Proceedings of the 9th International Conference

# PATH INTEGRALS

## NEW TRENDS AND PERSPECTIVES

Dresden, Germany September 23 – 28, 2007

*editors*

**Wolfhard Janke**

*Universität Leipzig, Germany*

**Axel Pelster**

*Universität Duisburg-Essen, Germany*

**World Scientific**

NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI

# NONUNIVERSAL FINITE-SIZE EFFECTS NEAR CRITICAL POINTS

V. DOHM

*Institute for Theoretical Physics, RWTH Aachen University,*
*D-52056 Aachen, Germany*
*E-mail: vdohm@physik.rwth-aachen.de*

We study the finite-size critical behavior of the anisotropic $\varphi^4$ lattice model with periodic boundary conditions in a $d$-dimensional hypercubic geometry above, at, and below $T_c$. Our perturbation approach at fixed $d = 3$ 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)]. 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. 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 *anti-ferromagnetic* NNN coupling and the existence of a Lifshitz point at a larger value of this coupling. 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.

*Keywords*: Anisotropy; Excess free energy; Binder cumulant; Finite-size scaling; Universality; Monte Carlo simulation; Ising model.

## 1. Introduction

A major achievement of the renormalization-group (RG) theory is the proof that the *bulk* critical behavior of thermodynamic quantities has the property of scaling and two-scale factor universality.[1] This is summarized by the asymptotic (small reduced temperature $t = (T - T_c)/T_c$, small ordering field $h$) scaling form of the singular part of the bulk free energy density

$$f_{s,b}(t,h) = A_1|t|^{d\nu}\, W_{\pm}(A_2 h|t|^{-\beta\delta}) \tag{1}$$

with universal critical exponents $\nu, \beta, \delta$ and the universal scaling function $W_{\pm}(z)$ above $(+)$ and below $(-)$ $T_c$. Equation (1) is valid for both isotropic and anisotropic systems below $d = 4$ dimensions. For *confined* systems with a characteristic length $L$, two-scale factor universality is no longer valid if the system is spatially anisotropic as described by a $d \times d$ anisotropy matrix $\mathbf{A}$.[2,3] This is summarized by the asymptotic (large $L$, small $t$, small $h$) finite-size scaling form[4] of the singular part of the free energy density

$$f_s(t,h,L) \;=\; L^{-d}\,\mathcal{F}(C_1' t L'^{1/\nu}, C_2' h' L'^{\beta\delta/\nu}; \bar{\mathbf{A}})\,, \tag{2}$$

with the finite-size scaling function $\mathcal{F}$ where $L' = L(\det\mathbf{A})^{-1/(2d)}$, $h' = h(\det\mathbf{A})^{1/4}$, and with the reduced anisotropy matrix $\bar{\mathbf{A}} = \mathbf{A}/(\det\mathbf{A})^{1/d}$, $\det\mathbf{A} > 0$. In the isotropic case, $\mathbf{A} = c_0\mathbf{1}$ and $\bar{\mathbf{A}} = \mathbf{1}$. In addition to the two nonuniversal amplitudes $C_1', C_2'$, the matrix $\bar{\mathbf{A}}$ contains up to $d(d+1)/2-1$ nonuniversal anisotropy parameters. As a consequence of (2), the critical amplitude $\mathcal{F}(0,0;\bar{\mathbf{A}})$, the critical Binder cumulant[1,5]

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

and the critical amplitude of the thermodynamic Casimir force are nonuniversal as well. In this contribution we report very recent results[4] on $\mathcal{F}(\tilde{x},0;\bar{\mathbf{A}})$ and $U(\bar{\mathbf{A}})$ based on RG finite-size perturbation theory at fixed $d=3$ . We shall also mention briefly nonuniversal effects on the *bulk* order-parameter correlation function and nonuniversal finite-size effects due to subleading long-range (van der Waals type) interactions in isotropic systems. This diversity of asymptotic critical behavior[4] suggests to distinguish subclasses of interactions within a universality class (see Fig. 1).

