a perturbation part

\[
H'_2 = v' \left( \sum_{j=1}^N \left[ 6u'_0(\Phi'^2 - M'_0^2)\sigma_j^2 + 4u'_0\Phi'\sigma_j^3 + u'_0\sigma'_j^4 \right] \right).
\]

The crucial point is to incorporate the lowest-mode average

\[
M'_0(r_0, u'_0, L') = \frac{\int d\Phi' \Phi'^2 \exp(-H'_0)}{\int d\Phi' \exp(-H'_0)}
\]

into the parameter

\[
r'_0L(r_0, u'_0, L') = r_0 + 12u'_0M'_0
\]

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 [81] 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 \( L' \), \( M'_0 \) and \( r'_0L \) interpolate smoothly between the mean-field bulk limits above and below \( T_c \)

\[
\lim_{L' \to \infty} M'_0 \equiv M'^2_{mf} = \begin{cases} 0 & \text{for } r_0 \geq 0, \\ -r_0/(4u'_0) & \text{for } r_0 \leq 0. \end{cases}
\]

\[
\lim_{L' \to \infty} r'_0L \equiv r_{mf} = \begin{cases} r_0 & \text{for } r_0 \geq 0, \\ -2r_0 & \text{for } r_0 \leq 0. \end{cases}
\]

The contribution of \( H'_1 \) to \( L^{-d} \Gamma''(\Phi'^2) \) is (compare Eq. (15) in Appendix B)

\[
- \frac{1}{L^{d/2}} \ln \left[ \prod_{k' \neq 0} \int \frac{d\tilde{\Phi}'(k')}{(\nu')^d L^{d/2}} \exp(-H'_1) = - \frac{N - 1}{2L^{d/2}} \ln(2\pi)
\]

\[
+ \frac{1}{2\pi^{d/2}} \sum_{k' \neq 0} \ln \left\{ \left[ r'_0L + \delta \tilde{K}'(k') \right](\nu')^{2/d} \right\}.
\]\n
The leading contributions of the perturbation term \( 6u'_0(\Phi'^2 - M'_0^2)\sigma_j^2 \) of \( H'_2 \) to \( L^{-d} \Gamma''(\Phi'^2) \) read

\[
6u'_0(\Phi'^2 - M'_0^2)S_1(r'_0L) - 36u'_0(\Phi'^2 - M'_0^2)^2S_2(r'_0L)
\]

\[
+ O(u'_0^3(\Phi'^2 - M'_0^2)^3)
\]

where

\[
S_m(r'_0L) = L'^{-d} \sum_{k' \neq 0} \left\{ \left[ r'_0L + \delta \tilde{K}'(k') \right]^{-m} \right\}.
\]

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. (4.10) as it contains the coupling between the fluctuations \( \Phi'^2 - M'_0^2 \) of the lowest mode and those of the higher modes \( \Phi' \). For a discussion of the order of the neglected terms see also Refs. [66, 81].

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

\[
f' = L'^{-d} \Gamma'(0) - L'^{-d} \ln \left\{ \frac{L'^{d/2}}{(\nu')^d} \int_{-\infty}^{\infty} d\Phi' \exp[-H'^{eff}] \right\}
\]

\[
= - \frac{N - 1}{2L^{d/2}} \ln(2\pi)
\]

\[
+ \frac{1}{2\pi^{d/2}} \sum_{k' \neq 0} \ln \left\{ \left[ r'_0L + \delta \tilde{K}'(k') \right](\nu')^{2/d} \right\}
\]

\[
- \frac{1}{L'^{-d}} \ln \left\{ \frac{L'^{d/2}}{(\nu')^d} \int_{-\infty}^{\infty} d\Phi' \exp[-H'^{eff}] \right\}
\]

\[
- 6u'_0M'_0^2S_1(r'_0L) - 36u'_0M'_0^2S_2(r'_0L),
\]

\[
H'^{eff} = L'^{d} \left( \frac{1}{2} u'_0^{eff} \Phi'^2 + u'_0^{eff} \Phi'^4 \right),
\]

\[
r'^{eff}_0 = r_0 + 12u'_0S_1(r'_0L) + 144u'_0^2M'_0^2S_2(r'_0L).
\]

Apart from the different form of the lattice interaction \( \delta \tilde{K}'(k') \) and the different vectors \( k' \), Eq. (4.13) 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
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 (4.13) in App. C and (4.33)-(4.35)]. (ii) In (4.18) there are the additive logarithmic finite-size terms

$$-\frac{N - 1}{2L^d} \ln(2\pi) - \frac{1}{L^d} \ln L^{d/2}$$

$$= -\frac{1}{2v} \ln(2\pi) + \frac{1}{2L^d} \ln \frac{2\pi}{L^d}$$  \hspace{1cm} (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 r.h.s. of (4.22) is an unimportant nonsingular bulk part, the second term yields a nonnegligible contribution to the universal value of the finite-size scaling function $\mathcal{F}^{ex}$ 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 (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, 35, 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 $\Phi'^2 - M'^2$ of the lowest mode amplitude around its average $M'^2$ 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 $\Phi'^2$ around zero. Setting $M'^2 = 0$ 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 (4.18) for large $L'$ below $T_c$ is

$$\lim_{L' \to \infty} - L'^{-d} \ln \left\{ \frac{L'^{d/2}}{(v')^{1/d}} \int_{-\infty}^{\infty} d\Phi' \exp \left[ -H'^{eff} \right] \right\}$$

$$= -\frac{r'^{\text{eff}}}{16u'^{\text{eff}}}$$  \hspace{1cm} (4.23)

which, after expansion of $(u'^{\text{eff}})^{-1}$ with respect to $u'^{\text{eff}}$, would produce arbitrary large powers of $u'^{\text{eff}}$. On the other hand it is clear at the outset that, because of neglecting the terms $\sim u'^{\text{eff}} \sigma'^{2} \sigma'^{3}$ and $\sim u'^{\text{eff}} \sigma'^{4}$ of $H'^{eff}$, the neglected terms in (4.18) are bulk terms of $O(u'^{\text{eff}})$ corresponding to two-loop terms. Therefore it is necessary to further improve the perturbation expression (4.18). Here our reformulation of the $\int d\Phi' e^{-H'^{eff}}$ term will be guided by the requirement that higher-order powers of $u'^{\text{eff}}$ are neglected already at the level of $H'^{eff}$, before integrating over $\Phi'$. For this purpose we rewrite the logarithm of the integral over the lowest mode as

$$\ln \left\{ \frac{L'^{d/2}}{(v')^{1/d}} \int_{-\infty}^{\infty} d\Phi' \exp \left[ -H'^{eff} \right] \right\}$$

$$= \ln \int_{-\infty}^{\infty} ds \exp \left[ -\frac{r'^{\text{eff}} L'^{d/2}}{2u'^{2}S_{1}(r'_{0L})^{1/2}} \frac{s}{s^{4}} \right]$$

$$+ \frac{1}{2} \ln \left[ \frac{L'^{d/2}}{(v')^{2/d}u'^{2}S_{1}(r'_{0L})^{1/2}} \right].$$  \hspace{1cm} (4.24)

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

$$(u'^{\text{eff}})^{-1/2} = u'^{-1/2} + 18u'^{1/2}S_{2}(r'_{0L}) + O(u'^{3/2}).$$  \hspace{1cm} (4.25)

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

$$f' = -\frac{N - 1}{2L^{d}} \ln(2\pi)$$

$$+ \frac{1}{2L^{d}} \sum_{k' \neq 0} \ln \left\{ \left[ r'_{0L} + \delta \hat{K}'(k') \right] \left( v' \right)^{1/2d} \right\}$$

$$- \frac{1}{L^{d}} \ln \int_{-\infty}^{\infty} ds \exp \left( -\frac{1}{2} \frac{r'^{\text{eff}} S_{2}(r'_{0L})^{1/2}}{v'^{2}S_{2}(r'_{0L})^{1/2}} \right)$$

$$- \frac{1}{2L^{d}} \ln \left[ \frac{L'^{d/2}u'^{2}S_{2}(r'_{0L})^{1/2}}{v'^{d/2}} \right]$$

$$- 36u'^{2}M'^{2}S_{2}(r'_{0L})$$  \hspace{1cm} (4.26)

with

$$y'^{\text{eff}} = L'^{d/2}u'^{-1/2}\{ r'[1 + 18u'^{1/2}S_{2}(r'_{0L})] + 12u'^{1/2}S_{1}(r'_{0L}) \} + 144u'^{2}M'^{2}S_{2}(r'_{0L})$$  \hspace{1cm} (4.27)

$$w'^{\text{eff}} = u'^{-1/2}[1 + 18u'^{1/2}S_{2}(r'_{0L})].$$  \hspace{1cm} (4.28)

Now, because of $u'^{2}M'^{2} \sim O(v'^{1/2})$ at $T_c$, $y'^{\text{eff}}$ and $w'^{\text{eff}}$ and the last two terms in (4.26) contain terms only up to $O(v'^{1/2})$ at $T_c$. One can verify that in the bulk limit below $T_c$ the last two terms $-6u'^{2}M'^{2}S_{1}$ and
\(-36u_0^2M_{04}^2S_2\) of (4.26) which are of \(O(1)\) are exactly cancelled by the \(O(1)\) terms of the saddle-point contribution \(-y^{\text{eff}}_{\lambda}/(16L^d)\) of the integral term of (4.26). Thus Eq. (4.26) correctly contains the bare bulk free energy density \(f'_b\) in one-loop order [i.e., up to \(O(1)\)]

\[
f'_b^+ = -\frac{\ln(2\pi)}{2\nu'} + \frac{1}{2} \int_{\mathbf{k}'} \ln\{|r_0 + \delta\tilde{K}'(\mathbf{k}')|v'\}^{2/d} + O(u'_0),
\]

\[
f'_b^- = \frac{1}{2} r_0 M_{04}^2 + u'_0 M_{04}^4 - \frac{\ln(2\pi)}{2\nu'} + \frac{1}{2} \int_{\mathbf{k}'} \ln\{|-2r_0 + \delta\tilde{K}'(\mathbf{k}')|v'\}^{2/d} + O(u'_0)
\]

above and below \(T_c\), respectively, where

\[
\int = (\det \mathbf{A})^{1/2} \int_{\mathbf{k}} \equiv (\det \mathbf{A})^{1/2} \prod_{\alpha=1}^{d} \int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk_\alpha}{2\pi}.
\]

We shall rewrite (4.26) in terms of \(r_0 - r_{0c}\) where

\[
r_{0c} = -12u'_0 \int_{\mathbf{k}'} \frac{1}{\delta\tilde{K}'(\mathbf{k}')}) = -12u'_0 \int_{\mathbf{k}} \frac{1}{\delta\tilde{K}(\mathbf{k})}
\]

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 \(0 \leq |t(L/\xi_0)^{1/v'}| \lesssim O(1)\) above, at, and below \(T_c\), i.e., the regime (b) mentioned above. If applied to the regime \(L/\xi_0 \gg 1\) 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

\[
f'(r_0 - r_{0c}, u'_0, L', K_{i,j}, v') = f'_{\text{ns,b}}(r_0 - r_{0c}, u'_0, K_{i,j}, v') + \delta f'(r_0 - r_{0c}, u'_0, L', K_{i,j}, v'),
\]

where \(f'_{\text{ns,b}}\) is a non-singular bulk part up to linear order in \(r_0 - r_{0c}\),

\[
f'_{\text{ns,b}}(r_0 - r_{0c}, u'_0, K_{i,j}, v') = \frac{-\ln(2\pi)}{2v'} + \frac{1}{2} \int_{\mathbf{k}'} \ln\{|\delta\tilde{K}'(\mathbf{k}')|v'\}^{2/d} + \frac{r_0 - r_{0c}}{2} \int_{\mathbf{k}'} |\delta\tilde{K}'(\mathbf{k}')|^{1/d} \cdot
\]

As expected from bulk theory [82], 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 \(\tilde{A}\) rather than on \(A\)

\[
\lim_{v' \to 0} \delta f'(r_0 - r_{0c}, u'_0, L', K_{i,j}, v') = \delta f'(r_0 - r_{0c}, u'_0, L', \tilde{A})
\]

The r.h.s. of (4.33) can be further decomposed as

\[
\delta f'(r_0 - r_{0c}, u'_0, L', \tilde{A}) = f'_{\text{ns,b}}(r_0 - r_{0c}, u'_0) + f'_s(r_0 - r_{0c}, u'_0, L', \tilde{A}),
\]

where \(f'_{\text{ns,b}}\) is a non-singular bulk part proportional to \((r_0 - r_{0c})^2\) [82]. 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 non-singular 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 (4.20) give rise only to corrections to scaling. However, although the limit (4.33) 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 Section X.

