

Violation of finite-size scaling in three dimensions

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Abstract. We reexamine the range of validity of finite-size scaling in the φ^4 lattice model and the φ^4 field theory below four dimensions. We show that general renormalization-group arguments based on the renormalizability of the φ^4 theory do not rule out the possibility of a violation of finite-size scaling due to a finite lattice constant and a finite cutoff. For a confined geometry of linear size L with periodic boundary conditions we analyze the approach towards bulk critical behavior as $L \rightarrow \infty$ at fixed ξ for $T > T_c$ where ξ is the bulk correlation length. We show that for this analysis ordinary renormalized perturbation theory is sufficient. On the basis of one-loop results and of exact results in the spherical limit we find that finite-size scaling is violated for both the φ^4 lattice model and the φ^4 field theory in the region $L \gg \xi$. The non-scaling effects in the field theory and in the lattice model differ significantly from each other.

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1 Introduction

One of the fundamental achievements of the renormalization-group (RG) theory of critical phenomena is the elucidation and proof of universality and scaling near critical points [1–3]. These predictions have been shown to be asymptotically exact sufficiently close to criticality of infinitely large systems. For finite or partially finite systems, the field-theoretic version of RG theory has also provided an apparently exact prediction of universal finite-size scaling for systems with periodic boundary conditions [4], in accord with phenomenological considerations [5] and with numerous analytical and numerical studies in statistical and elementary particle physics in the past decades [3–12]. Thus the validity of finite-size scaling appears to be well established.

Consider, for example, the susceptibility $\chi(t, L)$ of a ferromagnetic system for $t = (T - T_c)/T_c \geq 0$ in a d -dimensional finite geometry with a characteristic size L . For large L and small t the property of finite-size scaling means that χ has the asymptotic form

$$\chi(t, L) = \chi(t, \infty) f(L/\xi) \quad (1)$$

where $\chi(t, \infty) = A_\chi t^{-\gamma}$ is the bulk susceptibility and $\xi = \xi_0 t^{-\nu}$ is the bulk correlation length. For a given geometry and periodic boundary conditions the scaling function $f(x)$ was found [4] to be universal for $d < 4$ which implied that the relative deviation from bulk critical behavior

$$\Delta\chi \equiv \frac{\chi(t, \infty) - \chi(t, L)}{\chi(t, \infty)} = g(L/\xi) \quad (2)$$

is universal as well in the entire range $0 \leq L/\xi \leq \infty$ with $g(\infty) = 1 - f(\infty) = 0$. This result, if correct, agrees with the scaling hypothesis [5] which implies that the approach towards bulk critical behavior ($L/\xi \rightarrow \infty$ at fixed $\xi < \infty$ above T_c) can be embodied in the scaling function $g(L/\xi)$ [5]. Universality in this context means that the shape of the scaling function $g(x)$ depends on the geometry and on the boundary conditions but does not depend on any nonuniversal parameter, in particular not on the lattice constant \tilde{a} of lattice models or on the cutoff Λ of field theories. As a consequence it was generally accepted that finite-size scaling functions such as $g(x)$ can be calculated on the basis of field theories in the limit $\Lambda \rightarrow \infty$ [3, 4, 7–50].

Brézin's RG analysis [4] started from the φ^4 lattice model with a finite lattice spacing \tilde{a} . The RG arguments, however, were presented within the renormalized theory after the limit $\tilde{a} \rightarrow 0$ was taken. This limit is usually considered in studies of renormalized field theory of *bulk* systems for $d < 4$ [3, 13, 51] where cutoff and lattice effects are known to yield only subleading corrections to the leading critical temperature dependence. The asymptotic unimportance of cutoff and lattice effects also for *confined* systems appeared to be a plausible assumption that was not questioned in reference [4] but is checked now and found to be invalid.

Very recently we have shown [52] that this latter assumption is not generally justified in the $O(n)$ symmetric φ^4 field theory of confined systems with periodic boundary conditions. Specifically it was shown in the large- n limit for $2 < d < 4$ that a finite cutoff Λ implies a violation of finite-size scaling in the region $L/\xi \gg 1$ above T_c ,

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with a non-exponential and nonuniversal approach $\Delta\chi \propto (AL)^{-2}$ towards zero, even arbitrarily close to T_c . This behavior was traced back to the $(\nabla\varphi)^2$ term in the field-theoretic φ^4 Hamiltonian which approximates the more general interaction $(\varphi_i - \varphi_j)^2$ of the φ^4 lattice model. In the latter model an exponential size dependence in the region $L/\xi \gg 1$ was found [52], in accord with previous results for exactly solvable model systems [5, 6, 14, 53–57]. The possibility of a violation of finite-size scaling in the φ^4 lattice model at finite lattice spacing, however, was not yet analyzed in our recent work [52]. Thus the important question remained open whether the violation of finite-size scaling found in the φ^4 field theory [52] is an artifact of the field-theoretic continuum approximation or whether finite-size scaling breaks down more generally for $L/\xi \gg 1$ in confined lattice systems with a finite lattice constant.

