Nonuniversal finite-size scaling in anisotropic systems

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(Received 22 April 2004; published 30 November 2004)

We study the bulk and finite-size critical behavior of the O(n) symmetric φ^4 theory with spatially anisotropic interactions of noncubic symmetry in $d<4$ dimensions. In such systems of a given (d,n) universality class, two-scale factor universality is absent in bulk correlation functions, and finite-size scaling functions including the Privman-Fisher scaling form of the free energy, the Binder cumulant ratio, and the Casimir amplitude are shown to be nonuniversal. In particular it is shown that, for anisotropic confined systems, isotropy cannot be restored by an anisotropic scale transformation.

DOI: 10.1103/PhysRevE.70.056136 PACS number(s): 64.60.−i, 05.70.Jk, 75.40.−s

A basic tenet in the physics of critical phenomena is the notion of a universality class. It is characterized by the dimensionality d of the system and by the number n of the components of the order parameter. (See, e.g., the review article [1].) Within a certain (d,n) universality class, the universal quantities (critical exponents, amplitude ratios, and scaling functions) are independent of microscopic details, such as the particular type of (finite-range or van der Waals type) interactions or the lattice structure [2]. This implies that a given universality class includes both spatially isotropic and anisotropic systems.

Once the universal quantities of a universality class are known the asymptotic critical behavior of very different systems (e.g., fluids and magnets) is believed to be known completely provided that only *two* nonuniversal amplitudes A_1 and A_2 are given. This property is known as *two-scale factor universality* or *hyperuniversality* [1,3,4]. In terms of the singular part of the reduced bulk free energy density $F_s/Vk_BT \equiv f_s(t,h)$ above T_c,

$$f_s(t,h) = A_1 t^{d\nu} W(A_2 h t^{-\beta\delta}) \tag{1}$$

with $W(0)=1$ and $t=(T-T_c)/T_c \ll 1$, this property can be stated as [5]

$$\lim_{t\to 0+} f_s(t,0)\xi^d = Q(d,n) = \text{universal}. \tag{2}$$

Thus the amplitude $\xi_0=(Q/A_1)^{1/d}$ of the correlation length $\xi=\xi_0 t^{-\nu}$ at zero ordering field h is not an independent amplitude but is universally related to A_1. The validity of two-scale factor universality has been established by the renormalization-group (RG) theory on the basis of an *isotropic* Hamiltonian with short-range interactions below the upper critical dimension $d^*=4$ [4] but no general proof has been given for the anisotropic case.

In this paper we study the critical behavior of systems with a spatial anisotropy of noncubic symmetry within a given (d,n) universality class. An example is an Ising ferromagnet with an isotropic nearest-neighbor (NN) coupling $J>0$ and an anisotropic next-nearest-neighbor (ANNN) coupling J' on a simple-cubic lattice. In some range of J'/J this model has the same type of critical behavior as the ordinary $(J'=0)$ Ising model. We shall show that for such systems Eq. (2) must be generalized to

$$\lim_{t\to 0+} f_s(t,0)\prod_{i=1}^{d}\xi^{(i)} = Q(d,n) = \text{universal}, \tag{3}$$

where $\xi^{(i)}=\xi_0^{(i)}t^{-\nu}$ are the correlation lengths associated with the principal directions of the anisotropic system and where $Q(d,n)$ is the same universal quantity for both isotropic and anisotropic systems. (For $d=2$, $n=1$, this is already known for the Ising model with anisotropic NN (ANN) interactions $J_x \neq J_y$ [3].) There are, in general, $d+1$ nonuniversal bulk amplitudes $\xi_0^{(1)},\ldots,\xi_0^{(d)}$, A_2 whose ratios are also nonuniversal. Note that there still exists a unique critical exponent $\nu(d,n)$ that is identical for isotropic and anisotropic systems within the same (d,n) universality class [6–10].

A different type of critical behavior exists in the so-called *strongly* anisotropic systems [11–14] where not only *amplitudes* depend on the spatial directions but also the critical exponents (e.g., $\nu_\parallel$ and $\nu_\perp$) depend on the direction. These systems do not belong to the (d,n) universality class of ordinary critical points and our analysis will not include such types of anisotropy.

While Eq. (3) is a natural generalization of Eq. (2) we shall call attention to the intriguing problem of *finite-size* effects in anisotropic systems. For simplicity we shall confine ourselves to the case of periodic boundary conditions in rectangular $L_1\times L_2\times\cdots\times L_d$ block geometries (including L^d cubic geometry and $\infty^{d-1}\times L$ film geometry). There have been several studies of this problem in the past [5,13,15–18]. We shall only briefly comment on the more complicated case of anisotropic confined systems with nonperiodic boundary conditions [17,19–23].