### D. Bare perturbation result

The calculation of \(\delta f'\) is outlined in App. B and C for the power-law regime \(|r_0 - r_{0c}| \lesssim O(u'_0 L^{-d/2})\), \(L' \gg (v')^{1/d}, |r_0 - r_{0c}|^{1/d} (v')^{1/d} \ll 1\). The result reads for \(2 < d < 4\)

\[
\delta f'(r_0 - r_{0c}, u'_0, L', \tilde{A}) = \frac{-1}{L^d} \left\{ \ln \int_{-\infty}^{\infty} ds \exp\left(-\frac{1}{2} u'_0 \frac{\xi_{\text{eff}}(\tilde{A})}{L'} s^2 - s^4 \right) \right\}
\]

\[
- \frac{3}{2\pi^2} \left( \frac{M_0^2 L'^2}{2\pi} \right) I_1(\nu_0 L'^2, \tilde{A}) = \frac{9}{2\pi^4} L' I_2(\nu_0 L'^2, \tilde{A})
\]

with

\[
y_{0\text{eff}}(\tilde{A}) = \left( \frac{V'}{u'_0} \right)^{1/2} \left[ 1 + \frac{18u'_0}{2\pi} \left( \frac{A_d(d-2)}{2\pi} \right)^{-1/2} + \frac{L'^{2-d}}{16\pi^4} L' I_2(\nu_0 L'^2, \tilde{A}) \right]
\]

\[
+ 12u'_0 \left( \frac{A_d(d-2)}{2\pi} \right) \left( \frac{L'^{2-d}}{16\pi^4} L' I_2(\nu_0 L'^2, \tilde{A}) \right)
\]

\[
+ \frac{144u'_0^2 M_0^2}{\nu_0} \left( \frac{A_d(d-2)}{2\pi} \right) \left( \frac{L'^{2-d}}{16\pi^4} L' I_2(\nu_0 L'^2, \tilde{A}) \right)
\]

(4.38)
\[ w_0^{eff}(\mathbf{A}) = u_0^{-1/2} \left[ 1 + 18u_0' \left( \frac{A_d(d-2)}{2\varepsilon} \right) (r'_{0L})^{-\varepsilon/2} \right. \\
\left. + \frac{L^d}{16\pi^4} I_2(r'_{0L}L^2, \mathbf{A}) \right] , \quad (4.39) \]

\[ r'_{0L}(r_0-r_0c, u_0', L') = r_0 - r_0c + 12u_0'M_0^2 , \quad (4.40) \]

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

\[ y'_0 = (r_0 - r_0c)(V'/u_0')^{1/2} , \quad (4.42) \]

\[ \vartheta(y_0) = \int_0^\infty ds \, s^m \exp \left(-\frac{3}{2}y_0 s^2 - s^4\right) , \quad (4.43) \]

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

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

\[ K_d(y, \mathbf{A}) = \sum_n \exp(-yn \cdot \mathbf{A}n) \quad (4.46) \]

with \( n = (n_1, n_2, ..., n_d), n_\alpha = 0, \pm 1, ..., \pm \infty \). The behavior of the functions \( J_0, J_1, \) and \( J_2 \) for small and large arguments \( r'_{0L}L^2 \) is given in App. C.

The crucial information on the anisotropy is contained in the sum (4.46). By means of the Poisson identity \[ 83 \] [see also (13.9)] one can show that this function satisfies

\[ K_d(y, \mathbf{A}) = (\det \mathbf{A})^{-1/2} \left( \frac{\pi}{y} \right)^{d/2} K_d \left( \frac{\pi}{y}, \mathbf{A}^{-1} \right) . \]

The sum (4.46) could formally be rewritten in \( k' \) space as \( \sum_{k'} \exp(-yk' \cdot k') \) with \( y = L^2/(4\pi^2) \) but in practice there is no advantage of using the more complicated \( k' \) vectors (see the example (2.22) in Sect. II). For this reason the sums in the three-dimensional calculations in Sect. VIII will be performed in \( k \) 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 \( t \neq 0 \) the small-\( t \) behavior is \( \delta f'_t \sim |t|^{d/2} \) rather than \( \sim |t|^d \). (ii) At \( t = 0 \) the leading large-\( L' \) behavior is \( \delta f' \sim L'^{-d/4} \) 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 \( \delta f'_{\mu} \) 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 \[ 84 \]. 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 \[ 63, 81 \]. 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 \( \varepsilon \) expansion \[ 62 \]. This approach has already been successfully employed in previous finite-size studies \[ 63, 64, 67, 68, 69, 70 \] 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

\[ u' = \mu^{-\varepsilon} A_d Z_{u'}^{-1} Z_\varphi^2 u_0' \]

and \( r = Z_{r^{-1}}(r_0 - r_0c) = at, \varphi' = Z_{\varphi^{-1/2}} \varphi' \) with an arbitrary inverse reference length \( \mu \). \( L' \) is not renormalized. Furthermore, the reduced anisotropy matrix \( \mathbf{A} \) 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 \( h' \), (2.19), the additional renormalization \( h'_R = Z_{h'}^{1/2} h' \) is necessary \[ 69 \].

The geometric factor of bulk theory [see (5.1)]

\[ A_d = \frac{\Gamma(3-d/2)}{2^{d-2} \pi^{d/2} (d-2)} = S_d \Gamma(3 + \varepsilon/2) \Gamma(1 - \varepsilon/2) \quad (5.2) \]

appears naturally in Eqs. (4.37) - (4.39) rather than the more commonly used factor \( S_d = 2^{1-d^2/2} \pi^{d/2}(d/2)^{-1} \). The perturbation results of amplitudes and scaling functions depend on the choice of the geometric factor in (5.1) \[ 62, 63, 66, 72, 83 \] (see, e.g., the universal ratio \( Q_1 \) in (6.19) below, see also the comment after (5.10) 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 (3.1), in contrast to the factor \( S_d \). For this reason we have incorporated \( A_d \) in the definition of the renormalized coupling \( u' \), (5.1). Any other choice, such as \( S_d \) instead of \( A_d \), would introduce artificial \( d \) dependences into the perturbation results. For the same reason we employ \( A_d \) in the definition of the multiplicatively and additively renormalized free energy density

\[ f'_R(r, u', L', \mu, \mathbf{A}) = \delta f'(Z_r r, \mu^{-\varepsilon} Z_u u' Z_{\varphi^{-1/2}}^{1/2} A_d A(u', \varepsilon)) \]

\[ - \frac{1}{8} \mu^{-\varepsilon} A_d A(u', \varepsilon) . \quad (5.3) \]
Because of relations such as (3.1) the Z factors $Z_r(u', \varepsilon)$, $Z_w(u', \varepsilon)$, and $Z_{\varphi}(u', \varepsilon)$ depend on $u'$ in the same way as the usual $Z$ factors depend on $u$ in the standard isotropic $\phi^4$ theory. The same statement holds for the additive renormalization constant $A(u', \varepsilon)$ because of

$$
\int_0^\infty \ln(r_0 + k \cdot A k) = (\det A)^{-1/2} \int_0^\infty \ln(r_0 + k' \cdot k') = - (\det A)^{-1/2} \frac{2A_d}{d\varepsilon} r_0^{d/2} .
$$

(5.4)

Thus the renormalization constants read up to one-loop order $Z_r(u', \varepsilon) = 1 + 12u'/\varepsilon$, $Z_w(u', \varepsilon) = 1 + 36u'/\varepsilon$, $Z_{\varphi}(u', \varepsilon) = 1$, $A(u', \varepsilon) = -2/\varepsilon$. The $Z$ factors $Z_w$ and $Z_r$ are sufficient to renormalize $y^{\text{eff}}_0$, (4.27), and $w^{\text{eff}}_0$, (4.28), whereas the additive renormalization constant $A(u', \varepsilon)$ is needed to absorb the pole term $\sim -A_0(r_0 - r_{0c})^2/(\varepsilon^2)$ in the square brackets of (4.37). After substituting these renormalization constants one verifies that the resulting renormalized free energy density $f^R$ has a finite limit for $\varepsilon \to 0$ at fixed $u' > 0$.

We define the dimensionless amplitude function

$$
F^R_R(r/\mu^2, u', L', \mu, \bar{\mu}) = \mu^{-d} A_d f^R_R(r, u', \mu, L', \bar{\mu}) .
$$

(5.5)

From the $\mu$ independence of $\delta f^R(r_0 - r_{0c}, u'_0, L', \bar{\mu})$ one can derive the renormalization-group equation (RGE) for the amplitude function

$$
\left( \mu \partial_{\mu} + r \zeta \partial_r + \beta_r \partial_{u'} + d \right) F^R_R(r/\mu^2, u', L', \mu, \bar{\mu}) = - \frac{r^2}{(2\mu^4)} B(u') ,
$$

(5.6)

where the field-theoretic functions $\beta_r(u', \varepsilon), \zeta_r(u')$, and $B(u')$ are defined as usual [62, 63]. Eq. (5.6), however, differs from the corresponding bulk RGE (119) of [82] since here we are using $r$ rather than the bulk correlation lengths $\xi_0^{\mu}$ as the appropriate measure of the temperature variable. Using $r$ rather than $\xi_0^{\mu}$ is of advantage in finite-size theories where a single finite-size scaling function is derived for both $r \geq 0$ and $r < 0$. The functions $\zeta_r(u')$, $\beta_r(u', 1)$ and $B(u')$ as well as the fixed point value $u^* = u'$ are accurately known [63, 86] from Borel resummations. Integration of the RGE yields

$$
F^R_R \left( \frac{r}{\mu^2}, u', L', \mu, \bar{\mu} \right) = \mu^d \left\{ F^R_R \left( \frac{r(l)}{\mu_{l}^2}, u'(l), L_{l} \mu, \bar{\mu} \right) + \frac{r(l)^2}{2l^2 \mu^2} \int_1^{l} B(u'(t)) \left\{ \exp \left[ \int_{t}^{l} \left[ 2\zeta_r(u'(t')) - \varepsilon \right] \frac{dt'}{t'} \right] + \frac{l}{t} \int_{t}^{l} \right\} \right\} .
$$

(5.7)

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

Eqs. (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 $r'_0$ will appear in the form of the effective renormalized counterpart

$$
\begin{align*}
\rho^R_0(l) &\equiv r_0^R(r(l), l^2 \mu^2 A_d^{-1} u'(l), L') = r(l) + 12(\mu l)^2 A_d^{-1} u'(l)^{1/2} (L')^{-d/2} \partial_2(y'(l)) ,
\end{align*}
$$

(5.8)

$$
\begin{align*}
y'(l) &= r(l) \mu^{-2} l^{-2} (L' \mu l)^{d/2} A_d^{-1} u'(l)^{-1/2} .
\end{align*}
$$

(5.9)

Correspondingly, the effective renormalized counterparts of $y^{\text{eff}}_0$ and of $w^{\text{eff}}_0$ appearing in the renormalized form of the logarithmic part of $\delta f^R$ are given by

$$
\begin{align*}
y^{\text{eff}}(l, \bar{\mu}) &= (\mu l L')^{d/2} A_d^{-1} u'(l)^{-1/2} \times \left\{ \frac{r(l)}{\mu l^2} \left[ 1 + 18u'(l) R_2 \left( \frac{r(l)}{\mu l^2}, l \mu L, \bar{\mu} \right) \right] \\
&+ 12u'(l) R_1 \left( \frac{r(l)}{\mu l^2}, l \mu L, \bar{\mu} \right) \\
&+ 144(\mu l L')^{-d/2} A_d^{-1} u'(l)^{-1/2} \partial_2(y'(l)) \times R_2 \left( \frac{r(l)}{\mu l^2}, l \mu L, \bar{\mu} \right) \right\} ,
\end{align*}
$$

(5.10)

$$
\begin{align*}
w^{\text{eff}}(l, \bar{\mu}) &= u'(l)^{-1/2} \left[ 1 + 18u'(l) R_2 \left( \frac{r(l)}{\mu l^2}, l \mu L, \bar{\mu} \right) \right] ,
\end{align*}
$$

(5.11)

$$
\begin{align*}
R_1(q, p, \bar{\mu}) &= \varepsilon^{-1} q[1 - q^{-\varepsilon/2}] + p^{\varepsilon/2} (4\pi^2 A_d)^{-1} I_1(q p^2, \bar{\mu}) ,
\end{align*}
$$

(5.12)

$$
\begin{align*}
R_2(q, p, \bar{\mu}) &= - \varepsilon^{-1} [1 - q^{-\varepsilon/2}] - \frac{1}{2} q^{\varepsilon/2} + p^{\omega} (16\pi^4 A_d)^{-1} I_2(q p^2, \bar{\mu}) .
\end{align*}
$$

(5.13)

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

$$
\begin{align*}
l^R_0(l) = \mu^2 l^2 .
\end{align*}
$$

(5.14)

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

$$
\lim_{L \to \infty} \mu \mu_L^2 = \left\{ \begin{array}{ll}
\mu_L^2 = r_0(l_+) & \text{for } T > T_c , \\
\mu_L^2 = -2r_0(l_-) & \text{for } T < T_c ,
\end{array} \right.
$$

(5.15)

and appropriately implies $\mu \propto L'^{-1}$ for large finite $L'$ at $T = T_c$. As a natural choice for the reference length $\mu^{-1}$ we take $\mu^{-1} = \xi_0^+, \xi_0^-$ where [62]

$$
\xi_0^+ = \left[ Z_r(u', \varepsilon) a_0^{-1} Q' \exp \left( \int_{u'}^{u''} \frac{\zeta_r(u''') - \zeta_r(u''')}{\beta_r(u''', \varepsilon)} \frac{du'''}{u'''} \right) \right]^{1/2} .
$$

(5.16)
is the asymptotic amplitude of the second-moment bulk correlation length of the isotropic system above $T_c$, as defined in (5.6). 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 $A_d$, (5.2) and the $O(u')$ term of $Q(1, u', d)$ and the $O(u')$ term of $Q^*$ vanish [63, 82, 87], similar to the vanishing of the order-parameter amplitude function at $O(u')$ [63]. The same observation was recently made for the correlation-length amplitude within the $\epsilon$ expansion [51] where the same geometric factor $A_d$ was employed (apart from a harmless factor of 2). In three dimensions the amplitude $Q^*$ it is accurately known from Borel re-summations [87].

Eqs. (5.8) and (5.11) 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 non-critical region.