It is the purpose of the present paper to take up this problem for the $O(n)$ symmetric φ^4 lattice model at finite lattice constant \tilde{a} in the context of a detailed RG analysis, without taking the limit $\tilde{a} \rightarrow 0$. We assume renormalizability in terms of bulk renormalizations and thus work for dimensionality d below the upper critical dimension which is 4 in our case. Thus this may become relevant to real three-dimensional systems. We shall show that the renormalizability of the φ^4 model in a confined geometry implies the asymptotic ($L \rightarrow \infty, \xi \rightarrow \infty$) validity of finite-size scaling for $d < 4$ at any fixed finite ratio $L/\xi < \infty$, in agreement with the proof of Brézin [4], but does not rule out a violation of finite-size scaling in the limit $L/\xi \rightarrow \infty$ at finite $\tilde{a}/\xi > 0$. On the basis of one-loop results for general n and of exact results in the large- n limit we indeed find such a violation: instead of (2) the more general form

$$\Delta\chi = g(L/\xi) [1 + R(L/\xi, \tilde{a}/\xi)] \quad (3)$$

must be considered where $g(x)$ is universal but where the nonuniversal function R contains a nontrivial dependence on the lattice constant \tilde{a} . Although R vanishes for fixed finite ratio $L/\xi < \infty$ in the asymptotic region,

$$\lim_{(L,\xi) \rightarrow \infty} R(L/\xi, \tilde{a}/\xi) = R(L/\xi, 0) = 0, \quad L/\xi \text{ fixed}, \quad L/\xi < \infty, \quad (4)$$

it exhibits a singular behavior in approaching the bulk limit $L/\xi \rightarrow \infty$ at any fixed $\tilde{a}/\xi > 0$,

$$\lim_{x \rightarrow \infty} R(x, \tilde{a}/\xi) = \infty, \quad \tilde{a}/\xi \text{ fixed}, \quad \tilde{a}/\xi > 0. \quad (5)$$

This implies that for sufficiently large L/ξ the leading size dependence

$$\Delta\chi \sim g(L/\xi)R(L/\xi, \tilde{a}/\xi), \quad L/\xi \gg 1, \tilde{a}/\xi > 0, \quad (6)$$

is nonuniversal and violates finite-size scaling. We emphasize that this violation is not a subleading non-asymptotic property but occurs in leading order at any finite $\xi < \infty$, even arbitrarily close to T_c where “corrections to scaling” or corrections of *bulk* properties due to a finite lattice constant are completely negligible. (Here and in the

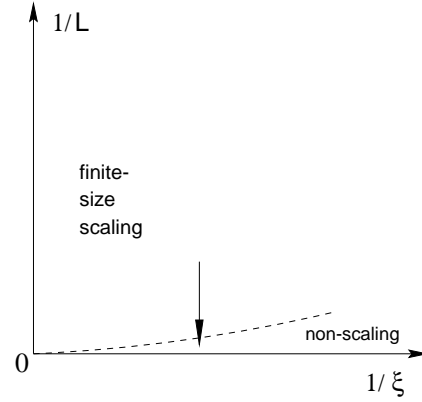


Fig. 1. Asymptotic $L^{-1} - \xi^{-1}$ plane in units of the lattice constant \tilde{a} above T_c (schematic plot) for the φ^4 lattice model below four dimensions where L is the system size and ξ is the bulk correlation length. Nonuniversal lattice effects become nonnegligible in the non-scaling region below the dashed line where finite-size scaling is violated. This crossover line is determined by equation (107). Well above this line the dependence on the lattice spacing \tilde{a} is negligible in equation (3). The arrow indicates an approach towards bulk critical behavior at constant $0 < t \ll 1$ through the non-scaling region where equation (106) is valid. A corresponding non-scaling region exists also for the field-theoretic φ^4 model at finite cutoff where the crossover line is determined by equation (123) and the non-scaling effect is described by equation (122), compare Figure 1 of reference [52]. A corresponding crossover line should be added to Figure 1 of reference [63].

following the symbol \sim means asymptotic behavior including the amplitude, *i.e.*, $\Delta\chi \sim G(x)$ for $x \gg 1$ means $\lim_{x \rightarrow \infty} \Delta\chi/G(x) = 1$.)