It has been hypothesized [5] that two-scale factor universality holds not only for *bulk* systems but also for *confined systems*, except that the finite-size scaling functions depend on the geometry and on the boundary conditions. For example, for a system in a cube of volume L^d with periodic boundary conditions, the singular part of the reduced free energy density $f_s(t,h,L)$ near bulk T_c was predicted to have the asymptotic scaling form for large L [5]

$$f_s(t,h,L) = L^{-d} Y_{cube}(C_1 t L^{1/\nu}, C_2 h L^{\beta\delta/\nu}), \tag{4}$$

where the function $Y_{cube}(x,y)$ is universal and where C_1 and C_2 are the only nonuniversal parameters. A similar ansatz was made for the correlation length $\xi_\parallel$ in an $L^{d-1}\times\infty$ cylinder [5]. As a consequence, the amplitude $Y_{cube}(0,0)$ and the Binder cumulant ratio [1,24,25]

$$U = \frac{1}{3}[(\partial^4 Y_{cube}/\partial y^4)/(\partial^2 Y_{cube}/\partial y^2)^2]_{y=0,x=0} \tag{5}$$

are predicted to be universal. (For example, they should be independent of the ratio J'/J.) The scaling form (4), if extended to realistic geometries and boundary conditions, has far-reaching consequences for measurable quantities [1,26]. In particular the prediction of a universal character of the Casimir amplitude

$$\Delta = (d-1) Y_{film}(0,0) \tag{6}$$

is of interest, e.g., for fluid [27], superfluid [28], and superconducting [29] films.

The universality of the scaling functions Y of Eqs. (4) or (6) was supposed to be valid for all systems in a given universality class [1,5] including anisotropic lattice systems provided that an appropriate rescaling of the lattice spacings (or length L) is performed [5]. This appears to be consistent with existing studies of finite-size effects in anisotropic systems where it was stated that isotropy can be restored asymptotically by an anisotropic scale transformation [11,13,16,18–21,23,30].

We have found that this picture of finite-size effects in anisotropic systems, though valid in special cases, is, in general, not correct. In the present paper we show, for periodic boundary conditions, that Eqs. (4)–(6), though valid for isotropic systems and for systems with cubic symmetry in the range $L/\xi \lesssim O(1)$ [31], are not universally valid for the anisotropic systems of the type described above (e.g., spin models with NN and ANNN interactions on simple-cubic lattices) although these systems belong to the same universality class as isotropic systems. In such anisotropic systems the finite-size scaling functions depend, in general, on additional nonuniversal parameters (apart from C_1 and C_2), even after a rescaling of the lattice spacing or of the length L. Thus, in general, two-scale factor universality and isotropy cannot be restored and the notion of a universality class is only of restricted relevance for the scaling functions of confined systems.

We shall prove our claims within the O(n) symmetric φ^4 field theory with the spatially anisotropic Hamiltonian (at $h=0$)

$$H(r_0,u_0,\Lambda;\mathbf{A};V;\varphi) = \int_V d^d x \left(\frac{r_0}{2}\varphi^2 + \sum_{\alpha,\beta}^{d} \frac{A_{\alpha\beta}}{2} \frac{\partial\varphi}{\partial x_\alpha}\frac{\partial\varphi}{\partial x_\beta} + u_0(\varphi^2)^2 \right) \tag{7}$$

for the n-component field $\varphi(\mathbf{x})$. The sum runs over the components x_α of the spatial coordinates $\mathbf{x}$, $\alpha=1,\ldots,d$. The $d\times d$ anisotropy matrix $\mathbf{A}\equiv(A_{\alpha\beta})$ is assumed to be real, symmetric, and positive definite. This model has a critical point at some value $r_0=r_{0c}(\mathbf{A};u_0,\Lambda)$ where Λ is a (sharp or smooth) cutoff in $\mathbf{k}$ space. In addition to the three parameters r_0, u_0, and Λ of the standard isotropic ($\mathbf{A}=\mathbf{1}$) model, our model has $d(d+1)/2$ nonuniversal parameters contained in the matrix $\mathbf{A}$. Below we shall argue that the nondiagonality of the anisotropy matrix $\mathbf{A}$ is a generic case of real anisotropic systems. For simplicity we assume a cubic volume, $V=L^d$, $0\leqslant x_\alpha \leqslant L$, with periodic boundary conditions.

First we prove that the model defined by Eq. (7) belongs to the same bulk universality class as the standard isotropic Landau-Ginzburg-Wilson model with $\mathbf{A}=\mathbf{1}$. The characteristic properties of the matrix $\mathbf{A}$ are described in terms of the d eigenvalues $\lambda_i>0$ and eigenvectors $\mathbf{e}_i$ defined by $\mathbf{A}\mathbf{e}_i=\lambda_i\mathbf{e}_i$. A rotation by the orthogonal matrix $\mathbf{U}$ yields the diagonal matrix $\mathbf{U}\mathbf{A}\mathbf{U}^{-1}=\boldsymbol{\lambda}$ with diagonal elements λ_i. After the transformation of the spatial coordinates

$$\mathbf{x}' = \boldsymbol{\lambda}^{-1/2}\mathbf{U}\mathbf{x} \tag{8}$$

and of the field

$$\varphi'(\mathbf{x}') = (\det \mathbf{A})^{1/4}\varphi(\mathbf{U}^{-1}\boldsymbol{\lambda}^{1/2}\mathbf{x}'), \tag{9}$$

$$\det \mathbf{A} = \prod_{i=1}^{d} \lambda_i > 0, \tag{10}$$

the Hamiltonian (7) becomes

$$H(r_0,u_0,\Lambda;\mathbf{A};V;\varphi) = H'(r_0,u_0',\Lambda';V';\varphi') \tag{11}$$