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

$$f_R'(r(l), u'(l), l \mu, \bar{\Lambda}) = 2(2) \frac{l^2}{(\mu^2)^2} \int B(u'(l')) \left\{ \exp \left[ \int \frac{2 \zeta_r(u'(l'))}{l} \right] + 1 \right\} dl' \frac{d}{dl'},$$

(5.17)

above and below $T_c$, respectively, where $l_+$ and $l_-$ are determined by Eq. (5.15). The last integral term in (5.17) contains both a contribution $\propto l^{2-\alpha/\nu}$ to the singular finite-size part $f_s'$ and a contribution $\propto l^2$ to the nonsingular bulk part $f_{ns,b}'$ of $\delta f'$ [see Eq. (4.30), compare also Eqs. (6.5) 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 $F$ we consider (5.17) - (5.20) the limit of small $t \ll 1$ or $l \to 0$. In this limit we have $u'(l) \to u'(0) = u^*$, $r(l)/(\mu^2)^2 \to Q^* t^{-\alpha/\nu}$,

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

(6.1)

$$\tilde{x} = t(\mu L')^{\nu} = t(L'/\xi_0)^{1/\nu}.$$  

(6.2)

In (6.1) we have used the hyperscaling relation

$$2 - \alpha = d \nu.$$  

(6.3)

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

$$\tilde{y} + 12 \vartheta_{2}(\tilde{y}) = \tilde{t}^{d/2} A_d^{1/2} u^*^{-1/2},$$

(6.4)

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

(6.5)

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

$$w^{eff}(l, \bar{x}) \to W(\bar{x}, \bar{\Lambda}) = u^*^{-1/2} \left[ 1 + 18 u^* R_2(1, \bar{\Lambda}) \right],$$

(6.6)

$$y^{eff}(l, \bar{x}) \to Y(\bar{x}, \bar{\Lambda}) = \tilde{t}^{d/2} A_d^{1/2} u^*^{-1/2} \times \left\{ Q^* \tilde{x} \tilde{l}^{-1/\nu} \left[ 1 + 18 u^* R_2(1, \bar{\Lambda}) \right] + 12 u^* R_1(1, \bar{\Lambda}) \right\} + 144 u^*^{3/2} \tilde{t}^{-d/2} A_d^{-1/2} \vartheta_{2}(\tilde{y}) R_2(1, \bar{\Lambda}).$$

(6.7)

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

$$\int B(u'(l')) \left\{ \exp \left[ \int \frac{2 \zeta_r(u'(l'))}{l} \right] - \frac{d}{dl'} \right\} dl' \quad \to \quad -\frac{\nu}{\alpha} B(u^*) + O(\mu^2/\nu).$$

(6.8)

is known from bulk theory [82]. In (6.8) the subleading term $O(\mu^2/\nu)$, together with the prefactor $r(l)^2/(l \mu)^2$ in


This result is valid for $2 < d < 4$ in the range $L' \gg \bar{a}$ and $0 \leq |\bar{x}| \lesssim O(1)$ above $a$, and at below $T_c$ (but not for the exponential regime $|\bar{x}| \gg 1$, see Sect. X). It incorporates the correct bulk critical exponents $\alpha$ and $\nu$ 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 $\xi^+_{b*}$ of the scaling variable $\bar{x}$. (6.2). For finite $L'$, $f_{s,b}'(t, L')$ is an analytic function of $t$ near $t = 0$, in agreement with general analyticity requirements. From previous studies at finite external field [32] [58] we infer that the extension of (6.9) to $h' \neq 0$ has the structure

$$
\begin{align*}
 f_{s,b}'(t, h', L') = L'^{-d} F(\bar{x}, h', h'|\xi^+_{b*}; \vec{A})
\end{align*}
$$

where $\xi^+_{b*}$ is defined after (6.14). Thus the constants $C_1'$ and $C_2'$ in (6.13) and (6.14) can be chosen most naturally as $C_1' = (\xi^+_{b*})^{-1/\nu}$ and $C_2' = (\nu^+_{b*})^{-\beta/\nu}$.

Of particular interest is the finite-size amplitude

$$
\begin{align*}
 F(0, \vec{A}) = F_c(\vec{A})
\end{align*}
$$

where $F_c(\vec{A})$ is the free energy density of the isotropic system at $h' = 0$ obtained from $f_{s,b}'(t, 0, L')$, in the limit of small $t$ as

$$
\begin{align*}
 f_{s,b}'(t, L') \rightarrow f_{s,b}'(t, 0, L') = L'^{-d} F(\bar{x}, \vec{A})
\end{align*}
$$

where the finite-size scaling function is given by

$$
\begin{align*}
 F(\bar{x}, \vec{A}) &= -A_d \left[ \frac{\nu}{4d} + \frac{\nu^* Q^{2+2:2}}{2\alpha} B(u^*) \right] \\
&+ \frac{18u^* |\varphi_{2}(\bar{y})|^2}{2} - \frac{1}{2} \ln \left( \frac{2\pi A_{d}^{1/2} W(\bar{x}, \vec{A})}{\bar{t}^{1/2}} \right) \\
&- \ln \int_{-\infty}^{\infty} ds \exp \left[ -\frac{1}{2} \varphi_{2}(\bar{y}) \right] s^2 - s^4 \\
&+ \frac{1}{2} J_0(\bar{t}^2, \vec{A}) - \frac{3 \bar{t}^2}{2\pi^2 A_{d}^{1/2}} \varphi_{2}(\bar{y}) I_1(\bar{t}^2, \vec{A}) \\
&+ \frac{9 \bar{t}^2 u^*}{4\pi^4 A_{d}^{1/2}} |\varphi_{2}(\bar{y})|^2 I_2(\bar{t}^2, \vec{A})
\end{align*}
$$

This result is valid for $2 < d < 4$ in the range $L' \gg \bar{a}$ and $0 \leq |\bar{x}| \lesssim O(1)$ above $a$, and at below $T_c$ (but not for the exponential regime $|\bar{x}| \gg 1$, see Sect. X). It incorporates the correct bulk critical exponents $\alpha$ and $\nu$ 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 $\xi^+_{b*}$ of the scaling variable $\bar{x}$. (6.2). For finite $L'$, $f_{s,b}'(t, L')$ is an analytic function of $t$ near $t = 0$, in agreement with general analyticity requirements. From previous studies at finite external field [32] [58] we infer that the extension of (6.9) to $h' \neq 0$ has the structure

$$
\begin{align*}
 f_{s,b}'(t, h', L') = L'^{-d} F(\bar{x}, h', h'|\xi^+_{b*}; \vec{A})
\end{align*}
$$

where $\xi^+_{b*}$ is defined after (6.14). Thus the constants $C_1'$ and $C_2'$ in (6.13) and (6.14) can be chosen most naturally as $C_1' = (\xi^+_{b*})^{-1/\nu}$ and $C_2' = (\nu^+_{b*})^{-\beta/\nu}$.

Of particular interest is the finite-size amplitude $F(0, \vec{A}) = F_c(\vec{A})$ at $t = 0$,

$$
\begin{align*}
 F_c(\vec{A}) &= \left( 18 - \frac{36}{d} \right) u^* |\varphi_{2}(0)|^2 - \frac{1}{2} \ln \left( \frac{2\pi A_{d}^{1/2} W(\vec{A})}{\bar{t}^{1/2}} \right) \\
&- \ln \int_{-\infty}^{\infty} ds \exp \left[ -\frac{1}{2} \varphi_{2}(\bar{y}) \right] s^2 - s^4 \\
&+ \frac{1}{2} J_0(\bar{t}^2, \vec{A}) - \frac{3 \bar{t}^2}{8\pi^2} I_1(\bar{t}^2, \vec{A}) - \frac{3 \bar{t}^4}{64\pi^4} I_2(\bar{t}^2, \vec{A})
\end{align*}
$$

where $\bar{t}^{1/2} = 12u^* A_{d}^{-1/2} |\varphi_{2}(0)|$ and

$$
\begin{align*}
 W(\vec{A}) &= u^{-1/2} \left[ 1 + 18u^* |\varphi_{2}(\vec{A})|^2 \right]
\end{align*}
$$

with $\theta_{2}(0) = \Gamma(3/4) / \Gamma(1/4)$ and

$$
\begin{align*}
 R_1(1, \vec{A}) &= \frac{1}{2} \bar{t}_c(4\pi^2 A_{d})^{-1} \varphi_{2}(1, \vec{A}) \\
 R_2(1, \vec{A}) &= -\frac{1}{2} \bar{t}_c(16\pi^2 A_{d})^{-1} \varphi_{2}(1, \vec{A})
\end{align*}
$$

In the bulk (large $|\bar{x}|$) limit Eqs. (6.9) and (6.10) yield

$$
\begin{align*}
 f_{s,b}'(t, L') = -A_d Q^{*} \left( \frac{1}{4d} + \frac{\nu}{2\alpha} B(u^*) \right) \xi^+_{b*} |t|^{d\nu},
\end{align*}
$$

above and below $T_c$, respectively, with the universal bulk amplification ratios

$$
\begin{align*}
 f_{s,b}'(t) \xi^+_{b*} \equiv Q_1 &= -A_d Q^{*} \left( \frac{1}{4d} + \frac{\nu}{2\alpha} B(u^*) \right),
\end{align*}
$$

(For $Q_1$ compare (5.12).) Here we have used the bulk identifications

$$
\begin{align*}
 \mu_d = \left\{ \begin{array}{ll}
 \mu_d^+ = Q^{*} \xi^+_{b*} & \text{for } T > T_c, \\
 \mu_d^- = Q^{*} \xi^+_{b*} (2|t|)^{\nu} & \text{for } T < T_c,
\end{array} \right.
\end{align*}
$$

as implied by the choice (5.15). As noted in Sect. III, a complete two-loop calculation would yield further bulk contributions of $O(u^*)$ in $f_{s,b}'(t)$ Owing to the truncation (4.25) no terms of $O(u'^{2})$ and higher order appear in

$$
\begin{align*}
 (6.18) \text{and (6.20).}
\end{align*}
$$

In order to present the scaling function

$$
\begin{align*}
 F^c(\bar{x}; \vec{A}) = F(\bar{x}; \vec{A}) - F_{b}^{c}(\bar{x})
\end{align*}
$$

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

$$
\begin{align*}
 F_{b}^{c}(\bar{x}) = \left\{ \begin{array}{ll}
 L^d f_{s,b}^{+} = \bar{Q}_1 \bar{x}^{d\nu} & \text{for } T > T_c, \\
 L^d f_{s,b}^{-} = \bar{Q}_1 |\bar{x}|^{d\nu} & \text{for } T < T_c,
\end{array} \right.
\end{align*}
$$

(6.23)
with $Q^{-} = (A^{-}/A^{+})Q_{1}$, representing the large $|\bar{x}|$ behavior of $F(\bar{x}, \bar{A})$. It should be noted that it is not obvious how to interpret the $d \times d$ matrix $\bar{A}$ for the case of non-integer dimensions $d$.

In the spirit of the fixed $- d$ minimal subtraction approach \cite{02}, we shall evaluate $F(\bar{x}, \bar{A})$ and $F^{\epsilon}(\bar{x}, \bar{A})$ in $d = 3$ dimensions without any further expansion with respect to $\bar{u}$. This is in contrast to the $\epsilon$ expansion which is a double expansion with respect to $\bar{u}^{*}$ and $\epsilon = 4 - d$.

### B. Epsilon expansion

Considering $\bar{u}^{*}$ as a smallness parameter and using the results of App. C we obtain from (6.12) at fixed $2 < d < 4$

$$F_{c}(\bar{A}) = \frac{1}{2} \ln \left\{ \left( \frac{12}{24\pi A^{d}_{d} \Gamma(1/4)^{d}} \right)^{2/d} \frac{\Gamma(\epsilon/d)}{\Gamma(3/4)^{d}} u^{2/d} + \frac{1}{8\pi^{2}} \left( \frac{12}{A^{d}_{d}} \Gamma(1/4)^{d} \right) I_{1}(0, \bar{A}) + O(u^{4/d}) \right\}$$

(6.24)

Substituting $u^{*} = \epsilon/36 + O(\epsilon^{2})$ and expanding all $d$ dependent quantities with respect to $\epsilon = 4 - d$ yields the $\epsilon$-expansion result at $T_{c}$

$$F_{c}(\bar{A}) = \frac{1}{4} \ln \epsilon + f_{0}(\bar{A}) + f_{1}(\bar{A}) \epsilon^{1/2} + O(\epsilon),$$

(6.25)

$$f_{0}(\bar{A}) = -\frac{1}{4} \ln 18 - \frac{1}{2} I_{1}(0, \bar{A})$$

$$+ \frac{1}{2} \int_{0}^{\infty} dy \left[ \frac{\pi}{y} \right]^{2} - K_{4}(y, \bar{A}) + 1 - e^{-y},$$

(6.26)

$$f_{1}(\bar{A}) = \frac{\Gamma(1/4)}{\pi \Gamma(3/4) \sqrt{2}} \int_{0}^{\infty} dy \left[ K_{4}(y, \bar{A}) - \left( \frac{\pi}{y} \right)^{2} - 1 \right],$$

(6.27)

where now $\bar{A}$ denotes a $4 \times 4$ matrix. The $\epsilon$ expansion result (6.24) - (6.27) is independent of which renormalization scheme and which kind of perturbation scheme is used. The same result is obtained if one starts with the effective Hamiltonian of Brézin and Zinn-Justin \cite{64} or with the cumulant expansion of Rudnick et al. \cite{32}. Because of the strict expansion with respect to $u^{*}$ and $\epsilon$, the exponential structure of the distribution $\sim \exp[-H^{eff}]$ is destroyed. As expected, the $\epsilon$ - expansion term $\sim \ln \epsilon$ is not well behaved for $\epsilon \to 0$ since at $d = 4$ the finite lattice constant $\hat{a}$ must not be neglected.

A nontrivial question arises if the $\epsilon$-expansion result is applied to three-dimensional anisotropic systems with a matrix $\bar{A} \neq 1$. It appears that, to some extent, it is ambiguous how the physical $3 \times 3$ matrix $\bar{A}$ (which, in general, has 5 independent nonuniversal matrix elements) should be continued to $d = 4$ in order to evaluate the coefficients $f_{0}(\bar{A})$ and $f_{1}(\bar{A})$. This matrix $\bar{A}$ in (6.25) is necessarily a $4 \times 4$ matrix which, in general, has 9 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 $f_{0}(\bar{A})$ and $f_{1}(\bar{A})$ 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

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

(6.28)

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

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

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

A corresponding problem would arise in an $\epsilon$ expansion in $d = 2 + \epsilon$ dimensions. In Sect. 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 $\bar{A}$ in an $\epsilon$ expansion.