Our results imply that the property of finite-size scaling (for confined systems with periodic boundary conditions) which was previously believed to be exact for $d < 4$ in the asymptotic ($L \gg \tilde{a}, \xi \gg \tilde{a}$) region of the $L^{-1} - \xi^{-1}$ plane (Fig. 1) is not valid in a small but important part of this region (below the dashed line in Fig. 1). The nonuniversal function R is negligible at $T = T_c$ for sufficiently large L but it increases as L/ξ increases above T_c at fixed $\tilde{a}/\xi > 0$. The approach to the bulk limit (arrow in Fig. 1) corresponds to a crossover from the scaling region to a non-scaling region where nonuniversal effects due to the finite lattice constant dominate the finite-size deviations from bulk behavior. The location of the (smooth) crossover region may be characterized by the line along which $R(L/\xi, \tilde{a}/\xi) \simeq 1$, *i.e.*, where the scaling and non-scaling contributions to $\Delta\chi$ are equally large. This requirement defines the dashed line in Figure 1. A similar line should exist below T_c . Explicit results for R will be given in Sections 4 and 5 for the φ^4 lattice model for $2 < d \leq 4$.

Essential features of these results will remain valid even for $d > 4$ [58] such that the finite-size scaling form of Privman and Fisher [59,60] will be violated for $L \gg \xi$. In particular, the lowest-mode approach of Brézin and Zinn-Justin [16] and the phenomenological single-variable

scaling form of Binder *et al.* [61,62] fail qualitatively for $L \gg \xi \gg \tilde{a}$ where these theories predict a *universal power-law* behavior $\Delta\chi \propto L^{-d}$ above four dimensions, rather than a *non-universal exponential* behavior [52] $\Delta\chi \propto e^{-cL}$ as derived in Sections 4 and 5 of the present paper. Such striking *structural* differences [63] between the lowest-mode approximation and the effects of the higher modes cannot be regarded only as “corrections” [64].

For comparison we also calculate the function $R_{\text{field}}(L/\xi, \Lambda\xi)$ for the field-theoretic φ^4 model at finite sharp cutoff Λ (with periodic boundary conditions). For $d < 4$ we find a violation of finite-size scaling [52] due to a divergence of $R_{\text{field}}(L/\xi, \Lambda\xi)$ in the limit $L/\xi \rightarrow \infty$ at fixed $\Lambda\xi < \infty$, analogous to (5) for the lattice model. The form of R_{field} of the φ^4 field theory, however, differs significantly from that of R for the φ^4 lattice model. Even the *sign* of $R_{\text{field}} < 0$ is different from that of $R > 0$. Thus the φ^4 field theory based on the standard Landau-Ginzburg-Wilson continuum Hamiltonian does not predict the correct structure of the leading finite-size deviation from bulk critical behavior of lattice systems at any $T > T_c$ (and presumably at any $T < T_c$) for $d < 4$. We show that this statement remains valid also for $d = 4$ which may be relevant to elementary particle physics [10,12,30], to disordered systems [65], and more generally to systems at their upper critical dimension [2]. For $d > 4$ the failure of the continuum approximation is even more severe as it pertains to the entire $L^{-1} - \xi^{-1}$ plane [58,63,66–68].

From a purely quantitative point of view, the non-scaling behavior of χ is a small effect that occurs predominantly in a region where the total finite-size contributions are exponentially small (for periodic boundary conditions). From a more fundamental point of view, however, the violation of finite-size scaling below four dimensions is a matter of principle, regardless of how small this effect might be. In particular, our RG analysis for the simplest case of *periodic* boundary conditions raises considerable doubt about the validity of finite-size scaling in the more complicated cases of *non-periodic* boundary conditions where additional renormalizations and nonuniversal length scales come into play. They imply that general RG arguments are less compelling since additional assumptions would be needed. Furthermore, possible non-scaling effects for non-periodic boundary conditions may no longer be exponentially small. This may open up the prospect of resolving the long-standing and recent problems concerning the interpretation [11] of experimental data for confined ${}^4\text{He}$ near the superfluid transition [69–80]. Work in this direction is in progress.