$$= \int_{V'} d^d x' \left(\frac{r_0}{2}\varphi'(\mathbf{x}')^2 + \frac{1}{2}(\boldsymbol{\nabla}'\varphi')^2 + u_0'(\varphi'^2)^2 \right) \tag{12}$$

with the changed four-point coupling

$$u_0' = (\det \mathbf{A})^{-1/2} u_0, \tag{13}$$

with the changed (noncubic) volume

$$V' = \prod_{i=1}^{d} L_i' = (\det \mathbf{A})^{-1/2} V, \tag{14}$$

$$L_i' = L\lambda_i^{-1/2}, \tag{15}$$

with a transformed cutoff Λ' in $\mathbf{k}'$ space, $\mathbf{k}'=\boldsymbol{\lambda}^{1/2}\mathbf{U}\mathbf{k}$, and with a critical point at

$$r'_{0c}(u'_0,\Lambda') = r_{0c}(\mathbf{A};u_0,\Lambda). \quad (16)$$

The temperature variable $r_0 - r_{0c} = r_0 - r'_{0c} = a_0 t$ remains invariant under the transformation (8) and (9).

According to Eq. (12), the bulk critical behavior of the *anisotropic* model H with the coupling u_0, Eq. (7), can be calculated within the minimally renormalized *isotropic* bulk theory $(V' \to \infty, \Lambda' \to \infty)$ for H' with the coupling u'_0 in $2 < d < 4$ dimensions [32], provided that $u'_0 > 0$. Specifically, the renormalized quantities of the Hamiltonian H' are defined as

$$u' = \mu^{-\varepsilon} Z_{u'}^{-1} Z_{\varphi'}^{2} A_d u'_0, \quad (17)$$

$$\varphi'_R = Z_{\varphi'}^{-1/2} \varphi', \quad (18)$$

$$r = Z_r^{-1}(r_0 - r'_{0c}) \quad (19)$$

with $A_d = \Gamma(3-d/2) 2^{2-d} \pi^{-d/2} (d-2)^{-1}$ and

$$r'_{0c} = (u'_0)^{2/\varepsilon} S(\varepsilon), \quad (20)$$

$\varepsilon = 4-d$, where $S(\varepsilon)$ and the Z factors $Z_i(u',\varepsilon)$ depend on ε and u' in the same way as they depend on ε and u in the standard $(\mathbf{A}=\mathbf{1}, V\to\infty, \Lambda\to\infty)$ theory [32], with an identical fixed point value $u'^* = u^*$. This statement applies also to the field-theoretic functions $\zeta_r(u')$ and $\zeta_{\varphi'}(u')$ which determine the critical exponents ν and η. This proves that the critical behavior of H and H' belongs to the same universality class in the whole range of $\mathbf{A}$ where det $\mathbf{A} > 0$.

Our model, Eq. (7) with $\mathbf{A} \neq c_0 \mathbf{1}$, can be considered as the continuum version of a φ^4 lattice Hamiltonian $H_{lattice}$ with short-range interactions J_{ij} [see, e.g., Eq. (50) below for a lattice model with a single lattice constant $\tilde{a}$]. Noncubic anisotropies may arise either from a noncubic lattice structure or from noncubic interactions on a cubic lattice [as an example see Eq. (51) below] or from both types of anisotropies. In some range of $\mathbf{A}$ near $\mathbf{A} \approx c_0 \mathbf{1}$ with $c_0 > 0$, $H_{lattice}$ and H belong to the same universality class. Note, however, that in general $r_{0c,lattice}(J_{ij};u_0,\tilde{a}) \neq r_{0c}(\mathbf{A};u_0,\Lambda)$.

In order to elucidate the effect of the nondiagonality of the anisotropy matrix $\mathbf{A}$ we first discuss the bulk order-parameter correlation function for $T \geq T_c$

$$G(\mathbf{x};\mathbf{A},u_0) \equiv \langle \varphi(\mathbf{x}) \varphi(0) \rangle_H, \quad (21)$$

where $\langle \cdots \rangle_H$ means an average with the exponential weight e^{-H}. Equations (8), (9), and (12) imply

$$G(\mathbf{x};\mathbf{A},u_0) = (\det \mathbf{A})^{-1/2} G'(\mathbf{x}';u'_0), \quad (22)$$

where

$$G'(\mathbf{x}';u'_0) \equiv \langle \varphi'(\mathbf{x}') \varphi'(0) \rangle_{H'}. \quad (23)$$

The second-moment bulk correlation length $\xi'(u'_0)$ associated with H' is defined by

$$\xi'(u'_0) = \left(\frac{1}{2d} \lim_{V'\to\infty} \frac{\int d^d x' \, \mathbf{x}'^2 G'(\mathbf{x}';u'_0)}{\int d^d x' \, G'(\mathbf{x}';u'_0)} \right)^{1/2}. \quad (24)$$