### C. Large - n limit

For comparison with the case $n = 1$ we also present the exact result for the finite-size scaling function $F_{\infty}$ of the free energy density per component $f_{\infty}(t, L)$ of the $\varphi^{4}$ 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. 89 we have

$$f_{\infty}(t, L) = \lim_{n \to \infty} \{- (nV)^{-1} \ln Z(t, 0, L)\}$$

$$= \hat{f}_{0} - \frac{(r_{0} - \chi^{-1}_{\infty})^{2}}{16u_{0n}} + \frac{1}{2V} \sum_{k} \ln \{|\chi^{-1}_{\infty} + \delta K(k)|^{2}\}$$

(6.30)

where $Z(t, 0, L)$ is defined by (2.29) and $\chi^{-1}_{\infty}$ is determined implicitly by $\chi^{-1}_{\infty} = r_{0} + 4u_{0n}L^{-1} \sum_{k}|\chi^{-1}_{\infty} + \delta K(k)|^{-1}$. The additive constant in (6.30) is $\hat{f}_{0} = -[\ln(2\pi)]/(2\hat{a})$. Using the results of App. C leads to the singular part of
\( f_\infty \) in the regime \( L' \gg \bar{a} \) and \( 0 \leq |\bar{x}| \lesssim O(1) \) at \( h = 0 \)
for \( 2 < d < 4 \)
\( f_{\infty, \star}(t, L; \bar{A}) = L^{-d} F_{\infty}(\bar{x}; \bar{A}) \), \hfill (6.31)
\[ F_{\infty}(\bar{x}; \bar{A}) = \frac{1}{2} G_0(P^2; \bar{A}) + \frac{A_d}{2(4-d)} \left[ \bar{x} P^2 - \frac{2}{d} P^d \right], \hfill (6.32) \]
\[ P^{d-2} = \bar{x} - \frac{4 - d}{A_d} G_1(P^2; \bar{A}), \hfill (6.33) \]
\[ G_x(P^2; \bar{A}) = (4\pi^2)^{-1} \int_0^\infty dy \frac{y^{-1}}{2} \exp \left( \frac{-P_y^2}{4\pi^2} \right) \times \left\{ \left( \frac{\pi}{y} \right)^{d/2} - K_d(y, \bar{A}) \right\} \hfill (6.34) \]

Here \( \bar{x} = t(L'/\xi_0 + 1)^{1/\nu} \) with \( \nu = (d - 2)^{-1} \), \( L' = (\delta A)^{-1/(2d)} L, \) \( \xi_0^{+} = (4\pi^2 u_A^2 / c^\gamma / \nu)^{1/\nu} \), and \( u_0 = (\delta A)^{-1/2} u_0 \). We note that the geometric factor \( A_4 \), \( \delta \xi_0 \), appears in \( (6.31) - (6.33) \) in a natural way.

The reason is that only diagrammatic contributions of single-loop structures contribute to the large \( -n \) limit. The function \( (1/2)G_0(\bar{x}; \bar{A}) \) with \( \bar{x} = r_0 L'^2 \) is the scaling function of the excess free energy density of the Gaussian model (see (B.13) - (B.17) of App. B). For \( T \geq T_c \) the function \( P(\bar{x}; \bar{A}) \) determines the finite-size scaling form of the susceptibility per component in the limit \( n \to \infty \)
\[ \chi_\infty^{\pm}(t, L; \bar{A}) = L'^{\gamma/\nu} g(\bar{x}; \bar{A}), \gamma/\nu = 2, \hfill (6.35) \]
where \( g(\bar{x}; \bar{A}) = [P(\bar{x}; \bar{A})]^{-2} \). Below we shall present the relative anisotropy effect
\[ \Delta \chi_{\infty, c}(\bar{A}) = \frac{g(0; \bar{A}) - g(0; 1)}{g(0; 1)} \hfill (6.36) \]
on \( \chi_{\infty}^{\pm} \) 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 \cite{11}) and corrects Eq. (44) of \cite{12} where the term \( -\log(2) / 2 \) should be dropped.

The scaling function of the excess free energy density above, at, and by \( T_c \) is given by
\[ F_{\infty, c}(\bar{x}) = F_{\infty}(\bar{x}; \bar{A}) - F_{\infty, c}(\bar{x}) \hfill (6.37) \]
with the bulk part
\[ F_{\infty, c}(\bar{x}) = \left\{ \begin{array}{ll}
Y \bar{x}^{d-2} & \text{for } T > T_c, \\
0 & \text{for } T < T_c,
\end{array} \right. \hfill (6.38) \]
where \( Y = (d-2)A_d / [2d(4-d)] \). At \( T_c \) the finite-size amplitude is given by
\[ F_{\infty}(0; \bar{A}) = \frac{1}{2} G_0(P^2; \bar{A}) - \frac{A_d}{d(4-d)} P^d, \hfill (6.39) \]
where \( P_c(\bar{A}) \equiv P(0; \bar{A}) \) is determined by
\[ P_c^{d-2} = \frac{4 - d}{A_d} G_1(P^2; \bar{A}) \hfill (6.40) \]

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 \cite{12, \[13, 14, 15]}. Within our \( \varphi^4 \) 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 \( \chi^+ = V < \Phi^2 >, \chi^- = V(< \Phi^2 > - < |\Phi|^2>) \), and the Binder cumulant
\[ U = 1 - \frac{1}{3} < \Phi^4 > - < \Phi^2 > \hfill (7.1) \]
where \( \Phi = N^{-1} \sum_j \varphi_j \) (see, e.g., \cite{68}). These quantities remain invariant under the transformation defined in Sect. II \cite{13}, \( \chi^{\pm} = (\chi^{\pm})' \), \( U = U' \). As a consequence we find that, in the regime (b) defined in Section IV.A, the finite-size scaling forms of these quantities are
\[ \chi^+(t, L; \bar{A}) = (\chi^+)'(t', L; \bar{A}) = (L'/\xi_0)^{\nu/\nu} P_{\chi}^+(\bar{x}; \bar{A}), \hfill (7.2) \]
\[ U(t, L; \bar{A}) = U'(t', L'; \bar{A}) = U(\bar{x}; \bar{A}), \hfill (7.3) \]
where the scaling functions \( P_{\chi}^+ \) and \( U \) are obtained from those of \cite{68} by the replacements \( Y \to Y(\bar{x}; \bar{A}) \) and \( R_2 \to R_2(1, \bar{1}, \bar{A}) \). Note that the functions \( P_{\chi}^+ \) are nonuniversal even for \( \bar{A} = 1 \) since they still contain nonuniversal overall amplitudes \( c^\chi \) proportional to the bulk amplitudes of \( \chi^\pm \) (see also \cite{68}). Here we consider only the relative anisotropy effect
\[ \Delta \chi_{\chi}^{\pm}(\bar{A}) = \frac{P_{\chi}^+(0; \bar{A}) - P_{\chi}^+(0; 1)}{P_{\chi}^+(0; 1)} \hfill (7.4) \]
on the susceptibilities \( \chi^+(0, L; \bar{A}) \) at \( T_c \). The analytic expressions are in \( 2 < d < 4 \) dimensions
\[ P_{\chi}^+(0; \bar{A}) = c^+ \left[ 1 - 18u^* R_2(1, \bar{1}, \bar{A}) \right]^{-1} \varphi_2(Y(\bar{A})) \hfill (7.5) \]
\[ P_{\chi}^-(0; \bar{A}) = c^- \left[ 1 - 18u^* R_2(1, \bar{1}, \bar{A}) \right]^{-1} \times \left\{ \varphi_2(Y(\bar{A})) - [\varphi_1(Y(\bar{A}))]^2 \right\}, \hfill (7.6) \]
where the constants \( c^\chi \) are independent of \( \bar{A} \) and drop out of the ratio \( (7.4) \). For \( Y(\bar{A}) \) and \( R_2(1, \bar{1}, \bar{A}) \) see \cite{64} and \cite{65}, for \( \varphi_{\bar{n}}(Y) \) see \cite{43}. The anisotropy effect on the Binder cumulant \( U(0; \bar{A}) \) at \( T_c \) will be described by the difference
\[ \Delta U_{\bar{n}}(\bar{A}) = U(0; \bar{A}) - U(0; 1) \hfill (7.7) \]
where
\[ U(0; \bar{A}) = 1 - \frac{1}{3} \varphi_4(Y(\bar{A})) [\varphi_2(Y(\bar{A}))]^{-2}. \hfill (7.8) \]
VIII. QUANTITATIVE RESULTS AND PREDICTIONS

For the application to three dimensions we shall employ the same values as previously [66, 72], $A_3 = (4\pi)^{-1}$, $
u = 0.6335$, $u^* = 0.0412$, $Q^* = 0.945$, $B(u^*) = 0.50$. For reasons of consistency, a slightly different value will be used for $\alpha = 2 - 3\nu = 0.0955$ 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 (8.14)]

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

This can be compared with the series expansion results for the three-dimensional Ising model by Liu and Fisher [72] who calculated the amplitude ratios $(R_+^3)^3 = 0.0188 \pm 0.0001$ 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 [73]). The relation between $R_+^3$ and $Q_1$ is $(R_+^3)^3 = -\alpha(1-\alpha)(2-\alpha)Q_1$. This yields the central values of the Ising model based on series expansions

$$Q_{1|\text{Ising}} = -0.1099, \quad A^-/A^+_{|\text{Ising}} = 1.91.$$  (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 (8.2) are in acceptable agreement with (8.1). As seen from (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, (5.1). The results (8.1) demonstrate the appropriateness of the choice of $A_d$, (6.2).

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 $\tilde{A} = 1$, $\xi_{d+} = \xi_{0+}$, where accurate MC data by Mon [34], [37], [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 $\xi_{0+}$ but both belong to the subclass of (asymptotically) isotropic systems with $\tilde{A} = 1$. Within the error bars, the MC results for the finite-size amplitude $F_c(1)$ of the free energy density at $T_c$ [34]

$$F_c(1)_{\text{MC}} = \begin{cases} -0.657 \pm 0.03 & (\text{sc lattice}) \\ -0.643 \pm 0.04 & (\text{bcc lattice}) \end{cases}$$  (8.3)

are consistent with the universality hypothesis. Subsequently the more accurate MC result at $T_c$ was obtained [33]

$$F_c(1)_{\text{MC}} = -0.625 \pm 0.005 \quad (\text{sc lattice})$$  (8.4)

which is also consistent with (8.2).

In three dimensions the numerical values of the quantities $\tilde{I}_c, J_0, I_1$, and $I_2$ in our analytical result (6.12) are $\tilde{I}_c = 2.042$, $J_0(I_2, 1) = 1.6430$, $I_1(I_2, 1) = -4.1581$, and $I_2(I_2, 1) = -15.1032$. This yields the theoretical prediction for the finite-size amplitude

$$F_c(1)_{d=3} = -0.6315,$$  (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 $\varepsilon$ expansion (0.25). For isotropic systems ($\tilde{A} = 1$) the coefficients in (0.25) are well defined. The numerical values are

$$f_0(1) = -0.3302, \quad f_1(1) = -0.4218,$$  (8.6)

where $\mathbf{1}$ denotes the $4 \times 4$ unity matrix. For $\varepsilon = 1$ the terms up to $O(\varepsilon^{1/2})$ of (0.25) yield

$$F_c(1)_{\varepsilon=1} = -0.7520,$$  (8.7)

which is in less good agreement with the MC results [8.3] and [8.4]. (Fig. 5)
In three dimensions the numerical evaluation of the scaling function \( F^{ex}(\tilde{x}; 1) \), as given in (6.22), (6.10), and (6.28), 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 Sect. IV A. A minimum with \( F^{ex}(\tilde{x}_{min}; 1)_{d=3} = -0.701, \tilde{x}_{min} = -0.910 \) (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 \( F^{ex}(\tilde{x}_{min}; 1)_{d=3} \) are predicted to be universal numbers. This can be tested by MC simulations for families of three-dimensional Ising models with \( \bar{A} = 1 \), (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 \( \xi_{0+} \). 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 \( F^{ex}(\tilde{x}; 1)_{d=3} \) 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 Sect. IV A, as expected.

For comparison we also present the exact result for the scaling function \( F^{cc}(\tilde{x}; 1) \) in the large - \( n \) limit in three dimensions. For \( \bar{A} = 1 \) and \( d = 3 \) the numerical solutions of (6.40) and (6.39) at \( T = T_c \) are \( P_c(1) = 1.946 \) and

\[
F^{cc}(0; 1) = F^{cc}(\tilde{x}; 1) = -0.526. \quad (8.9)
\]

In Fig. 6 the scaling function \( F^{cc}(\tilde{x}; 1) \), (8.32), is shown in three dimensions (dashed curve). Unlike the case \( n = 1, F^{ex}(\tilde{x}; 1) \) does not have a minimum at finite \( \tilde{x} \) below \( T_c \) but has a slow monotonic decrease towards a finite negative constant \( F^{ex}_{\infty}(\tilde{x}; 1) = -3.18 \). Above \( T_c \) it decays exponentially to zero (but not with the correct exponential form, see Sect. X.).

C. Three-dimensional anisotropy

In the following we present quantitative predictions for the nonuniversal effect of a non-cubic anisotropy on the finite-size scaling functions in three dimensions. We illustrate the three-dimensional anisotropy effects for the example of \( \bar{A} \) and \( \bar{A} \) given in (2.13) and (2.15) of Sect. II. In this example, \( \bar{A}(w) \) depends only on the single anisotropy parameter \( w \), (2.16), \(-\frac{1}{2} < w < 1 \). The crucial anisotropy function is given by (4.16) which enters the functions \( J_0, I_1, \) and \( I_2 \) defined in (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

\[
\Delta F_c(\bar{A}(w)) = F(0; \bar{A}(w)) - F(0; 1), \quad (8.10)
\]

\[
\Delta F_{c,\infty}(\bar{A}(w)) = F_{\infty}(0; \bar{A}(w)) - F_{\infty}(0; 1), \quad (8.11)
\]

where \( F(0; \bar{A}) \) and \( F_{\infty}(0; \bar{A}) \) are given by (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 \( w_{max} = 0.500 \), with \( \Delta F_{c,max} = 0.0167 \) and \( \Delta F_{c,\infty,max} = 0.0165 \), respectively, for \( n = 1 \). The slight difference of the two heights is presumably not a consequence of the approximations made for \( n = 1 \); such
The free energy it is predicted to be of remarkably larger than that on the Binder cumulant. For $w < \omega$, the range of the anisotropic three-dimensional Ising model in the corresponding relative effect on the Binder cumulant $\chi$ results for the Binder cumulant (see also [43]).