Our paper is organized as follows. In Section 2 we describe the renormalization scheme for the bulk φ^4 lattice model at finite lattice spacing. In Section 3 we extend this scheme to the confined system and show that the RG arguments do not rule out a violation of finite-size scaling in the limit $L \gg \xi$. In Section 4 we calculate $\Delta\chi$ for $d \leq 4$ in one-loop order for general n . The exact result for this quantity in the large- n limit is derived in Section 5. A summary and further discussion of our results is given in Section 6.

2 Lattice model: bulk properties at finite lattice constant

In this Section we introduce our notation and define the renormalization of bulk quantities of the φ^4 lattice model at finite lattice spacing above T_c . This will serve as the framework for the renormalization-group analysis of finite-size effects at finite lattice spacing in the subsequent Sections. A detailed formulation of the theory at finite lattice spacing is indispensable for clearly distinguishing lattice effects of the finite system from ordinary non-asymptotic Wegner [82] corrections to scaling.

We consider a φ^4 lattice Hamiltonian H for the variables φ_i on the lattice points \mathbf{x}_i of a simple-cubic lattice in a cube with volume $V = L^d$ and with periodic boundary conditions. (Generalizations to different geometries will be considered in the subsequent Sections.) We assume the statistical weight $\propto e^{-H}$ with

$$H = \tilde{a}^d \left\{ \sum_i \left[\frac{r_0}{2} \varphi_i^2 + u_0 (\varphi_i^2)^2 \right] + \sum_{i,j} \frac{1}{2\tilde{a}^2} J_{ij} (\varphi_i - \varphi_j)^2 \right\} \quad (7)$$

where \tilde{a} is the lattice constant. The variables φ_i have n components $\varphi_{i\alpha}$ with $\alpha = 1, 2, \dots, n$ which vary in the range $-\infty \leq \varphi_{i\alpha} \leq \infty$. The couplings J_{ij} are dimensionless quantities whereas the variables φ_i have the dimension $[\tilde{a}^{(2-d)/2}]$ and \tilde{a} has the dimension of a length.

2.1 Unrenormalized theory

The renormalization-group treatment of this model in the bulk limit $V \rightarrow \infty$ is well known which is usually carried out in the limit of zero lattice spacing $\tilde{a} \rightarrow 0$ or in the limit of infinite cutoff $\Lambda \rightarrow \infty$ in the continuum version (see (54) below) [3,13,51]. Here we shall formulate the renormalization of bulk quantities at finite \tilde{a} . Similar to the previous formulation of the bulk theory at fixed $d < 4$ [81] we shall express the bare theory in terms of the bulk correlation length ξ before turning to the renormalized theory.

We start from the bulk two-point vertex function [3,13,51]

$$\Gamma^{(2)}(\mathbf{k}, r_0, u_0, \tilde{a}, d) = \chi_b(\mathbf{k})^{-1} \quad (8)$$

where $\chi_b(\mathbf{k})$ is the bulk susceptibility at finite wavevector \mathbf{k} above T_c

$$\chi_b(\mathbf{k}) = \lim_{L \rightarrow \infty} \frac{\tilde{a}^{2d}}{L^d} \sum_{i,j} \langle \varphi_i \varphi_j \rangle e^{-i\mathbf{k} \cdot (\mathbf{x}_i - \mathbf{x}_j)}. \quad (9)$$

It serves to define the bulk correlation length ξ above T_c according to

$$\xi^2 = \chi_b(\mathbf{0}) \frac{\partial}{\partial k^2} [\chi_b(\mathbf{k})]_{|\mathbf{k}=\mathbf{0}}^{-1}. \quad (10)$$

We shall also consider the four-point vertex function $\Gamma^{(4)}$ of the bulk theory [3,13,51] at vanishing external wavenumber.

The parameter r_0 in H is taken to be a linear function of the reduced temperature

$$t = (T - T_c)/T_c, \quad r_0 = r_{0c} + a_0 t, \quad (11)$$

with $a_0 > 0$. The critical value r_{0c} of r_0 is determined by $\chi_b(\mathbf{0})^{-1} = 0$, *i.e.*

$$\Gamma^{(2)}(\mathbf{0}, r_{0c}, u_0, \tilde{a}, d) = 0, \quad (12)$$

which provides an implicit definition of the function

$$r_{0c} = r_{0c}(u_0, \tilde{a}, d) \quad (13)$$

at finite lattice spacing \tilde{a} . (Note that $r_{0c}(u_0, \tilde{a}, d)$ does not have an expansion in integer powers of u_0 , unlike the vertex functions $\Gamma^{(N)}(r_0, u_0, \tilde{a}, d)$ [81].)