## 2. Anisotropic $\varphi^4$ Lattice Model

We consider the $O(n)$ symmetric $\varphi^4$ lattice Hamiltonian

$$H = \tilde{a}^d\left[\sum_{i=1}^{N}\left(\frac{r_0}{2}\varphi_i^2 + u_0(\varphi_i^2)^2 - h\varphi_i\right) + \sum_{i,j=1}^{N}\frac{K_{i,j}}{2}(\varphi_i-\varphi_j)^2\right] \tag{4}$$

on a simple-cubic lattice with lattice constant $\tilde{a}$ in a hypercubic geometry with volume $V = L^d$ and with periodic boundary conditions. For simplicity we assume $n=1$. A variety of anisotropies may arise through the couplings $K_{i,j}$. They manifest themselves on macroscopic length scales via the $d\times d$ anisotropy matrix $\mathbf{A} = (A_{\alpha\beta})$ as given by the second moments[3]

$$A_{\alpha\beta} = A_{\beta\alpha} = N^{-1}\sum_{i,j=1}^{N}(x_{i\alpha}-x_{j\alpha})(x_{i\beta}-x_{j\beta})K_{i,j}\,, \tag{5}$$

where $x_{i\alpha}$ are the components of the lattice points $\mathbf{x}_i$.

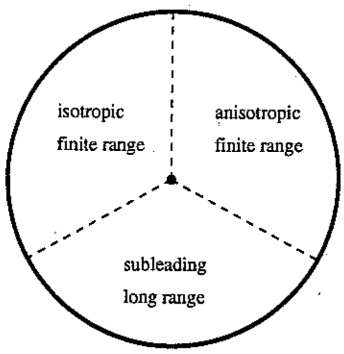


Fig. 1. Schematic representation of subclasses of systems with different types of interactions within a universality class. The subclasses have the same critical exponents and the same thermodynamic bulk scaling functions but, for given geometry and boundary conditions, different finite-size scaling functions, different bulk correlation functions, different bulk amplitude relations,[3] and a different number of nonuniversal parameters entering the asymptotic critical behavior.

As an example we consider isotropic NN couplings $K > 0$ and an anisotropic NNN coupling $J \neq 0$ in the $x - y$ planes, and an additional NN coupling $K_0 > 0$ in the $z$ direction (see Fig. 2 (b)). The corresponding anisotropy matrix is

$$\mathbf{A} = 2\tilde{a}^2 \begin{pmatrix} K+J & J & 0 \\ J & K+J & 0 \\ 0 & 0 & K_0 \end{pmatrix} . \qquad (6)$$

The matrix $\mathbf{A}$ enters the long-wavelength form of

$$\delta\widehat{K}(\mathbf{k}) = 2[\widehat{K}(\mathbf{k}) - \widehat{K}(\mathbf{0})] = \sum_{\alpha,\beta=1}^{d} A_{\alpha\beta}\, k_\alpha k_\beta + O(k^4) \qquad (7)$$

where $\widehat{K}(\mathbf{k})$ is the Fourier transform of the interaction $K_{i,j}$

$$\widehat{K}(\mathbf{k}) = N^{-1} \sum_{i,j} e^{-i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)} K(\mathbf{x}_i - \mathbf{x}_j) . \qquad (8)$$

In perturbation theory, $r_0 + \delta\widehat{K}(\mathbf{k})$ plays the role of an inverse propagator.

A characteristic feature of spatial anisotropy with non-cubic symmetry is the fact that there exists no unique bulk (second-moment) correlation length $\xi_\pm$ above and below $T_c$ but rather $d$ different correlation lengths $\xi_\pm^{(\alpha)}$ in the directions $\alpha = 1, ..., d$ of the $d$ principal axes. Such systems still have a single correlation-length exponent $\nu$ provided that $\det \mathbf{A} > 0$.