The corresponding anisotropy effect on the Binder cumulant for $n = 1$ at $T_c$ is shown in Fig. 8 as described by the difference $\Delta U_c(A(w))$, (2.17) [90]. Figs. 7 and 8 imply that the relative anisotropy effect on the free energy $\Delta F_c(A(w))/F_c(1)$ 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 $\Delta U_c(A(w))/U(0; 1)$ 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 [42], and in the regime $w > 0.8$. Previous MC simulations [42] of the anisotropic three-dimensional Ising model in the range $-0.48 \leq w \leq 0$ 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 $\chi^*$ and $\chi^-$ for $n = 1$ and on $\chi^*_\infty$ 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 $\chi^*$ and $\chi^*_\infty$ the corresponding effect on the susceptibility $\chi^-$ is only of $O(0.1\%)$. Previous MC simulations [42, 43] on $\chi^-$ did not resolve this small anisotropy effect.

Our prediction of the anisotropy effect on the finite-size scaling function $F^{ex}(\xi; A(w))$ for $n = 1$ near the minimum below $T_c$ is shown in Fig. 10 for several $w$. While the position of the minimum $\xi_{min}$ depends only weakly on the anisotropy the value $F^{ex}(\xi_{min}; 1)$ 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 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 two-dimensional Ising model has been provided recently by MC simulations of Selke and Shchur [14]. 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 non-monotonic dependence of $U$ on the ratio $J/K$ (as shown...
in Fig. 4 of Ref. [44].

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

$$\mathbf{A}_2 = 2a^2 \begin{pmatrix} K+J & J \\ J & K+J \end{pmatrix} \quad (8.12)$$

with the reduced anisotropy matrix

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

and with the single anisotropy parameter

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

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

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

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

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

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 $\varphi_i$ on decoupled one-dimensional chains with ferromagnetic NN interactions.

In its present form the matrix $\mathbf{A}_3$, (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 $2 \times 2$ 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 $\tilde{\mathbf{A}}_3 = \mathbf{A}_3 / (\det \mathbf{A}_3)^{1/3}$ that governs the anisotropy effect according to the results of the preceding sections. This matrix is given by

$$\tilde{\mathbf{A}}_3 = \left[\mathbf{K}_0(1-s^2)\right]^{-1/3} \begin{pmatrix} 1 & s & 0 \\ s & 1 & 0 \\ 0 & 0 & K_0 \end{pmatrix}, \quad (8.17)$$

$$\mathbf{K}_0 = \frac{K_0}{(K+J)} = \frac{K_0}{K}(1-s). \quad (8.18)$$

We see that the $J$ dependence of $\tilde{\mathbf{A}}_3$ differs qualitatively from that of $\tilde{\mathbf{A}}_2$ because of the additional $s$ dependence of $\mathbf{K}_0$ 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 $\mathbf{A}_1$ (8.25). This is achieved by the choice $\mathbf{K}_0 = 1$ or $K_0 = K + J$. Then the reduced anisotropy matrix becomes

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

with the same anisotropy parameter $s$ as in (8.13), (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 $\mathbf{A}_3$ would become $(\mathbf{A}_3)_{zz} = (1 - s^2)^{-1/3}(1 - s^2)^{-2/3}$ which would produce a qualitatively different anisotropy effect that is not an even function of $s$.

We have evaluated numerically the expressions (7.8), (4.33), (6.14) in three dimensions for the Binder cumulant $U(0; \mathbf{A}_3(s))$ at $T_c$ using the matrix $\mathbf{A}_3(s)$, (8.19). The result is shown in Fig. 12 in the range $-0.8 < s < 0.8$. The range $0 < s < 0.8$ corresponds to the range $0 < J/K < 4.0$ studied by Selke and Shchur [44].

The anisotropy effect shows up as a non-monotonic dependence on $s$. It is an even function of the anisotropy parameter $s$ and exhibits two maxima of equal height at $s_{\text{max}} = \pm 0.461$ corresponding to $J/K = 0.855$ and $J/K = -0.316$. This symmetry is a consequence of the symmetry property $K_3(y, \mathbf{A}_3(s)) = K_3(y, \mathbf{A}_3(-s))$ of the function (4.36). 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 $U(0; 1) = U(0; \mathbf{A}_3(0)) = 0.417$ for the isotropic three-dimensional $\varphi^4$ theory differs somewhat from the MC result $0.465$ of the three-dimensional Ising model on a $sc$ lattice and is, of course, far from the MC result $0.6107$ 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 $U(0; 1)$ 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 $\Delta U_c(\mathbf{A}_3(s))$, (7.7), as a function of $J/K$ together with the corresponding difference of the MC data of Fig. 4 by Selke and Shchur [44]. The theoretical maximal value is $\Delta U_{c,\text{max}} = 0.0010$ at $J/K = 0.855$ and $J/K = -0.316$. 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 $J/K = -0.3815$. We see that for positive $J/K$ there is remarkable agreement between the MC data in two dimensions and the anisotropic $\varphi^4$ 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 $\varphi^4$ 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 non-monotonicity 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 $J$ [34]. 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 have been 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 $0.0056 \pm 0.00015$ for $J/K = -0.25$ indeed confirms the predicted increase of $\Delta U_c$ for small negative $J/K$ according to Fig. 13. More quantitatively, there is indeed reasonable agreement with our theoretical result $\Delta U_c = 0.0073$ at $J/K = -0.25$ (as shown in Fig. 13) corresponding to $s = -1/3$. 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 $\Delta F_c(\mathbf{A}_3(s))$ 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 $s_{\text{max}} = \pm 0.450$ corresponding...
to $J/K = 0.818$ and $J/K = -0.310$. The theoretical maximal value is $\Delta F_{c,max} = 0.0060$ for $n = 1$. The corresponding effect for $n = \infty$ (dashed curve) as computed from the exact result $\Delta F_{c,\infty}$ 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 [14], 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 $\varphi^4$ theory in three dimensions with the reduced anisotropy matrix $\langle 8.19 \rangle$ we predict that this curve should be close to the difference $\Delta F_c(\bar{A}_2(s))$ of the free energy density of the two-dimensional Ising model with the reduced anisotropy matrix $\langle 8.13 \rangle$. 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 $F_{cx}$ for the reduced anisotropy matrix $\langle 8.19 \rangle$ near the 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.

![Figure 14: Differences $\Delta F_c(\bar{A}_2(s))$, $\langle 8.10 \rangle$, and $\Delta F_{c,\infty}(\bar{A}_2(s))$, $\langle 8.11 \rangle$, of the finite-size amplitudes $\langle 6.12 \rangle$ and $\langle 6.39 \rangle$ of the free energy density of anisotropic systems with the reduced anisotropy matrix $\bar{A}_2(s)$, $\langle 8.19 \rangle$, 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 $s$, $\langle 8.13 \rangle$.](image)

![Figure 15: Scaling function $F_{cx}(\tilde{x}; \bar{A}_3(s))$, $\langle 6.42 \rangle$, $\langle 6.11 \rangle$, $\langle 6.24 \rangle$, of the excess free energy density of anisotropic systems with the reduced anisotropy matrix $\bar{A}_3(s)$, $\langle 8.19 \rangle$, for $n = 1$ in a cubic geometry in three dimensions as a function of the scaling variable $\tilde{x} = t(L/\xi_0)_1^{1/\nu}$ for several values of the anisotropy parameter $s$, $\langle 8.14 \rangle$: $s = 0.45$ (solid line), $s = 0.80$, $-0.80$ (dot-dashed line), $s = 0$ (dotted line). (A similar discussion could be given for the three-dimensional Ising model on a sc lattice [35].)](image)

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

In Subsections C and D we have 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 $\Delta U_c$ and $\Delta F_c$ 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 discussion could be given for the model shown in Fig. 3 in the limits $w \to 1, w \to -1/2$.)

(i) According to $\langle 8.14 \rangle$, the limit $s \to 1$ can be performed as $K \to 0_+$ at fixed $J > 0$ and $K_0 > 0$ (keeping $\lambda_3 > 0$ and $\lambda_3 > 0$ positive while $\lambda_3 > 0_+$. 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 $\varphi^4$ 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, $q = U_3 \tilde{k}$, by means of the orthogonal matrix determined by the eigenvectors $\langle 8.10 \rangle$,

$$U_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}.$$  \hspace{1cm} (8.20)

Correspondingly the inverse propagator $r_0 + \delta \vec{K}(k)$ of the Hamiltonian $\langle 2.7 \rangle$ is transformed to $r_0 + \delta \vec{K}(q)$, where $\delta \vec{K}(q) \equiv \delta \vec{K}(U_3^{-1}q)$ with the interaction part

$$\delta \vec{K}(q) = \sum_{\alpha = 1}^{3} \lambda_\alpha \tilde{q}_\alpha^2 + \sum_{\alpha, \beta, \gamma, \delta} \tilde{B}_{\alpha,\beta,\gamma,\delta} q_\alpha q_\beta q_\gamma q_\delta + O(q^6)$$  \hspace{1cm} (8.21)

where $\lambda_\alpha$ is given after $\langle 8.15 \rangle$.

On the level of Landau theory a Lifshitz point exists at $\lambda_1 = 0$ corresponding to $s = -1$ or $J/K = -1/2$.
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 \( \lambda_1 = \lambda_{1LP} \) that depends on nonuniversal details of the model. [Similarly, \( v_{0c} \) depends on all details of the interaction, see (4.22).] This corresponds to a shifted coupling ratio \( (J/K)_{LP} = -1/2 + \lambda_{1LP}/(2\bar{\phi}^2) \), presumably with \( \lambda_{1LP} < 0 \). To describe the critical behavior near the Lifshitz point would require to introduce a renormalized shifted eigenvalue according to \( \lambda_R = Z\lambda (\lambda_1 - \lambda_{1LP}) \). 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 "\( \lambda \)-line" \( T = T_c(J/K) \) as \( J/K \to (J/K)_{LP} \). 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) - (6.14), (6.22), (6.32), (7.3), and (7.8) depend on the nonuniversal anisotropy matrix \( \tilde{\mathbf{A}} \) but are independent of the bare coupling \( u_0 \), of the lattice spacing \( \bar{\phi} \), of the cutoff of \( \varphi^4 \) field theory, and of the fourth-order moments \( B_{\alpha \beta \delta} \) etc.. We anticipate that the finite-size scaling functions would also remain independent of higher-order couplings, such as those of \( \varphi^6 \) terms and of higher-order gradient terms etc., if they were included in the Hamiltonian. A special matrix \( \tilde{\mathbf{A}} \) with given matrix elements \( \tilde{A}_{\alpha \beta} \) can be obtained from various different lattice structures with a large variety of different couplings, both in \( O(n) \) symmetric \( \varphi^4 \) lattice models and in \( O(n) \) symmetric fixed-length spin models. We expect that \( F(\bar{x}, \tilde{\mathbf{A}}) \) and \( U(\bar{x}, \tilde{\mathbf{A}}) \) are the same for all those systems whose geometry and boundary conditions are the same and whose reduced anisotropy matrix \( \tilde{\mathbf{A}} \) 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 \( \tilde{\mathbf{A}} \) 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 (ii) of Sect. II A with the three couplings \( K, J, \) and \( \overline{K} \) as described by the matrix

\[
\mathbf{A} = 2\bar{\phi}^2 \begin{pmatrix}
D & J + \overline{K} & J + \overline{K} \\
J + \overline{K} & D & J + \overline{K} \\
J + \overline{K} & J + \overline{K} & D
\end{pmatrix},
\]

with \( D = K + 2J + \overline{K} \) and with the reduced matrix \( \tilde{\mathbf{A}} \), (2.13). For a given fixed value of the anisotropy parameter \( w \), (2.10), a family of anisotropic spin models with different couplings \( K, J, \) and \( \overline{K} \) are predicted to have the same finite-size scaling functions if the third-NN coupling \( \overline{K} \) is chosen as

\[
\overline{K} = \frac{1}{1 - w} [wK - (1 - 2w)J]
\]

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

\[
J = \frac{w}{1 - 2w} K
\]

along which, at a given fixed value of \( w \), \(-1/2 < w < 1/2\), 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 (9.3) (in the range \( K + J > 0, K + 4J > 0 \)).