Instead of r_0 we shall substitute

$$r_0 = r_0 - r_{0c} + r_{0c}(u_0, \tilde{a}, d) \quad (14)$$

into $\Gamma^{(N)}$ and consider $\Gamma^{(N)}$ (at $\mathbf{k} = \mathbf{0}$) as well as the correlation length ξ as functions of $r_0 - r_{0c}, u_0, \tilde{a}, d$,

$$\Gamma^{(N)} = \Gamma^{(N)}(r_0 - r_{0c}, u_0, \tilde{a}, d), \quad (15)$$

$$\xi = \xi(r_0 - r_{0c}, u_0, \tilde{a}, d). \quad (16)$$

Since ξ is a monotonic function of $r_0 - r_{0c}$, equation (16) can be inverted to define $r_0 - r_{0c}$ as a function of ξ ,

$$r_0 - r_{0c} = h(\xi, u_0, \tilde{a}, d). \quad (17)$$

Finally we may substitute (17) into (15) which leads to bare vertex functions $\tilde{\Gamma}^{(N)}$ at finite \tilde{a} in terms of ξ ,

$$\tilde{\Gamma}^{(N)}(\xi, u_0, \tilde{a}, d) = \Gamma^{(N)}(h(\xi, u_0, \tilde{a}, d), u_0, \tilde{a}, d). \quad (18)$$

These definitions are parallel to those at infinite cutoff in reference [81]. (In particular, the functions $\tilde{\Gamma}^{(N)}$ have an expansion in integer powers of u_0 .) We illustrate these definitions by the one-loop results

$$h(\xi, u_0, \tilde{a}, d) = J_0 \xi^{-2} \left\{ 1 + 4(n+2)u_0 \times \int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}}(\hat{J}_{\mathbf{k}} + J_0 \xi^{-2}) \right]^{-1} + O(u_0^2) \right\}, \quad (19)$$

$$\tilde{\Gamma}^{(2)}(\mathbf{k}, \xi, u_0, \tilde{a}, d) = \hat{J}_{\mathbf{k}} + J_0 \xi^{-2} + O(u_0^2), \quad (20)$$

$$\tilde{\Gamma}^{(4)}(\xi, u_0, \tilde{a}, d) = 24u_0 \left\{ 1 - 4(n+8)u_0 \times \int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}} + J_0 \xi^{-2} \right]^{-2} + O(u_0^2) \right\} \quad (21)$$

where

$$\hat{J}_{\mathbf{k}} = \frac{2}{\tilde{a}^2} [J(0) - J(\mathbf{k})] \quad (22)$$

with

$$J(\mathbf{k}) = (\tilde{a}/L)^d \sum_{i,j} J_{ij} e^{-i\mathbf{k} \cdot (\mathbf{x}_i - \mathbf{x}_j)}. \quad (23)$$

We assume a finite-range pair interaction J_{ij} such that its Fourier transform has the small \mathbf{k} behavior

$$\hat{J}_{\mathbf{k}} = J_0 \mathbf{k}^2 + O(k_i^2 k_j^2) \quad (24)$$

with a finite constant

$$J_0 = \frac{1}{d} (\tilde{a}/L)^d \sum_{i,j} (J_{ij}/\tilde{a}^2) (\mathbf{x}_i - \mathbf{x}_j)^2 > 0. \quad (25)$$

The dependence of the quantities (19)-(21) on \tilde{a} comes from the integration limit of the bulk integral

$$\int_{\mathbf{k}} \equiv \int \frac{d^d k}{(2\pi)^d} \quad (26)$$

with $|k_j| \leq \pi/\tilde{a}, j = 1, 2, \dots, d$. Because of the super-renormalizability of the φ^4 theory [3,13,51] the bare functions $\tilde{\Gamma}^{(N)}$ remain finite in the limit $\tilde{a} \rightarrow 0$ at fixed ξ and u_0 for $d < 4$.