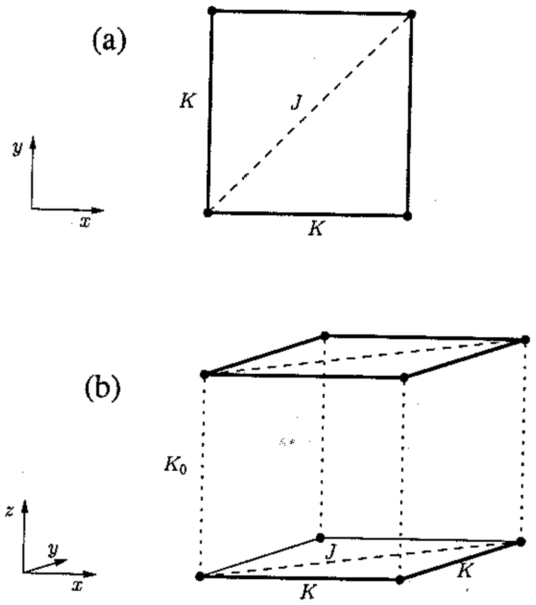


Fig. 2. Lattice points of (*a*) a square lattice, (*b*) a simple-cubic lattice, with isotropic NN couplings $K_x = K_y = K$ (solid lines), with an anisotropic NNN coupling $J$ in the $x-y$ planes (dashed lines), and a NN coupling $K_0$ in the $z$-direction (dotted lines). The corresponding anisotropic matrix $\mathbf{A}$ is given by Eq. (6).

## 3. Perturbation Approach

There exist three different types of finite-size critical behavior of $f_s$: (a) an exponential $L$ dependence for large $L/\xi_+^{(\alpha)} \gg 1$ at fixed temperature $T > T_c$, (b) the power-law behavior $\sim L^{-d}$ for large $L$ at fixed $L/\xi_\pm^{(\alpha)}$ ,$0 \leq L/\xi_\pm^{(\alpha)} \lesssim O(1)$, above, at and below $T_c$, (c) an exponential $L$ dependence for large $L/\xi_-^{(\alpha)} \gg 1$ at fixed temperature $T < T_c$. For the cases (a) and (c), ordinary perturbation theory with respect to $u_0$ is sufficient. For the case (b), a separation of the lowest mode and a perturbation treatment of the higher modes is necessary.[7–11] The case (b) corresponds to the central finite-size region above the dashed lines in Fig. 3. The cases (a) and (c) correspond to the regions below the dashed line. The latter regions are further divided[4] into a scaling region and a non-scaling region. The existence of the non-scaling region (shaded region in Fig. 3) has the following consequence. Unlike the bulk scaling function $W_\pm(z)$, (1), that is valid in the entire range $-\infty \leq z \leq \infty$ of the scaling argument $z$, the finite-size scaling functions such as $\mathcal{F}(x, y; \bar{\mathbf{A}})$ are valid only in a limited

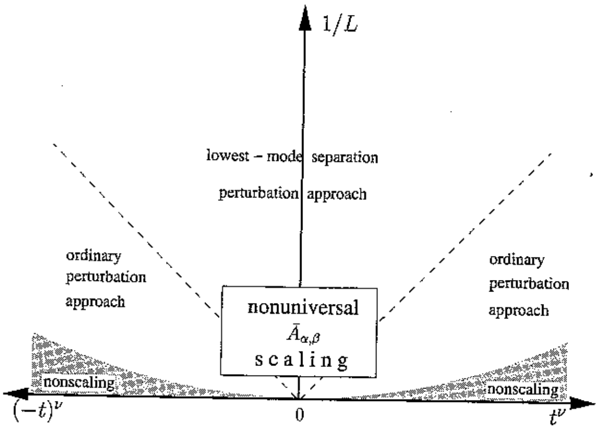


Fig. 3. Asymptotic part of the $L^{-1} - |t|^\nu$ plane at $h = 0$ for the anisotropic $\varphi^4$ theory in a cubic geometry with periodic boundary conditions. In the central finite-size region (above the dashed lines), the lowest mode must be separated whereas outside this region ordinary perturbation theory is applicable. Above the shaded region, finite-size scaling is valid but with scaling functions that depend on the anisotropy parameters $\bar{A}_{\alpha\beta}$. 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 $L^{-1} - h$ plane at $T = T_c$.