A non-trivial 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 \( \bar{\phi} = 1 \)

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

(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 class for periodic boundary conditions is known to very high accuracy \([39]\): \( U = 0.6118277 \pm 0.0000001 \). 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

\[
J = \frac{1}{3} (K_3 - K)
\]

(9.5)

according to (9.4) in which case

\[
\mathbf{A} = \frac{1}{2} \begin{pmatrix}
2K + 4K_3 & 0 \\
0 & 2K + 4K_3
\end{pmatrix}
\]

(9.6)

and \( \tilde{\mathbf{A}} = \mathbf{1} \). 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).
the bare free energy density (2.25) for \( n \) notation of ordinary perturbation theory is appropriate. Here we long to the asymptotic critical region. In these regimes we explicitly include the indices + and \( \bar{A} \), with \( \bar{A} \) = \( O \). 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 \( F^{\pm} \), \( f^{+} \), \( F^{\pm} \), 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 App. B)

\[
    f^{+} = f_0'(r_0, L', K_{i,j}, v') + O(u'_0), \tag{10.1}
\]

\[
    f^{-} = \frac{1}{2} r_0 M_{m,f}^2 + u'_0 M_{m,f}^2 + f_0(-2r_0, L', K_{i,j}, v') + O(u'_0) \tag{10.2}
\]

above and below \( T_c \), respectively, where \( M_{m,f}^2 \) is given by (4.43) and

\[
    f_0'(r_0, L', K_{i,j}, v') = -\frac{\ln(2\pi)}{2v'} + \frac{1}{2L'^2} \sum_{k'} \ln\{r_0 + \delta K'(k')(v')^{2/4}\}. \tag{10.3}
\]

Because of the \( k' = 0 \) term, the sum exists only for \( r_0 > 0 \). Rewriting these expressions in terms of \( r_0 - r_0c \) with \( r_0c \) given by (4.32) yields up to \( O(1) \)

\[
    f^{+} = f_0'(r_0 - r_0c, L', K_{i,j}, v'), \tag{10.4}
\]

\[
    f^{-} = -\frac{1}{64u'_0}[2(r_0 - r_0c)]^2 + \frac{3}{2}(r_0 - r_0c) \int_{k'} \delta K'(k') + f_0'(2(r_0 - r_0c), L', K_{i,j}, v'). \tag{10.5}
\]

We define the finite-size parts \( \delta f^\pm \) of \( f^\pm \) in the same way as \( \delta f^0 \) in (4.33) and (4.34). Calculating the sum in the continuum limit \( v' \to 0 \) at fixed \( |r_0 - r_0c| \neq 0 \) (see App. B and C) one obtains for \( 2 < d < 4 \)

\[
    \begin{align*}
    f^{+}(r_0, r_0c, u'_0, L', \bar{A}) & = -\frac{A_d}{d^2} (r_0 - r_0c)^{d/2} + \frac{1}{2L'^2} \mathcal{G}_0((r_0 - r_0c)L^2; \bar{A}) + O(u'_0), \tag{10.6} \\
    f^{-}(r_0, r_0c, u'_0, L', \bar{A}) & = -\frac{1}{64u'_0}[-2(r_0^2 - r_0c)^2 + \frac{A_d}{d^2} (-2(r_0 - r_0c))^{d/2} + \frac{1}{2L'^2} \mathcal{G}_0((r_0 - r_0c)L^2; \bar{A}) + O(u'_0) \tag{10.7}
    \end{align*}
\]

where \( \mathcal{G}_0 \) is given by (6.34). Eqs. (10.6) and (10.7) correspond to (4.37). The renormalized counterparts \( f^{\pm}_R \) of \( \delta f^{\pm} \) are defined in the same way as \( f^{\pm}_R \) in (5.3), (5.17). The explicit form of the functions \( f^{\pm}_R \) 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 \( \mu^{-1} = \xi'_0, \xi'_0 + \delta r + \xi'_0 + \xi'_0 = 2 - v + O(u^*) \) (the same choice will be made for the calculations in subsection B below). Then the functions \( f^{\pm}_R \) are given by

\[
    \begin{align*}
    f^{+}_R(r(l_+), u'(l_+), l_+\mu, L', \bar{A}) & = -A_d(l_+\mu)^{d}/(4d) + \frac{1}{2L'^2} \mathcal{G}_0(l_+^2, \mu^2 L^2; \bar{A}) + O(u'(l_+)), \tag{10.8} \\
    f^{-}_R(r(l_-), u'(l_-), l_-\mu, L', \bar{A}) & = -A_d(l_-\mu)^{d} \left\{ \frac{1}{64u'(l_-)} + \frac{1}{4d} \right\} + \frac{1}{2L'^2} \mathcal{G}_0(l_-^2, \mu^2 L^2; \bar{A}) + O(u'(l_-)). \tag{10.9}
    \end{align*}
\]

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

\[
    F^{\pm}_{1-\text{loop}}(\tilde{x}; \bar{A}) = \frac{1}{2} \mathcal{G}_0(L^2/\xi_{0+}^2; \bar{A}) + O(u^*), \tag{10.10}
\]

where \( \xi_{0+} = \xi_{0+}^- t^{-\nu} \) and

\[
    \xi_{0+}^- = \xi_{0+}^- |t|^{-\nu}, \xi_{0+}^- / \xi_{0+}^+ = 2 - \nu + O(u^*) \tag{10.11}
\]

are the bulk second-moment correlation lengths above and below \( T_c \), respectively (for \( \xi_{0+}^\pm \) see (5.10)). 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, \( F^{\pm}_{1-\text{loop}} \) diverges for
\( \hat{x} \to 0 \) at fixed finite \( L \) which originates from the \( k' = 0 \) term of (10.3). [This divergence could formally be suppressed by an \( L' \) dependent choice of \( \ell_\pm \) but this would not avoid a structurally incorrect nonanalytic \( t \) dependence at \( t = 0 \) for finite \( L' \).]

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

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

Nevertheless, \( F_{\text{1-loop}}^{\text{ex}, \pm}(\hat{x}; \tilde{A}) \) has the advantage of displaying the expected \textit{exponential} large \( |\hat{x}| \) behavior. The leading large \( \hat{x} \) behavior of \( G_0 \) for the isotropic case is (see App. B)

\[ G_0(\hat{x}^{2\nu}; 1) = -2d\left( \frac{\hat{x}^2}{2\pi} \right)^{(d-1)/2} \exp(-\hat{x}^\nu) + O(\exp(-2\hat{x}^\nu)). \]  

(10.12)

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

\[ F_{\text{1-loop}}^{\text{ex}, \pm}(\hat{x}; 1) = -\frac{3}{2\pi} (L/\xi_\pm) \exp(-L/\xi_\pm) + O(u^*), \]  

(10.13)

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

In 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 \( \tilde{A} \neq 1 \) 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 \( F_{\text{ex}}^{\text{ex}}(\hat{x}; \tilde{A}_3(s)) \) and \( F_{\text{1-loop}}^{\text{ex}, \pm}(\hat{x}; \tilde{A}_3(s)) \), with \( \tilde{A}_3(s) \) given by (8.19), for several examples of \( s \). In this case the scaling argument (horizontal axis of Fig. 17) needs to be replaced by \( t(L/\xi_{0,+})^{1/\nu} \).

**FIG. 17:** Scaling functions \( F_{\text{ex}}^{\text{ex}}(\hat{x}; 1), (6.22), (6.10), (6.23) \) for \( d = 3 \) (thick solid line), \( F_{\text{1-loop}}^{\text{ex}, \pm}(\hat{x}; 1), (10.10) \) for \( d = 3 \) (thin solid lines), and (10.13) (dashed lines) for the excess free energy density of isotropic systems as a function of the scaling variable \( \hat{x} = (L/\xi_{0,+})^{1/\nu} \). MC result (full circle) for the Ising model on a sc lattice [32]. No scaling function exists in the large - \(|\hat{x}|\) regions above and below \( T_c \) which are sensitive to all nonuniversal details of the model according to \( F_{\text{ex}, \pm}^{\text{ex}}(L/\xi_\pm; 1; \bar{\alpha}/\xi_\pm), (10.15) \), with (10.25).

**B. Non-scaling regime**

1. **Anisotropic \( \varphi^4 \) 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 \( \xi_{0,+}/\bar{\alpha} \gg 1 \) is sufficiently large. In earlier work [9] it was pointed out for the example of the susceptibility that the finite lattice constant \( \bar{\alpha} \) becomes non-negligible in the limit of large \( L/\bar{\alpha} \) at fixed \( T \neq T_c \) in the regime where the finite-size scaling function has an exponential form. Here we further discuss this issue 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 \( \bar{\alpha} \) and only NN couplings \( K \). In this case we have \( \tilde{A} = 2a^2 K_1 \), \( \bar{\alpha} = 1, L = (2a^2 K)^{1/2} L' \), \( \bar{\alpha} = (2a^2 K)^{1/2} a' \), and there exist well defined bulk second-moment correlation lengths \( \xi_\pm = (2a^2 K)^{1/2} \xi_\pm \) above and below \( T_c \) (for \( n = 1 \)). As shown in App. B, the excess free energy density in one-loop order attains the following form in the limit of large \( L/\bar{\alpha} = L'/a' \) at fixed arbitrary \( \bar{\alpha}/\xi_\pm > \) 0

\[ f_{\text{ex}, \pm}^{\text{ex}}(t, L) \underset{L/\bar{\alpha} \gg 1}{\longrightarrow} L^{-d} F_{\text{ex}, \pm}(L/\xi_\pm; 1; \bar{\alpha}/\xi_\pm) \]  

(10.14)

\[ F_{\text{ex}, \pm}(L/\xi_\pm; 1; \bar{\alpha}/\xi_\pm) = -d \left\{ \frac{\bar{\alpha}}{2\xi_\pm} \right\}^{2(d-1)/d} \]  

(10.15)
This result applies to the shaded region of Fig. 1. The exponential part of \((10.13)\) can be rewritten as 
\[ \exp(-L/\xi_{\pm}) \] 
with the exponential correlation lengths
\[ \xi_{\pm} = \frac{\tilde{a}}{2} \left[ \arcsinh \left( \frac{\tilde{a}}{2\xi_{\pm}} \right) \right]^{-1} \] (10.16)
above and below \(T_c\), respectively. As a nontrivial relation between bulk properties and finite-size effects \([10]\), the lengths \(\xi_{\pm}\) describe the exponential part of the bulk order-parameter correlation function \([76]\) 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 \(a\) dependence of \(\xi_{\pm}\) cannot be neglected even for small \(\tilde{a}/\xi_{\pm} \ll 1\) if \(L/\xi_{\pm} > [24 \ln 2] \left(\xi_{\pm}/\tilde{a}\right)^2\) is sufficiently large (see Fig. 1 of Ref. \([9]\)). The same argument now applies to the \(\tilde{a}\) dependence of the exponential part of \(\mathcal{F}^{\text{ex,±}}(L/\xi_{\pm}1; \tilde{a}/\xi_{\pm})\), \((10.13)\). This implies that finite-size scaling and universality are violated in the large - \(|\tilde{x}|\) tails of \(\mathcal{F}^{\text{ex,±}}\) at any \(\tilde{a}/\xi_{\pm} > 0\) even arbitrarily close to \(T_c\) because ultimately, for \(|\tilde{x}| \to \infty\) (i.e., for large \(L\) at fixed \(|t| \neq 0\)), the tails of \(\mathcal{F}^{\text{ex,±}}\) 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 \((12.2), (1.3),\) or \((1.4)\) with a single scaling argument \(\propto L^{1/\nu}\) and with a single nonuniversal amplitude \(C_1\) can be defined in this large - \(|\tilde{x}|\) region \([94]\). Higher-loop contributions cannot remedy this violation. It is obvious that an even larger variety of different nonscaling effects exist in the exponential finite-size region of systems with non-cubic anisotropies (\(\hat{A} \neq 1\)).

2. Isotropic \(\varphi^4\) field theory

The diversity of nonuniversal non-scaling 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 \(\varphi^4\) field theory based on the standard Hamiltonian
\[ H_{\text{field}} = \int d^dx \left[ \frac{\nu}{2} \varphi^2 + \frac{1}{2}(\nabla \varphi)^2 + u_0 \varphi^4 \right] \] (10.17)
in a cube with \(V = L^d\) and periodic b.c. and with some cutoff \(\Lambda\) in \(k\) space. Keeping the cutoff finite may be a convincingly tool for testing universality as has been convincingly demonstrated by Nicoll and Albright \([93]\) in the context of bulk universality \([8]\). In a similar spirit this was done in \([9, 10]\) with regard to finite-size universality in the large-\(n\) limit at and above \(T_c\). We shall show that \(\mathcal{F}^{\text{ex,±}}\) 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 \([11, 90]\) of the singular part of the excess free energy density at \(T_c\).

Since \(f^{\text{ex,±}}\) has a finite limit for \(\Lambda \to \infty\) we first we calculate \(f^{\text{ex,±}}\) at infinite cutoff \(\Lambda = \infty\) within the minimal renormalization scheme at fixed dimension \(2 < d < 4\) \([62, 63, 82]\). In one-loop order we obtain
\[ f^{\text{ex,±}}_{\Lambda = \infty}(t, L) = L^{-d} f^{\text{ex,±}}_{\Lambda = \infty}(L/\xi_{\pm}) \] (10.18)
where for large \(L/\xi_{\pm}\)
\[ f^{\text{ex,±}}_{\Lambda = \infty}(L/\xi_{\pm}) = -d \left( \frac{L}{2\pi \xi_{\pm}} \right)^{(d-1)/2} \exp \left\{ -\frac{L}{\xi_{\pm}} \right\} \] (10.19)
with the bulk second-moment correlation lengths
\[ \xi_{\pm}(t; u_0) = \xi_{0\pm}(u_0)|t|^{-\nu} \{ 1 + C_{\pm}(t, u_0) \} \] (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
\[ C_{\pm}(t, u) = \sum_{m=1}^{\infty} a^{(m)}_{\pm}(u) |t|^{\Delta m} \] (10.21)
with the universal Wegner exponent \(\Delta = \omega\nu, \omega = \partial \beta_u(u, \varepsilon)/\partial u|_{u=u_{\star}}\), and the Wegner amplitudes \(a^{(m)}_{\pm}(u)\) depending in the nonuniversal renormalized coupling \(u\). The latter is defined by
\[ u = A_d Z_u(u, \varepsilon)^{-1} Z_{\varphi}(u, \varepsilon)^2 u_0 \xi_{0\pm}^{-1} \] (10.22)
(with the choice \(\mu = \xi_{0\pm}^{-1}\)) where \(Z_u(u, \varepsilon)\) and \(Z_{\varphi}(u, \varepsilon)\) are the standard \(Z\) factors \([80]\). Equation \((10.22)\) determines \(u\) as an implicit function of \(u_0 \xi_{0\pm}^{-1}\). Although \(C_{\pm}\) is an negligible additive correction in \((10.20)\) for sufficiently small \(|t|\) this is not the case in the exponential part of \((10.19)\) which, for small \(C_{\pm}\), can be rewritten as
\[ \exp \left\{ -\frac{L}{\xi_{\pm}} \right\} = A(L, t, u) \exp \left( -\frac{L}{\xi_{0\pm}|t|^{-\nu}} \right), \] (10.23)
\[ A(L, t, u) = \exp \left\{ C_{\pm}(t, u) \frac{L}{\xi_{0\pm}|t|^{-\nu}} + O(C_{\pm}^2) \right\} \] (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 nonnegligible if \(L\) is sufficiently large, \(L \gg |C_{\pm}|^{-1} \xi_{0\pm}|t|^{-\nu}\). Thus the tails of the large \(L\) dependence of \(\mathcal{F}^{\text{ex,±}}_{\Lambda = \infty}\) 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 non-asymptotic form of the second-moment bulk correlation lengths at finite \(\tilde{a}\)
\[ \xi_{\pm}(t; u_0 \tilde{a}) = \xi_{0\pm}|t|^{-\nu} \{ 1 + C_{\pm}(t, u_0 \tilde{a}) \} \] (10.25)
in \((10.13)\) and \((10.16)\) and to include all correction terms in \(C_{\pm}(t,uq^2)\). The reasoning described above must also be extended to the case when a smooth cutoff \(\Lambda\) in \(k\) space is taken into account. This can be done by including an isotropic (Pauli-Villars type) term \(\frac{1}{2}(V^2\phi^2)/\Lambda^2\) in the Hamiltonian \((10.17)\). In this case the structure of \(\mathcal{F}_{ex,\pm}\) still remains exponential \(\propto \exp[-L/\xi_{e\pm}(\Lambda)]\) for large \(L/\xi_{e\pm}\) but the exponential correlation lengths

\[
\xi_{e\pm}(\Lambda) = \xi_{\pm}[1 - \frac{1}{2} \Lambda^{-2} \xi_{\pm}^{-2} + O(\Lambda^{-4} \xi_{\pm}^{-4})]\]