For $T \geq T_c$ and $|\mathbf{x}'|/\xi' \lesssim O(1)$ the asymptotic scaling form of $G'(\mathbf{x}';u'_0)$ reads [1,5] for $|\mathbf{x}'| \gg \Lambda'^{-1}, \xi' \gg \Lambda'^{-1}$,

$$G'(\mathbf{x}';u'_0,) = A_G |\mathbf{x}'|^{-d+2-\eta} \Phi(|\mathbf{x}'|/\xi') \quad (25)$$

with a universal scaling function Φ, a nonuniversal amplitude $A_G(u'_0,\Lambda')$, and with $\xi' = \xi'_0(u'_0) t^{-\nu}$, apart from corrections to scaling. Equations (8), (22), and (25) imply asymptotically

$$G(\mathbf{x};\mathbf{A},u_0) = A'_G |\boldsymbol{\lambda}^{-1/2} \mathbf{U}\mathbf{x}|^{-d+2-\eta} \Phi(|\boldsymbol{\lambda}^{-1/2} \mathbf{U}\mathbf{x}|/\xi') \quad (26)$$

with $A'_G = A_G (\det \mathbf{A})^{-1/2}$. Thus the anisotropy does not change the universal structure of the scaling *function* Φ but makes the scaling *argument* of Φ and the spatial behavior of G anisotropic, even right at $T_c(\mathbf{A})$ (see also [7–9]).

Choosing $\mathbf{x} = x_i \mathbf{e}_i$ along the principal direction $i, i = 1, \cdots, d$ defined by the eigenvector $\mathbf{e}_i$, we have $(\mathbf{U}\mathbf{x})_j = x_i \delta_{ij}$ and

$$G(x_i \mathbf{e}_i;\mathbf{A},u_0) = A'_G (|x_i|/\lambda_i^{1/2})^{-d+2-\eta} \Phi(|x_i|/\xi^{(i)}), \quad (27)$$

where

$$\xi^{(i)}(\mathbf{A},u_0) = \xi_0^{(i)} t^{-\nu} \quad (28)$$

are the *principal correlation lengths* of the anisotropic system with the nonuniversal amplitudes

$$\xi_0^{(i)}(\mathbf{A},u_0) = \lambda_i^{1/2} \xi'_0(u'_0). \quad (29)$$

(The amplitudes ξ'_0 and $\xi_0^{(i)}$ may depend, in general, also on the cutoff.) Their product

$$V_{corr}(\mathbf{A}) = \prod_{i=1}^{d} \xi^{(i)} \quad (30)$$

constitutes the appropriate measure of the correlation volume whose shape is ellipsoidal rather than spherical. This is seen by determining the singular part $F_s(t;\mathbf{A},u_0)/Vk_BT \equiv f_s(t;\mathbf{A},u_0)$ of the bulk free energy density $f = -\lim_{V\to\infty} V^{-1} \ln \int \mathcal{D}\varphi e^{-H}$ of the anisotropic system. Using Eqs. (10), (11), (14), and (15) we obtain

$$f_s(t;\mathbf{A},u_0) = (\det \mathbf{A})^{-1/2} f'_s(t;u'_0), \quad (31)$$

where $f'_s(t;u'_0)$ is the singular part of the bulk free energy density $f' = -\lim_{V'\to\infty} V'^{-1} \ln \int \mathcal{D}\varphi' e^{-H'}$ associated with H', Eq. (12). Together with Eq. (2) for the isotropic system, Eqs. (10), (14), and (28)–(31) lead to

$$\lim_{t\to 0+} f_s(t;\mathbf{A},u_0) V_{corr}(\mathbf{A}) = Q(d,n) = \text{universal}, \quad (32)$$

which is identical with Eq. (3).

From Eqs. (26)–(29) we see that a complete knowledge of the asymptotic behavior of the correlation function G requires the knowledge of the $d+1$ nonuniversal amplitudes A'_G and $\xi_0^{(i)}$ and of the $d(d-1)/2$ nonuniversal parameters characterizing the directions of the d eigenvectors $\mathbf{e}_i$. For real magnetic materials these quantities are unknown as they depend on all microscopic details. Furthermore, real magnetic materials may have lattice structures and anisotropic interactions (e.g., ANN, ANNN, and third ANN interactions) corresponding to a nondiagonal matrix $\mathbf{A}$. It is because of the nondiagonality of $\mathbf{A}$ that both a scale transformation and a rotation are necessary and that a simple rescaling of d amplitudes is not sufficient. Clearly two-scale factor universality is absent in the bulk correlation functions of such anisotropic systems (e.g., metamagnets [33]) although they belong to the same universality class as isotropic systems (e.g., fluids).

While the anisotropy does not destroy the universality of the scaling function Φ of the *bulk* correlation function G (in the nonexponential regime $r/\xi \lesssim O(1)$ [2]), a fundamental complication arises for *confined* systems since, in general, the principal directions $\mathbf{e}_i$ of the intrinsic anisotropy are totally unrelated to the orientation of the surfaces of the confining geometry (e.g., $L_1 \times L_2 \times \cdots \times L_d$ rectangular geometry). This introduces a source of nonuniversality that cannot be absorbed only by a transformation of the lengths L_i of the confining geometry or of the scaling argument. Within our model (7), a complete information of this source of nonuniversality requires, at $h=0$, the knowledge of $d+d(d-1)/2 = d(d+1)/2$ nonuniversal parameters (rather than d parameters). Within this model we shall show that this implies not only the absence of two-scale factor universality but the absence of universality itself for all finite-size scaling functions and finite-size amplitude ratios of anisotropic systems with noncubic symmetry. *In particular, two-scale factor universality and isotropy cannot be restored by an anisotropic scale transformation for confined systems in rectangular geometries with a nondiagonal anisotropy matrix* $\mathbf{A}$. This is the central general result of this paper to be demonstrated in the following on the basis of exact results in the large-n limit and of one-loop RG results for $n=1$, 2, 3.