range of $x$ and $y$, above the shaded region in Fig. 3. 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 nonuniversal length scales such as the lattice spacing $\tilde{a}$,[14] the inverse cutoff $\Lambda^{-1}$ of $\varphi^4$ field theory,[15] the length scale $u_0^{-1/\varepsilon}$ set by the four-point coupling,[4] and the van-der-Waals interaction-length $b^{1/(\sigma-2)}$ (see Section 4.3 below).[16,17] Furthermore the anisotropy parameters $\bar{A}_{\alpha\beta}$ are relevant in all regions. This diversity can be traced back[4,14] to a similar diversity of the large-distance ($r \gg \tilde{a}$) behavior of *bulk* correlation functions in the $r^{-1} - |t|^\nu$ plane corresponding to the $L^{-1} - |t|^\nu$ plane of Fig. 3.

It is appropriate to first transform $H$ to a Hamiltonian $H'$ such that the $O(k_\alpha k_\beta)$ terms of $\delta\widehat{K}(\mathbf{k})$ attain an isotropic form. This transformation consists of a rotation and rescaling of lengths in the direction of the principal axes.[3] This rescaling is equivalent to a shear transformation which distorts the geometry, the lattice structure, and the boundary conditions in a nonuniversal way. The advantage of the transformed system is that its bulk renormalizations are well known from the standard isotropic $\varphi^4$ field theory. Thus, in order to derive the scaling function $\mathcal{F}$, it is most appro-

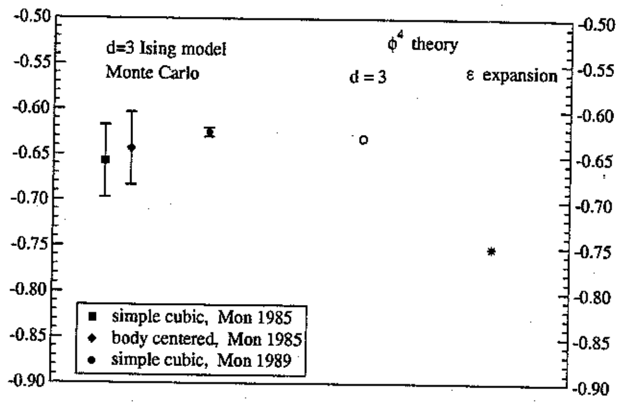


Fig. 4. Finite-size amplitude $\mathcal{F}(0,0;\mathbf{1})$ of the free energy density of isotropic systems in a cubic geometry at $T_c$ in three dimensions. Theoretical prediction[4] at $d=3$ (open circle), and at $\varepsilon = 1$ (star) of the $\varepsilon$ expansion. MC data for the $d=3$ Ising model on sc and bcc lattices.[12,13]

priate to develop perturbation theory within the transformed system with the Hamiltonian $H'$ for which a unique second-moment correlation length $\xi'_\pm$ is well defined.

## 4. Results

### 4.1. *Isotropic case*

For the purpose of calculating the finite-size free energy within the minimal renormalization scheme in three dimensions[6] we have further improved[4] the earlier finite-size perturbation approach[7–11] for the case of a one-component order parameter.

In order to test the reliability of our finite-size theory we first consider the isotropic case $K_0 = K, J = 0$, $\bar{\mathbf{A}} = \mathbf{1}$ where accurate MC data by Mon[12,13] for the $d = 3$ Ising model are available. Our theoretical result for the finite-size amplitude at $h = 0$ and $T = T_c$

$$\mathcal{F}(0,0;\mathbf{1})_{d=3} = -0.6315 \tag{9}$$

in excellent agreement with the MC results (see Fig. 4). The $\varepsilon = 4 - d$ expansion result $-0.7520$ is in less good agreement.