(10.26)

become cutoff dependent. This causes a cutoff dependent prefactor \(A(L,t,u,\Lambda)\) in \((10.27)\). As pointed out in \([12]\) there exists a close relation between the dependence of finite-size effects and the \(x\) dependence of the bulk order-parameter correlation function \(G_0\) discussed in Sect. III. In retrospect, the arguments presented above apply also to the exponential part of \(G_0 \propto |x|-d/2 \exp(-|x|/\xi_{e\pm})\) even if it is isotropic because here the same correlation lengths \(\xi_{e\pm}\) appear as in the large \(L\) decay of the finite-size quantities. No scaling functions \(\Phi_{\pm}\), \((3.5), (3.6), (3.19)\) can be defined in the exponential large-distance regime \(|x|/\xi_{e\pm} \gg 1\) (shaded region in Fig. 2). Thus the exponential tails of \(G_0(x;t)\) of the \(\phi^4\) 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 \(\mathcal{F}_{ex,\pm}/\mathcal{F}_{b}\) becomes arbitrarily large for sufficiently large \(L/\xi_{e\pm}\) this happens in a region where the magnitude of \(\mathcal{F}_{ex,\pm}\) 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 non-scaling finite-size effects in the presence of (effective) long-range correlations caused by a sharp momentum cutoff \(-\Lambda \leq k_\alpha < \Lambda\) used in \([3, 11]\). Such a cutoff has often been used in the formulation and application of the RG theory based on the \(\phi^4\) Hamiltonian \((10.17)\) (see, e.g., \([95, 98, 99]\)). 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 \(\phi^4\) 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 \([3, 11]\) have raised the question whether this remains true also for confined systems. It was found, for the susceptibility and for the excess free energy in the large-\(\alpha\) 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 \([11, 98]\) 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 \(G_{0}(x;t;\Lambda)\) \([11, 72]\) whose algebraically decaying non-scaling 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 \([28]\) whereas in \([11]\) no \(L\) dependent nonsingular part was defined. We find that, in the presence of a sharp cutoff \(\Lambda\) and for large \(L\), Eq. \((10.18)\) with \((10.19)\) is to be replaced by

\[
f_{ex,\pm}(t,L) = f_{ex,\pm}^{\Lambda,s}(t,L) + f_{ex,\pm}^{\Lambda,ns}(L),
\]

(10.27)

with the singular part

\[
f_{ex,\pm}^{\Lambda,s}(t,L) = L^{-2}\Lambda^{-d/2}\tilde{\Phi}_{d}(\xi_{\pm}^{-1}\Lambda^{-1}) + f_{\Lambda=\infty}^{ex,\pm}(t,L),
\]

(10.28)

\[
\tilde{\Phi}_{d}(z) = \int_{0}^{\infty} dy \left[ e^{-(1+z/2)^{2}} - e^{-y^{2}} \right] E_{d}(y),
\]

(10.29)

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

(10.30)

and the \(L\) dependent nonsingular part

\[
f_{\Lambda,ns}^{ex}(L) = L^{-2}\Lambda^{-d/2} \int_{0}^{\infty} dy e^{-y} E_{d}(y).
\]

(10.31)

Although our one-loop result \((10.27) - (10.31)\) for the total excess free energy density \(f_{ex,\pm}^{\Lambda,s}(t,L)\) is equivalent to equations \((8)\) and \((16)\) of \([11]\), there is a crucial difference with regard to singular part. In contrast to the nonvanishing function \(\tilde{\Phi}_{d}(z)\) 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 \(f_{\Lambda,ns}^{ex}(L) \propto L^{-d}\) 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 \(\alpha\) 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 \((10.28)\) dominates in the shaded region of Fig. 1 compared to the scaling part \(f_{\Lambda=\infty}^{ex,\pm} \propto L^{-d}\) but vanishes at \(T = T_c\) and is subleading in the central finite-size regime. Thus the leading finite-size contributions in the \(\phi^4\) 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 $T_c$ \cite{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 \cite{100}, as noted already in \cite{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. \cite{96}, the sharp cutoff implies an unphysical discontinuity of the slope of the interaction $\delta \hat{K}(k) = k^2$ at the boundary of the Brillouin zone which is the mathematical origin of the $L^{-2}$ terms. For the reasons given above, however, we disagree with the opinion expressed in \cite{96} that the concept of finite-size scaling as developed for systems with short range interactions does not apply to the $\varphi^4$ model \cite{101,102} with a sharp cutoff. The authors of \cite{96} did not perform an analysis based on a decomposition of the type \cite{25,27} and \cite{101,102}. Our analysis shows that, in spite of the mathematical artifact of $\hat{K}(k)$ 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 \cite{27} and \cite{29}. It was pointed out by Dantchev and Rudnick \cite{13} that it affects the finite-size susceptibility in the regime $L/\xi \gg 1$, similar to the effect caused by a sharp cutoff \cite{9}. The effect of this interaction on the excess free energy $f^{ex}_s$ and on the critical Casimir force in the case of film geometry was first studied by Chen and the present author \cite{11,18}. The asymptotic structure for $L/\xi \gg 1$ in one-loop order above $T_c$ at $h = 0$ is

$$ f^{ex}_s(t, L) = L^{-d} \left[ F^{ex}(L/\xi) + b L^{-2-\sigma} \Psi(L/\xi + \epsilon) \right]$$

which is similar to \cite{35}. 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 $\Psi_{cube}$ has an algebraic large-$L$ behavior $\sim (L/\xi)^{-2}$. The latter dominates the exponentially decaying scaling part $F^{ex, \pm}_s \propto \exp(-L/\xi_{cube})$ in the shaded region of Fig. 1. This implies that, in this region, two nonuniversal length scales $b^{1/(\sigma-2)}$ and $\xi_{cube}$ at $h = 0$ govern the leading singular part of the excess free energy density

$$ f^{ex, \pm}_s(t, L) \sim L^{-d} \left[ b^{1/(\sigma-2)} L^{-2-\sigma} \left( \xi_{cube} \right)^2 \right]$$

even arbitrarily close to criticality. In addition, there is the nonuniversal $u_0$ - dependent exponential tail of $F^{ex, \pm}_s$. In \cite{102}, both the amplitude $\sim b$ and the power $-d - \sigma$ of the $L$ dependence are nonuniversal. Thus the universal scaling form \cite{12}, with only one length scale $\tilde{C}_1^{\nu}$ 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 \cite{102} and \cite{103} and the corresponding structure for the critical Casimir force in film geometry has been confirmed in \cite{51,52,90}.

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Appendix A : Universal bulk amplitude relations

In this Appendix we present explicit expressions for the universal constants $Q_i$, $Q_3$, and $P_i$, \cite{35} - \cite{13}, in terms of universal scaling functions. Near $T_c$ the sum rule \cite{35} yields

$$ \chi'_b(t, h') = -A^1_2 t^d \partial^2 W_{\pm} (A^1_2 h')^{-\beta\delta} / \partial h'^2 $$

$$ = D^1 t^{2-n} \Phi_\pm (D^2_2 h')^{-\beta\delta} \quad (A.1) $$

with the universal function

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

At $t > 0, h' = 0$, \cite{A.3} yields $\chi'_b(0, 0) = \Gamma'_+ |t|^{-\gamma}$ with

$$ \Gamma'_+ = -A^1_1 A^2_2 W^2 = D^1 (\xi'_0)^2 \Phi_+(0) \quad (A.3) $$

where $W = \text{lim}_{y \rightarrow 0} \partial^2 W_\pm (y) / \partial y^2$.

At $t = 0, h' \neq 0$ we have from \cite{35,39} $\xi'_b(0, h') \equiv \xi'_b h'^{-\nu/\beta\delta}$ with

$$ \xi'_b = \xi'_0 (D^2_2)^{-\nu/\beta\delta} \tilde{X} $$

thus \cite{A.1} yields $\chi'_b(0, h') = \Gamma'_b |h'|^{-\nu/\beta\delta}$ with

$$ \Gamma'_b = -A^1_1 A^2_2^{1+1/\delta} W $$

$$ = D^1 \left[ \xi'_0 + (D^2_2)^{-\nu/\beta\delta} \tilde{X} \right]^{2-n} \Phi_+(\infty) \quad (A.5) $$

where $\Phi_+(\infty) \equiv \Phi_+ (\infty)$ and

$$ W = \lim_{y \rightarrow -\infty} \left\{ |y|^{\nu/\beta\delta} \partial^2 W_\pm (y) / \partial y^2 \right\} \quad (A.6) $$

$$ \tilde{X} = \lim_{y \rightarrow -\infty} \left\{ |y|^{\nu/\beta\delta} X_\pm (y) \right\} \quad (A.7) $$

\cite{A.3} and \cite{A.5} yield

$$ \Gamma'_b / \Gamma'_+ = A^1_1 A^2_2^{1-1/\delta} W_2 W^2 $$

$$ = D^1 [1/\Phi_+(0) \left[ (\tilde{X}^{2-n} \Phi_+(\infty))^{-1} \right]^2, (A.8) $$
thus we obtain the universal ratio
\[ P_2 = \frac{A'_2}{D_2'} = \left[ \frac{\hat{W} \Phi_+(0)}{W_2 X^{2-\eta} \Phi(\infty)} \right]^{\delta/(\delta-1)}. \] (A.9)

Eqs. (A.4) and (A.8) yield a universal ratio \( Q_2 \) different from \( P_2 \),
\[ Q_2 = \frac{\Gamma'_c}{\Gamma_c} \left( \frac{c'_e}{\xi_{01}^+} \right)^{2-\eta} = \frac{\Phi_+(0)}{\Phi(\infty)}, \] (A.10)

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 \( G_b'(x'_1, x'_2; t, h') = \lim_{V \to \infty} \langle \phi'(x'_1) \phi'(x'_2) \rangle' \) has the asymptotic scaling form
\[ G_b'(x'_1, x'_2; t, h') = D'_1 |x'|^{-d+2-\eta} Z_\pm \left( |x'|/\xi'_e, D'_2 h'|t|^{-\beta} \right) \] (A.11)
with the same constants \( D'_1 \) and \( D'_2 \) as in Eq. (3.3.5) and with a universal function \( Z_\pm(x, y) \). From (A.11), (2.11), and (3.3) we obtain the square of the bulk order parameter below \( T_c \)
\[ [m'_b(t)]^2 = \lim_{h' \to 0} \lim_{|x'| \to \infty} G_b'(x'_1, x'_2; t, h') = D'_1 \left( \xi_{00} ' - \xi_e' \right)^{2-\eta} W_2 / \Phi_+(0) \] (A.12)
\[ = (A'_1 A'_2)^2 |\xi_{00} ' - \xi_e' |^{-\eta} W_1 / \tilde{Z}. \] (A.13)

Together with (3.16) this yields the universal quantities
\[ Q_1 = A'_1 \left( \xi_{00} '+ \xi_e' \right)^d = -\tilde{Z} W_2 \left[ X_\pm(0) \right]^{-d+2-\eta} / \left[ W_1 \Phi_+(0) \right]. \] (A.14)

and
\[ P_3 = D'_1 A'_1 A'_2 \left( \xi_{00} '+ \xi_e' \right)^{-2-\eta} W_2 / \Phi_+(0). \] (A.15)

Finally we consider the universal ratio (3.14). The amplitude \( D'_\infty \) is given by \( D'_\infty = D'_1 \Phi_+(0, 0) \) with the universal constant [13, 101]
\[ \hat{C} = \frac{\hat{D}_\infty}{D_\infty} = \frac{\Phi_+(0, 0)}{\Phi_+(0, 0)} = \frac{(4\pi)^{d/2} \Gamma(2d/2)}{2^{d-2-\eta} \Gamma((d-2+\eta)/2)}. \] (A.16)

Together with (A.3) this yields a universal ratio \( Q_3 \) different from \( P_3 \),
\[ Q_3 = \hat{D}_\infty \left( \xi_{00} '+ \xi_e' \right)^{-2-\eta} / \hat{C}' = \Phi_+(0, 0) \hat{C}' / \Phi_+(0). \] (A.17)

The universal constant \( \hat{Q}_3 \) in (3.14) is
\[ \hat{Q}_3 = \frac{\Phi_+(0, 0)}{\Phi_+(0)}. \] (A.18)