First we consider the susceptibility χ (per component) of the field-theoretic model (7) above T_c in a finite cube with periodic boundary conditions. In the limit $n\to\infty$ at fixed $u_0 n$ it is determined by [34]

$$\chi^{-1} = r_0 + 4u_0 n L^{-d} \sum_{\mathbf{k}} (\chi^{-1} + \mathbf{k}\cdot\mathbf{A}\mathbf{k})^{-1} \tag{33}$$

with $\mathbf{k}\cdot\mathbf{A}\mathbf{k} \equiv \Sigma^d_{\alpha,\beta} A_{\alpha\beta} k_\alpha k_\beta$. The sum $\Sigma_{\mathbf{k}}$ runs over $\mathbf{k}$ vectors with components $k_\alpha = 2\pi m_\alpha / L, m_\alpha = 0, \pm 1, \ldots$ up to some cutoff Λ. For $2<d<4$ the asymptotic form of the correlation length ξ' defined by Eq. (24) is $\xi' = \xi'_0 t^{1/(2-d)}$ with

$$\xi'_0 = (4u'_0 n A_d a_0^{-1}/\varepsilon)^{1/(d-2)}. \tag{34}$$

For large $L \gg \Lambda^{-1}$ and small $0 \leqslant t \ll 1$ we find the asymptotic scaling form for $L'/\xi' \lesssim O(1)$

$$\chi(t,L;\mathbf{A}) = L'^{\gamma/\nu} g_{cube}(L'/\xi';\overline{\mathbf{A}}), \quad \gamma/\nu = 2, \tag{35}$$

with the rescaled length

$$L' = L(\det \mathbf{A})^{-1/2d} \tag{36}$$

and the normalized anisotropy matrix

$$\overline{\mathbf{A}} = \mathbf{A}/(\det \mathbf{A})^{1/d}, \tag{37}$$

where $g_{cube}(x;\overline{\mathbf{A}})$ is determined implicitly by

$$x^{d-2} - g_{cube}^{(2-d)/2} = (4-d) A_d^{-1} I_1(g_{cube}^{-1};\overline{\mathbf{A}}), \tag{38}$$

$$I_j(z;\overline{\mathbf{A}}) = \int_0^\infty ds (4\pi^2)^{-j} s^{j-1} P(s,\overline{\mathbf{A}}) e^{-zs/4\pi^2}, \tag{39}$$

with

$$P(s,\overline{\mathbf{A}}) = (\pi/s)^{d/2} - \sum_{\mathbf{m}} e^{-\mathbf{m}\cdot\overline{\mathbf{A}}\mathbf{m}s}. \tag{40}$$

The sum $\Sigma_{\mathbf{m}}$ runs over $\mathbf{m} = (m_1, \ldots, m_d)$ with all integers $m_\alpha = 0, \pm 1, \ldots$. For $\overline{\mathbf{A}} = \mathbf{1}, g_{cube}(x;\mathbf{1}) \equiv g_{cube,iso}(x)$ is the known scaling function of the isotropic case [34]. For $\overline{\mathbf{A}} \neq \mathbf{1}$, however, $g_{cube}(x;\overline{\mathbf{A}})$ is nonuniversal and depends on $\overline{\mathbf{A}}$ in a highly complicated way via the inhomogeneous $\mathbf{m} \neq \mathbf{0}$ modes, even after having introduced the rescaled length L', Eq. (36). The effect of these modes depends on the orientation of the eigenvectors $\mathbf{e}_i$ relative to the shape of the confining geometry. In general this anisotropy effect cannot be inferred from the knowledge of finite-size scaling functions of isotropic systems of the same universality class and cannot be described by a transformation of the argument x of $g_{cube,iso}(x)$ (unlike the case for the scaling function Φ of the bulk correlation function G) or by a rescaling of L.

Only in the special cases where $\mathbf{A} = \boldsymbol{\lambda}$ is diagonal at the outset and where the eigenvectors $\mathbf{e}_i$ happen to be parallel to the edges of the confining cube, the finite-size scaling function of the *anisotropic* system in a cubic geometry can be reexpressed in terms of the scaling function of the *isotropic* system in a $L'_1 \times \cdots \times L'_d$ block geometry, $L'_i = L\lambda_i^{-1/2}$. Such special cases with a diagonal matrix $\mathbf{A}$ are $d=2$ or $d=3$ spin models on sc cubic lattices with only NN couplings $J_x \neq J_y$ [3,13,23] or $J_x \neq J_y \neq J_z$ [18], respectively.