We have also calculated the scaling function $\mathcal{F}^{ex}(\tilde{x}, 0; \mathbf{1})$ of the excess free energy density $f_s^{ex}(t,0,L) = f_s(t,0,L) - f_s(t,0,\infty)$ for the isotropic case. The scaling argument is $\tilde{x} = t(L/\xi_{0+})^{1/\nu}$ where $\xi_{0+}$ is the asymptotic amplitude of the second-moment bulk correlation length above $T_c$. The

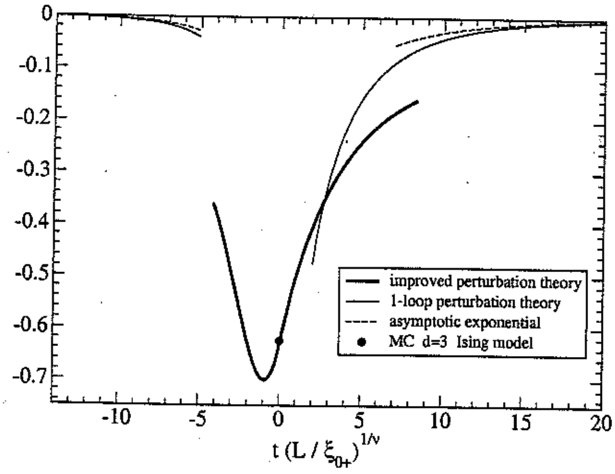


Fig. 5. Theoretical prediction of the scaling function $\mathcal{F}^{ex}(\tilde{x}, 0; 1)$ of the excess free energy density of isotropic systems for $d = 3$ (thick solid line). MC result (full circle) for the Ising model on a sc lattice at $t = 0$.[13] No scaling function exists in the large - $|\tilde{x}|$ regions above and below $T_c$ which are sensitive to all nonuniversal details of the model.

result is shown in Fig. 5 (thick solid line). The thin lines are the result of ordinary one-loop perturbation theory that breaks down at $T_c$.

### 4.2. *Anisotropic case*

Highly precise numerical information on the nonuniversal anisotropy effect on the critical Binder cumulant $U$ of the anisotropic two-dimensional Ising model, see Fig.2 (a), has been provided recently by MC simulations of Selke and Shchur.[18] In order to mimic the two-dimensional anisotropy within our three-dimensional $\varphi^4$ lattice model we choose $K_0 = K + J$. To exhibit the *deviations* from isotropy and for the purpose of a comparison with the MC data[18] for the anisotropic two-dimensional Ising model we have plotted in Fig. 6 our theoretical result for the *difference* $U(\bar{\mathbf{A}}) - U(1)$ as a function of $J/K$ together with the corresponding difference of the MC data.[18,19] We see that for positive $J/K$ there is remarkable agreement.

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[18] who found a *monotonic decrease* of $U$ when taking a weak antiferromagnetic coupling $J$.[20] We also predict the existence of a Lifshitz point near $J/K \lesssim -1/2$ with a wave vector instability in the $(1,1,0)$ direction. Very recently MC simulations have

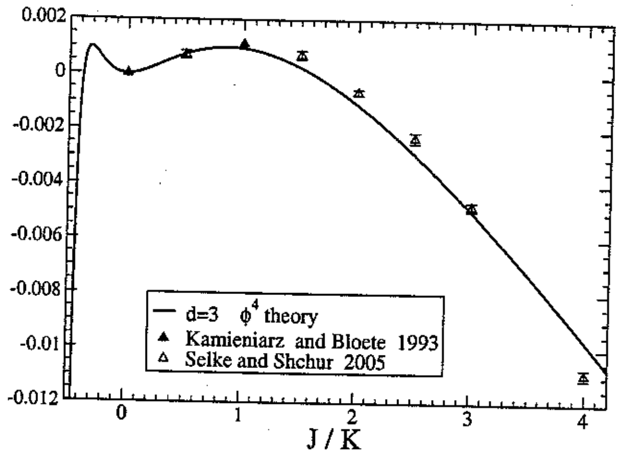


Fig. 6. Difference $U(\bar{\mathbf{A}}) - U(1)$ of the Binder cumulant plotted as a function of $J/K$ together with the corresponding difference of the MC data[18,19] for the two-dimensional Ising model of Fig. 2(a).