**Appendix B : Gaussian model with lattice anisotropy**

In order to derive the Gaussian part of (4.26) and the results of Sect. X we consider the Hamiltonian (2.1) and (2.7) for \( r_0 = a_0 t > 0, u_0 = 0 \) and \( h = h_0 \) with \( N \) scalar variables \( \varphi_j \) on a simple-cubic lattice with lattice constant \( a \) in a cubic volume \( V = L^d = Na^d \) with periodic boundary conditions. This Hamiltonian will be denoted by \( H^G \). The Jacobian of the linear transformation \( \varphi_j \to \tilde{\varphi}(k) \) is \( |\partial \varphi_j / \partial \tilde{\varphi}(k)| = (aL)^{-dN/2} \). The dimensionless partition function is
\[ Z^G = \prod_{k} \frac{1}{\mathcal{L}_{d/2}} \int d\tilde{\varphi}(k)^\d \exp(-H^G) \]
\[ = \prod_{k} \left( \frac{2\pi}{|r_0 + \delta \tilde{K}(k)|a^d} \right)^{1/2}. \] (B.1)

For the transformed system one obtains
\[ Z'^G = \prod_{k} \frac{1}{\mathcal{L}_{d/2}} \int d\tilde{\varphi}'(k)^\d \exp(-H'^G) \]
\[ = \prod_{k} \left( \frac{2\pi}{|r_0 + \delta \tilde{K}'(k)|a^d} \right)^{1/2}. \] (B.2)

with \( v' = (\det A)^{-1/2} a^d \). Eqs. (B.1) and (B.2) define the integration measure \( \int d\tilde{\varphi}(k) \) and \( \int d\tilde{\varphi}'(k) \). The Gaussian free energy densities divided by \( k_B T \) are
\[ f^G = -\frac{\ln(2\pi)}{2\mathcal{L}} + \frac{1}{2L^d} \sum_k \ln{|r_0 + \delta \tilde{K}(k)|a^d} \] (B.3)
\[ f'^G = -\frac{\ln(2\pi)}{2v'} + \frac{1}{2L^d} \sum_k \ln{|r_0 + \delta \tilde{K}'(k)|v'^{d/2}}. \] (B.4)

The correctness of the additive constant of \( f^G \) can be checked by performing the integrations of \( Z^G \) in real space for \( K_{i,j} = 0, \delta \tilde{K}(k) = 0 \),
\[ \prod_{j=1}^N \int_{-\infty}^{\infty} \frac{d\tilde{\varphi}_j}{a_1^{d/2}} \exp \left[ -a^d \sum_{j=1}^N \frac{r_0^2}{2d^2} \right] = \left( \frac{2\pi}{r_0 a^d} \right)^{N/2}. \] (B.5)

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 (B.3) we consider
\[ \Delta(r_0, L, K_{i,j}, a) = L^{-d} \sum_k \ln{|r_0 + \delta \tilde{K}(k)|a^d} \]
\[ - \int \ln{|r_0 + \delta \tilde{K}(k)|a^d} \] (B.6)
where the sum $\sum_k$ and the integral $\int_k$ have finite cutoffs $\pm \pi/\bar{a}$ for each $k_\alpha$ [see Eq. (B.31)]. Using the integral representation
\[
\ln w = \int_0^\infty \, \text{d}y y^{-1} \left[ \exp(-y) - \exp(-wy) \right] \quad (B.7)
\]
and interchanging the integration $\int \, \text{d}y$ with $\sum_k$ and $\int_k$ we obtain, because of $L^{-d} \sum_k 1 = \int_k 1$,
\[
\Delta(r_0, L, K_{i,j}, \bar{a}) = \int_0^\infty \, \text{d}y y^{-1} \exp\left[-\delta \tilde{K}(k)\bar{a}^2 y\right] \left[ \exp\left(-\delta \tilde{K}(k)\bar{a}^2 y\right) - L^{-d} \sum_k \exp\left(-\delta \tilde{K}(k)\bar{a}^2 y\right) \right].
\]
(B.8)
Since $\delta \tilde{K}(k)$ is a periodic function of each component $k_\alpha$ of $k$ the sum in (B.8) satisfies the Poisson identity
\[
L^{-d} \sum_k \exp\left(-\delta \tilde{K}(k)\bar{a}^2 y\right) = \sum_n \int_k \exp\left(-\delta \tilde{K}(k)\bar{a}^2 y + i k \cdot nL\right)
\]
(B.9)
where $n = (n_1, n_2, \ldots, n_d)$ and $k \cdot n = \sum_{\alpha=1}^d k_\alpha n_\alpha$. The sum $\sum_n$ runs over all integers $n_\alpha$, $\alpha = 1, 2, \ldots, d$ in the range $-\infty \leq n_\alpha \leq \infty$. This leads to the exact representation
\[
\Delta(r_0, L, K_{i,j}, \bar{a}) = -\int_0^\infty \, \text{d}y y^{-1} e^{-\bar{a}^2 y} \sum_n \int_k \exp\left(-\delta \tilde{K}(k)\bar{a}^2 y + i k \cdot nL\right). \quad (B.10)
\]
Note that here the integral $\int_k$ still has finite lattice cutoffs $\pm \pi/\bar{a}$. We shall evaluate $\Delta(r_0, L, K_{i,j}, \bar{a})$ for large $L/\bar{a} \gg 1$ and distinguish two regimes: (i) $L \bar{a}^{1/2} \lesssim O(1)$, $r_0 \bar{a}^{1/2} \ll 1$, and (ii) $L \bar{a}^{1/2} \gg 1$ for arbitrary fixed $r_0 \bar{a}^{1/2} > 0$.

In the regime (i), the large - $k$ dependence of $\delta \tilde{K}(k)$ does not matter. Therefore we may replace $\delta \tilde{K}(k)$ by its small - $k$ form $k \cdot A k$ and let the integration limits of $\int_k$ go to $\infty$. Furthermore it is useful to substitute the integration variable $z = 4\pi^2 \bar{a}^2 y/L^2$. Then we obtain
\[
\Delta(r_0, L, K_{i,j}, \bar{a}) \to \Delta(r_0, L; A) = -\int_0^\infty \, \text{d}z z^{-1} e^{-r_0 L^2 z/(4\pi^2)} \times \sum_{n \neq 0} \int_k \exp[-k \cdot A k L^2 z/(4\pi^2) + i k \cdot nL]. \quad (B.11)
\]
The Gaussian integral over $k$ yields
\[
\int_k \exp[-k \cdot A k L^2 z/(4\pi^2) + i k \cdot nL] = (\text{det} A)^{-1/2} \left( \frac{\pi}{L^2 \gamma} \right)^{d/2} \exp(-n \cdot A^{-1} \mathbf{n}^2 z) \quad (B.12)
\]
Eqs. (B.11) and (B.12) lead to
\[
\Delta(r_0, L; A) = L^{-d} G_0(r_0 L^2; \bar{A}) \quad (B.13)
\]
where $G_0$ and $K_d(y, \bar{A})$ are given by (3.34) and (4.16). Thus, in the regime (i), we derive from Eqs. (B.13), (B.8), and (B.13)
\[
f^G = f_b^G + \frac{1}{2} L^{-d} G_0(r_0 L^2; \bar{A}) \quad (B.14)
\]
with the bulk part $f_b^G$ obtained from (B.3) by the replacement $L^{-d} \sum_k \to \int_k$. 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 $H^{G^G}$ [Eqs. (2.29) and (2.33)] for $u' = 0, h' = 0$ for which the corresponding result reads
\[
f^{G^G} = f_b^{G^G} + \frac{1}{2} L^{-d} G_0(r_0 L^2; \bar{A}) \quad (B.15)
\]
with the bulk part $f_b^{G^G}$ given in (4.29) for $u'_0 = 0$. Now the parameter $r_0$ is related to the second-moment bulk correlation length of $H^{G^G}$ [see (4.14)]
\[
\xi^{G^G}_+ = \frac{1}{r_0^{1/2}} = \frac{\xi^{G^G}_0 t^{-1/2}}{\bar{a}}, \quad \xi^{G^G}_+ = \frac{2 K}{a_0^{1/2}} \quad (B.16)
\]
This leads to the identification of the scaling function of the Gaussian excess free energy density in the regime (i)
\[
\mathcal{F}^{G,ex}(\tilde{x}; \bar{A}) = \frac{1}{2} G_0(\bar{A}) \quad (B.17)
\]
with $\tilde{x} = t(L'/\xi^{G^G}_+)^{1/\nu}$, $\nu = 2$.

In the regime (ii), $\Delta(r_0, L, K_{i,j}, \bar{a})$ will attain an exponential $L$ dependence and the complete $k$ dependence of $\delta \tilde{K}(k)$ does matter. For simplicity we consider only nearest-neighbor couplings $K_{i,j} = K$ on a sc lattice, $\delta \tilde{K}(k) = 4K \sum_{\alpha=1}^d [1 - \cos(\bar{a} k_\alpha)]$, with the second-moment bulk correlation length of the Gaussian model
\[
\xi^{G^G}_+ = \bar{a} \left( \frac{2K}{a_0} \right)^{1/2} = \frac{\xi^{G^G}_0 t^{-1/2}}{\bar{a}}, \quad \xi^{G^G}_+ = \bar{a} \left( \frac{2K}{a_0} \right)^{1/2} \quad (B.18)
\]
At the level of the Gaussian model there exist no Wegner corrections to (B.18). Using (B.7) we obtain, similar to App. A of [77], the exact representation for (B.6)
\[
\Delta(r_0, L, K; \bar{a}) = \bar{a}^{-d} \int_0^\infty \, \text{d}y y^{-1} e^{-r_0 y} \times \left\{ \text{S}(\infty, y) \right\}^d - \left\{ \text{S}(L/\bar{a}, y) \right\}^d \quad (B.19)
\]
\[ S(L/\tilde{a}, y) = S(\infty, y) + 2 e^{-2y} \sum_{m=1}^{\infty} I_{mL/\tilde{a}}(2y) \] 

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

\[ I_M(2y) = (2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \cos(M\theta) e^{2y \cos \theta} \] 

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 (B.20) suffices to obtain the leading exponential behavior. Thus we substitute \( 2y = zL/\tilde{a} \) in (B.19) and use the asymptotic formulae for large \( L/\tilde{a} \) (see (9.7.7) and (9.7.1) of [104] and App. A of [10]).

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

(B.22)

\[ \Delta(r_0, L, K, \tilde{a}) = -\frac{2d}{L^d} \left( \frac{L/\tilde{a}}{2\pi} \right)^{(d-1)/2} e^{-L/\xi^G_+} \] 

(B.24)

with the exponential correlation length

\[ \xi^G_+ = \frac{\tilde{a}}{2} \left[ \arcsinh \left( \frac{\tilde{a}}{2\xi^G_+} \right) \right]^{-1}. \] 

(B.25)

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 (B.24) and (B.25).

Within a RG treatment of the \( \phi^4 \) 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 Sect. 2 and App. A of [3], 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 \( \tilde{a}/\xi^G_+ > 0 \).

For field theory with \( \delta \tilde{K}(k) = k^2 \) and a sharp cutoff \( -\Lambda \leq k_a < \Lambda \) the Gaussian excess free energy density is given by (1/2)\( \Delta \) where \( \Delta \) is given by (B.6) with \( \tilde{a} \) replaced by \( \Lambda^{-1} \). From (A.31) of App. A of [39] and a RG treatment at finite \( \Lambda \) we obtain [10,27] - [10,31].

Appendix C: Sums over higher modes

Using (B.6) and the integral representation (B.7) with \( w = rL^2/(4\pi^2) \) we obtain from (B.13) and (B.34)

\[ \frac{1}{2L^d} \sum_{k' \neq 0} \ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\} = \frac{1}{2} \int_{k'}^{\infty} \ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\} d\varepsilon \] 

\[ + \frac{1}{2L^d} \ln \left( \frac{L^2}{v^{r^2/d}4\pi^2} \right), \] 

(C.1)

\[ J_0(rL^2, \tilde{A}) = \int_0^\infty \frac{dy}{y} \left\{ \exp \left( -\frac{rL^2y}{4\pi^2} \right) \cdot \left\{ (\pi/y)^{d/2} - K_d(y, \tilde{A}) + 1 \right\} - \exp(-y) \right\}. \] 

(C.2)

The \( v' \) dependent finite-size part in (C.1) comes from the absence of the \( k' = 0 \) term and is exactly cancelled by the corresponding logarithmic term in (B.20). For \( d > 0 \) the function \( J_0(rL^2, \tilde{A}) \) is finite for all \( 0 \leq rL^2 < \infty \) and diverges for large \( rL^2 \) as \( J_0(rL^2, \tilde{A}) \sim -\ln[rL^2/(4\pi^2)] \).

By means of differentiation with respect to \( r \) we obtain

\[ S_m(r) = L^d \sum_{k' \neq 0} \frac{\ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\}}{rL^2 - \bar{A}}, \] 

(C.3)

\[ I_m(rL^2, \tilde{A}) = \int_0^\infty dy \frac{\ln(-rL^2y/(4\pi^2))}{y} \cdot \left\{ K_d(y, \tilde{A}) - (\pi/y)^{d/2} - 1 \right\}. \] 

(C.4)

For \( 2 < d < 4 \) the behavior of these functions for \( r \to 0 \) is \( I_1(r, \tilde{A}) \to I_1(0, \tilde{A}) = \infty \), \( r^2 I_2(r, \tilde{A}) \to -16\pi^4 \). For \( 2 < d < 4 \) and \( r > 0 \) the bulk integral in (C.1) is

\[ \ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\} = \int_{k'}^{\infty} \ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\} d\varepsilon \] 

\[ + \frac{r}{2L^d} \int_{k'}^{\infty} \ln \left\{ \left[ r + \delta \tilde{K}'(k') \right] v^{r^2/d} \right\} d\varepsilon \] 

(C.6)

apart from nonsuprimal corrections that depend on the bulk integrals in (C.3) follow by differentiation with respect to \( r \).