We note that a conclusive answer about the appropriate way of rescaling the length L cannot be inferred only on the basis of the result of $\chi(0,L;\mathbf{A})$ at T_c, without further knowledge. The same statement applies to the correlation length $\xi_\parallel(0,L;\mathbf{A})$ in a $L^{d-1}\times\infty$ cylinder. It would always be possible to rewrite χ at T_c in the form

$$\chi(0,L;\mathbf{A}) = \hat{L}^{\gamma/\nu} g_{cube,iso}(0) \tag{41}$$

with the amplitude $g_{cube,iso}(0)$ of the *isotropic* system if all anisotropy effects are formally absorbed in the length

$$\hat{L} = L'[g_{cube}(0;\overline{\mathbf{A}})/g_{cube,iso}(0)]^{\nu/\gamma}. \tag{42}$$

But after the calculation of a different physical quantity at T_c it becomes obvious that this length $\hat{L}$ is inappropriate as will be demonstrated in the following.

Next we present the anisotropy effect on the finite-size scaling function of the singular part of the reduced free energy density per component in the large-n limit for cubic geometry and periodic boundary conditions. For $L \gg \Lambda^{-1}$, $0 \leqslant t \ll 1$, $L'/\xi' \lesssim O(1)$ we find

$$f_s(t,L;\mathbf{A}) = L^{-d} Y_{cube}(L'/\xi';\overline{\mathbf{A}}), \tag{43}$$

$$Y_{cube}(x;\bar{\mathbf{A}}) = -\frac{\ln 2}{2} + \frac{(d-2)A_d}{2d(4-d)}[g(x;\bar{\mathbf{A}})]^{-d/2} + \frac{1}{8\pi^2}\int_0^\infty ds\left(\frac{4\pi^2}{s} + \frac{1}{g(x;\bar{\mathbf{A}})}\right)P(s,\bar{\mathbf{A}})e^{-s/(4\pi^2 g)}, \quad (44)$$

where $g(x;\bar{\mathbf{A}}) \equiv g_{cube}(x;\bar{\mathbf{A}})$ is determined implicitly by Eqs. (38)–(40). The scaling function $Y_{cube}(x;\bar{\mathbf{A}})$, including the amplitude $Y_{cube}(0;\bar{\mathbf{A}})$, is nonuniversal. Only on the level of a lowest-mode ($\mathbf{k}=\mathbf{0}$) approximation in Eq. (33) does the explicit dependence of Y_{cube} on $\bar{\mathbf{A}}$ disappear. The effect of the $\mathbf{m} \neq \mathbf{0}$ modes cannot be described simply by a transformation of the scaling variable x of $Y_{cube}(x;\mathbf{1}) \equiv Y_{cube,iso}(x)$ of the isotropic case and it depends on $d(d+1)/2-1$ nonuniversal parameters contained in $\bar{\mathbf{A}}$. [Equivalent parameters appear already in G, Eq. (26).] This holds, of course, also for the relevant case of general finite $n<\infty$ as can be shown [35] within a one-loop RG calculation for the model (7). The exact scaling function $Y_{cube}(x;\bar{\mathbf{A}})$ for general n remains unknown even if the exact scaling function $Y_{cube,iso}(x)$ were given for general n and if the exact matrix $\bar{\mathbf{A}}$ were given for a special anisotropic system.

We note that the same rescaled length L', Eq. (36), is employed in the scaling argument L'/ξ' of Y_{cube} as in g_{cube} but not in the leading L^{-d} power law of Eq. (43). At $T=T_c$, it would of course be possible to rewrite f_s in the form

$$f_s(0,L;\mathbf{A}) = \bar{L}^{-d} Y_{cube,iso}(0) \quad (45)$$

with the amplitude $Y_{cube,iso}(0)$ of the *isotropic* system if the anisotropy effect is formally absorbed in the length

$$\bar{L} = L[Y_{cube}(0;\bar{\mathbf{A}})/Y_{cube,iso}(0)]^{-1/d}. \quad (46)$$

This length $\bar{L}$ differs, however, from the length $\hat{L}$, Eq. (42), introduced formally for the susceptibility $\chi(0,L;\mathbf{A})$.

As seen from our results for $\chi(t,L;\mathbf{A})$ and $f_s(t,L;\mathbf{A})$, a possible ambiguity of defining a rescaled length disappears after calculating the complete temperature dependence of the finite-size scaling functions of the anisotropic system. At the same time such results clarify whether or not isotropy can be restored by a scale transformation. The exact analytic form of our results (35) and (43) for $T \geq T_c$ unambiguously answers this question for cubic geometry and periodic boundary conditions. An extension of our results to rectangular $L_1 \times L_2 \times \cdots \times L_d$ block geometry [35] confirms our findings, i.e., even after a rescaling of the lengths L_i the finite-size scaling functions remain nonuniversal for systems with a nondiagonal matrix $\mathbf{A}$.

We conclude that, for rectangular geometry and periodic boundary conditions, finite-size scaling functions are, in general, *not* universally determined only by the bulk universality class but do depend on nonuniversal parameters in a highly complicated way if the system is anisotropic in the sense specified above. In particular, within our model (7), if the matrix $\mathbf{A}$ is nondiagonal, isotropy cannot be restored by a rescaling of lengths [36].