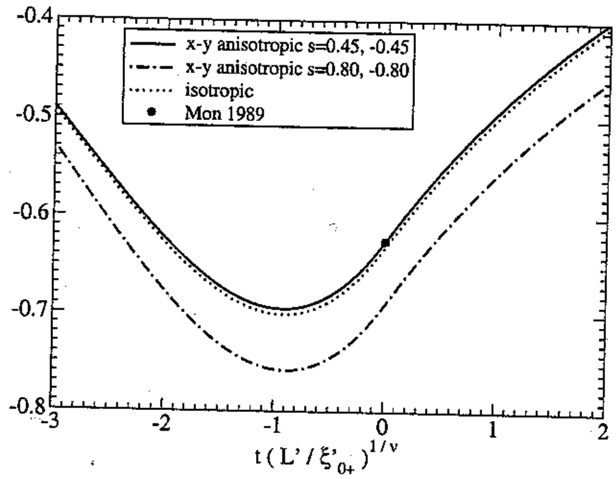


Fig. 7. Scaling function $\mathcal{F}^{ex}(\tilde{x}, 0; \bar{\mathbf{A}})$ of the excess free energy density of the anisotropic model with the anisotropy matrix (6) with $K_0 = K + J$ in a cubic geometry in three dimensions as a function of the scaling variable $\tilde{x} = t(L'/\xi'_{0+})^{1/\nu}$ for several values of the anisotropy parameter $s = (1 + K/J)^{-1}$ with $s = 0.45, -0.45$ (solid line), $s = 0.80, -0.80$ (dot-dashed line), $s = 0$ (dotted line, isotropic case). MC result (full circle) for the three-dimensional Ising model on a sc lattice.[13]

been started by Selke[21] in order to test these predictions in the regime of $J/K < 0$.

We have also calculated the nonuniversal anisotropy effect on the finite-size scaling function of $\mathcal{F}^{ex}$ for the anisotropy matrix (6) with $K_0 = K + J$ near the minimum below $T_c$ as shown in Fig. 7 for several values of

$$s = (1 + K/J)^{-1}. \tag{10}$$

Our theory predicts the finite-size effects to depend on $s^2$ rather than $s$. It would be interesting to test this symmetry property by MC simulations. As shown in Fig. 7, the anisotropy effect for $s = \pm 0.80$ corresponding to $J/K = 4$ and $J/K = -4/9$ is far outside the error bars of the MC data by Mon[13] for the isotropic case and may be be detectable in future MC simulations.

### 4.3. *Subleading long-range interactions*

Finally we discuss the case of an isotropic subleading long-range interaction of the van der Waals type as defined by the long-wavelength form[16,17,22,23]

$$\delta\widehat{K}(\mathbf{k}) = \mathbf{k}^2 \ - b\,|\mathbf{k}|^\sigma \ + \ O(k^4) \tag{11}$$

with $2 < \sigma < 4$, $b > 0$. It was pointed out by Dantchev and Rudnick[23] that it affects the finite-size susceptibility in the regime $L/\xi_+ \gg 1$, similar to the effect caused by a sharp cutoff.[15] The effect of the interaction (11) on the excess free energy $f_s^{ex}$ and on the critical Casimir force in the case of film geometry was first studied in Ref. 16,17. The asymptotic structure for $L/\xi_+ \gg 1$ in one-loop order above $T_c$ at $h = 0$ is[16,17]

$$f_s^{ex}(t,0,L) \ = L^{-d}\Big[\mathcal{F}^{ex}(L/\xi_+) + bL^{2-\sigma}\Psi(L/\xi_+)\Big]. \tag{12}$$