We expect that this conclusion holds also for nonperiodic boundary conditions and for nonrectangular geometries. For example, we expect that the universality of the amplitude u of the "corner" term $uL^{-d}\ln L$ of the $d=2$ and $d=3$ free energy density for free boundary conditions at T_c [37,38] is not generally valid for anisotropic systems. The universality of u was proven in [37] only for *isotropic* ($d=2$) systems whereas in [38] it was supposed to be valid "within a given RG universality class." Furthermore, there have been calculations [19–21,23] of edge exponents of anisotropic spin models in wedge geometries with free boundary conditions. It was found that the anisotropy enters explicitly into the exponents and that it was possible to rescale lengths anisotropically to bring the problem into an isotropic form. We expect, however, that this is, in general, not possible for the temperature-dependent finite-size scaling functions of lattice systems with edges whose continuum limit yields an effective Hamiltonian of the form of Eq. (7) with a *nondiagonal* matrix $\mathbf{A}$.

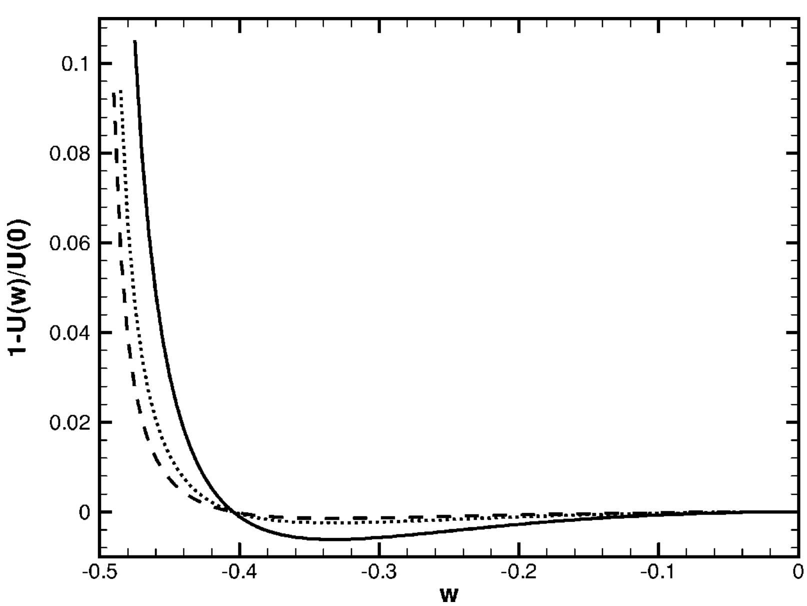

FIG. 1. Cumulant ratio $1-U(w)/U(0)$ vs coupling ratio $w=J'/(J+2J')$ of the field-theoretic model, Eq. (7), in three dimensions for $n=1$, 2, 3 (solid, dotted, dashed lines) according to Eqs. (53)–(57).

We briefly extend our analysis to $\infty^{d-1}\times L$ film geometry with periodic boundary conditions, with L being the thickness in the dth direction. In the large-n limit we find

$$f_{s,film}(t,L;\mathbf{A}) = L^{-d}[(\overline{\mathbf{A}}^{-1})_{dd}]^{-d/2}Y_{film,iso}(\tilde{x}), \tag{47}$$

where $Y_{film,iso}$ is the scaling function for the *isotropic* system, with a transformed argument $\tilde{x}=\tilde{L}/\xi'$,

$$\tilde{L} = [(\mathbf{A}^{-1})_{dd}]^{1/2}L \tag{48}$$

and where $(\mathbf{A}^{-1})_{dd}$ and $(\overline{\mathbf{A}}^{-1})_{dd}$ are the dth diagonal elements of the inverse of $\mathbf{A}$ and $\overline{\mathbf{A}}$, respectively [39]. In contrast with Eq. (4), a nonuniversal amplitude appears at bulk T_c and the Casimir amplitude

$$\Delta = (d-1)[(\overline{\mathbf{A}}^{-1})_{dd}]^{-d/2}Y_{film,iso}(0) \tag{49}$$

is nonuniversal. The simplicity of this anisotropy effect is due to the one-loop structure of diagrams contributing to the large-n limit. From finite-size theory at order u_0^2 [40] we infer a highly complicated $\overline{\mathbf{A}}$ dependence of $f_{s,film}$ for finite n. Furthermore we expect that the amplitudes [41] and scaling functions [42] of density profiles in film geometry are nonuniversal for anisotropic systems with noncubic symmetry. More generally, our results suggest that the feature of universality in the theory of boundary critical phenomena [43–45] as well as the notion of a "surface universality class" and of "(2+1)-scale factor universality" [45] need to be reconsidered for the case of anisotropic systems.

It would also be interesting to interpret finite-size effects in percolation problems of anisotropic systems [17,22] in the light of the results of the present paper.