We have verified that, for $n = 1$, the same structure is valid also for cubic geometry with periodic boundary conditions above and below $T_c$ where the function $\Psi_{cube}$ has an algebraic large-$L$ behavior $\sim (L/\xi_\pm)^{-2}$. The latter is dominant compared to the exponentially decaying scaling part $\mathcal{F}^{ex,\pm}$ in the shaded region of Fig. 3. This implies that, in this region, *two* nonuniversal length scales $b^{1/(\sigma-2)}$ and $\xi_\pm$ at $h = 0$ govern the *leading* singular part of the excess free energy density

$$f_s^{ex,\pm}(t,0,L) \ \sim \ L^{-d} \ \left[\frac{b^{1/(\sigma-2)}}{L}\right]^{\sigma-2} \ \left[\frac{\xi_\pm}{L}\right]^2, \tag{13}$$

even arbitrarily close to criticality. In addition, there is a nonuniversal $u_0$ dependent exponential tail[4] of $\mathcal{F}^{ex,\pm}$. In (13), both the amplitude $\sim b$ and the power $-d - \sigma$ of the $L$ dependence are nonuniversal. Thus, for isotropic systems with subleading long-range interactions, there exists no universal finite-size scaling form with only *one* reference length scale in the region $L/\xi_\pm \gg 1$ of the $L^{-1} - |t|^\nu$ plane although such systems are members of the same universality class as, e.g., Ising models with isotropic short-range interactions. The structure of (12) and (13) was confirmed and further studied by several authors.[24–26]

## Acknowledgments

I thank B. Kastening and W. Selke for useful discussions. Support by DLR under Grant No. 50WM0443 is gratefully acknowledged.

## References

1. V. Privman, A. Aharony, and P. C. Hohenberg, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1991), Vol. 14, p. 1.
2. X. S. Chen and V. Dohm, *Phys. Rev. E* **70**, 056136 (2004).
3. V. Dohm, *J. Phys. A* **39**, L 259 (2006).
4. V. Dohm, submitted to *Phys. Rev. E* [arXiv:0801.4096].
5. K. Binder, *Z. Phys. B* **43**, 119 (1981).
6. V. Dohm, *Z. Phys. B* **60**, 61 (1985); R. Schloms and V. Dohm, *Nucl. Phys. B* **328**, 639 (1989).
7. J. Rudnick, H. Guo, and D. Jasnow, *J. Stat. Phys.* **41**, 353 (1985).
8. E. Brézin and J. Zinn-Justin, *Nucl. Phys. B* **25** [**FS 14**], 867 (1985).
9. A. Esser, V. Dohm, M. Hermes, and J. S. Wang, *Z. Phys. B* **97**, 205 (1995).
10. A. Esser, V. Dohm, and X. S. Chen, *Physica A* **222**, 355 (1995).
11. X. S. Chen, V. Dohm, and N. Schultka, *Phys. Rev. Lett.* **77**, 3641 (1996).
12. K. K. Mon, *Phys. Rev. Lett.* **54**, 2671 (1985).
13. K. K. Mon, *Phys. Rev. B* **39**, 467 (1989).
14. X. S. Chen and V. Dohm, *Eur. Phys. J. B* **15**, 283 (2000).
15. X. S. Chen and V. Dohm, *Eur. Phys. J. B* **10**, 687 (2000).
16. X. S. Chen and V. Dohm, *Phys. Rev. E* **66**, 016102 (2002).
17. X. S. Chen and V. Dohm, *Physica B* **329-333**, 202 (2003).
18. W. Selke and L. N. Shchur, *J. Phys. A* **38**, L 739 (2005).
19. G. Kamieniarz and H. W. J. Blöte, *J. Phys. A* **26**, 233 (1988).
20. We have been informed by W. Selke that the preliminary simulations[18] for $J < 0$ were performed at $J/K = -0.5$ and $-0.75$.
21. W. Selke, private communication.
22. B. Widom, *J. Chem. Phys.* **41**, 74 (1964); R. F. Kayser and H. J. Raveché, *Phys. Rev. A* **29**, 1013 (1984).
23. D. Dantchev and J. Rudnick, *Eur. Phys. J. B* **21**, 251 (2001).
24. D. Dantchev, M. Krech, and S. Dietrich, *Phys. Rev. E* **67**, 066120 (2003).
25. D. Dantchev, H. W. Diehl, and D. Grüneberg, *Phys. Rev. E* **73**, 016131 (2006).
26. D. Dantchev, F. Schlesener, and S. Dietrich, *Phys. Rev. E* **76**, 011121 (2007).