We illustrate our theory by the example of the Binder cumulant ratio U for $L\to\infty$ at T_c, Eq. (5). We consider a φ^4 lattice model

$$H_{lattice} = \tilde{a}^d\left[\sum_i\left(\frac{r_0}{2}\varphi_i^2 + u_0(\varphi_i^2)^2\right) + \sum_{i,j}\frac{J_{ij}}{2\tilde{a}^2}(\varphi_i-\varphi_j)^2\right] \tag{50}$$

with an isotropic ferromagnetic interaction $J_{ij}=J>0$ between nearest neighbors but an anisotropic interaction $J_{ij}=J'$ with only six (rather than 12) next-nearest neighbors in the $+-(1,1,0)$, $+-(1,0,1)$, and $+-(0,1,1)$ directions on a simple-cubic lattice with a lattice constant $\tilde{a}$ in a cube with periodic boundary conditions. It is expected that a ferromagnetic critical point exists not only for $J>0$, $J'\geqslant 0$ but also for $J>0$, $J'<0$. In the continuum limit $(\tilde{a}\to 0)$ this model is reduced to Eq. (7) with

$$\mathbf{A} = c_0\begin{pmatrix}1 & w & w\\ w & 1 & w\\ w & w & 1\end{pmatrix}, \tag{51}$$

where $w=J'/(J+2J')\leqslant\frac{1}{2}$ and $c_0=2(J+2J')>0$. (Note that the matrix $\mathbf{A}$ is diagonal for a model with isotropic NNN interactions.) The positivity of c_0 requires $J'>-J/2$. For $w\neq 0$ the eigenvectors $\mathbf{e}_i$ are not parallel to the cubic axes. The constant c_0 can be absorbed in the bulk amplitude ξ_0' of ξ', Eq. (24), and does not appear in

$$\overline{\mathbf{A}}(w) = (1-3w^2+2w^3)^{-1/3}\begin{pmatrix}1 & w & w\\ w & 1 & w\\ w & w & 1\end{pmatrix}. \tag{52}$$

One of the eigenvalues of $\mathbf{A}$ vanishes at $w_c=-\frac{1}{2}$, i.e., $J'=-J/4$ (the two other eigenvalues vanish at $w=1$, $J'=-J$). Thus w may vary in the range $-\frac{1}{2}<w\leqslant\frac{1}{2}$ corresponding to a line of ferromagnetic critical points $T_c(w)$ terminating at a Lifshitz point $T_c(w_c)$ of the φ^4 continuum model (7) [but not necessarily of the φ^4 lattice model (50) whose line of critical points $T_c(w)$ may end at a value of w different from $-\frac{1}{2}$].

From a RG treatment of the model (7) within the minimal renormalization scheme in three dimensions [32] parallel to previous work [46] we obtain $U(w)$ for $L\to\infty$ at $T_c(w)$ in one-loop order for $n=1$ as

$$U(w) = 1 - \tfrac{1}{3}\vartheta_4(\tilde{Y})[\vartheta_2(\tilde{Y})]^{-2}, \tag{53}$$

where

$$\vartheta_m(\tilde{Y}) = \frac{\int_0^\infty ds\, s^m \exp\left(-\frac{1}{2}\tilde{Y}s^2 - s^4\right)}{\int_0^\infty ds\, \exp\left(-\frac{1}{2}\tilde{Y}s^2 - s^4\right)}. \tag{54}$$

Here the quantity $\tilde{Y}$ depends on w through $\overline{\mathbf{A}}(w)$,

$$\tilde{Y} = -b\left(\frac{4\pi}{\tilde{l}}[\tilde{l}^2 + I_1(\tilde{l}^2;\overline{\mathbf{A}})] + \frac{1}{2} + 4\pi\tilde{l}[\tilde{l}^4 + I_2(\tilde{l}^2;\overline{\mathbf{A}})]\right), \tag{55}$$

with

$$b = 144u'^*\vartheta_2(0), \tag{56}$$

$$\tilde{l} = [24\pi^{1/2}u'^{*1/2}\vartheta_2(0)]^{2/3}, \tag{57}$$

and $u'^*=u^*=0.0412$ where $I_j(z;\overline{\mathbf{A}})$ is given by Eq. (39). Clearly there is no way of eliminating the complicated *internal* dependence on the anisotropy matrix $\overline{\mathbf{A}}$ in Eq. (55); thus isotropy cannot be restored by means of a scale transformation.

We have also extended this result to general n [35]. While the w dependence is weak for $-0.4\lesssim w\leqslant\frac{1}{2}$ it becomes appreciable upon approaching $w_c=-\frac{1}{2}$, as shown in Fig. 1 for $n=1$, 2, 3. This proves the nonuniversality of $U(w)$. Similarly one can derive a w dependence of the Casimir amplitude $\Delta(w)$ and of other scaling functions. Note, however, that because of the *nonuniversal character* of $U(w)$ and $\Delta(w)$, these quantities may, in principle, differ, e.g., for the $(d=3,n=1)$ field-theoretic model [Eq. (7) with the matrix (51)], and the $(d=3,n=1)$ Ising model (with NN and ANNN couplings) even if the geometries and the boundary conditions are the same in both models.

This kind of nonuniversal finite-size effect should exist near critical points of real systems and should be detectable in Monte Carlo simulations of $d=2$ and $d=3$ spin models.

Support by NNSFC, by Max-Planck-Gesellschaft, by DLR, and by NASA is acknowledged.

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