2.2 Renormalization at finite lattice constant

As is well known, the perturbative results (19)-(21) of the bare theory do not provide a correct description in the critical region $\xi \gg \tilde{a}$ for $d \leq 4$. This problem is circumvented by turning to the renormalized theory which provides a mapping from the critical to the non-critical region where perturbation theory is applicable (see (44) below). We start from the bare N -point vertex functions $\tilde{\Gamma}^{(N)}$ as functions of the correlation length ξ where ξ is considered to be a given quantity. The explicit determination of ξ as a function of the reduced temperature t at finite \tilde{a} is a separate issue [81] that is postponed to Appendix A.

Since ξ does not require a renormalization it suffices to introduce only two renormalization factors Z_φ and Z_u to define multiplicatively renormalizable vertex functions $\tilde{\Gamma}_R^{(N)}$. We define the renormalized variable

$$\varphi_i^R = Z_\varphi^{-1/2} \varphi_i \quad (27)$$

and the renormalized coupling

$$u = J_0^{-2} \mu^{-\epsilon} Z_u^{-1} u_0 \quad (28)$$

with $\epsilon = 4 - d$. The reference length μ^{-1} is arbitrary. (It can be conveniently chosen as $\mu^{-1} = \xi_0$ where ξ_0 is the amplitude of the asymptotic bulk correlation length as specified in (A.17) of Appendix A.) The definitions (27) and (28) lead to the following renormalized vertex function $\tilde{\Gamma}_R^{(2)}$ (at finite \mathbf{k}) and $\tilde{\Gamma}_R^{(4)}$ (at vanishing wavenumber)

$$\tilde{\Gamma}_R^{(2)}(\mathbf{k}, \xi, u, \mu, \tilde{a}, d) = Z_\varphi \tilde{\Gamma}^{(2)}(\mathbf{k}, \xi, \mu^\epsilon J_0^2 Z_u u, \tilde{a}, d), \quad (29)$$

$$\tilde{\Gamma}_R^{(4)}(\xi, u, \mu, \tilde{a}, d) = Z_\varphi^2 \tilde{\Gamma}^{(4)}(\xi, \mu^\epsilon J_0^2 Z_u u, \tilde{a}, d). \quad (30)$$

The Z factors Z_φ and Z_u can be determined for $d \leq 4$ by standard renormalization conditions at $\xi = \mu^{-1}$

$$\left. \frac{\partial}{\partial k^2} \tilde{\Gamma}_R^{(2)}(\mathbf{k}, \mu^{-1}, u, \mu, \tilde{a}, d) \right|_{\mathbf{k}=\mathbf{0}} = J_0, \quad (31)$$

$$\tilde{\Gamma}_R^{(4)}(\mu^{-1}, u, \mu, \tilde{a}, d) = 24J_0^2 \mu^\epsilon u. \quad (32)$$

The Z factors are finite for $d \leq 4$ if $\tilde{a} > 0$ and remain finite for $d < 4$ if $\tilde{a} \rightarrow 0$ at fixed u and μ . The following analysis is valid for $d < 4$ and $d = 4$ since we keep the lattice spacing \tilde{a} finite. Substituting (20), (21), (24), (29) and (30) into (31) and (32) yields the Z factors in one-loop order

$$Z_\varphi(u, \mu\tilde{a}, d) = 1 + O(u^2), \quad (33)$$

$$Z_u(u, \mu\tilde{a}, d) = 1 + 4(n+8)uI(\tilde{a}\mu, d) + O(u^2) \quad (34)$$

where

$$I(\tilde{a}\mu, d) = \mu^{4-d} \int_{\mathbf{k}} \left[\mu^2 + \hat{J}_{\mathbf{k}}/J_0 \right]^{-2}. \quad (35)$$

We derive renormalization-group equations (RGE) for $\tilde{\Gamma}_R^{(N)}$ by taking the derivative of (29) and (30) with respect to μ at fixed u_0, \tilde{a} and $r_0 - r_{0c}$, *i.e.*, at fixed ξ . This yields (at $\mathbf{k} = \mathbf{0}$)

$$\left[\mu \partial_\mu + \beta_u \partial_u + \frac{N}{2} \zeta_\varphi \right] \tilde{\Gamma}_R^{(N)}(\xi, u, \mu, \tilde{a}, d) = 0 \quad (36)$$

with

$$\zeta_\varphi(u, \mu\tilde{a}, d) = (\mu \partial_\mu \ln Z_\varphi^{-1})_0, \quad (37)$$

$$\beta_u(u, \mu\tilde{a}, d) = (\mu \partial_\mu u)_0, \quad (38)$$

where the index 0 means differentiation at fixed parameters of the bare theory. The formal solution of (36) reads

$$\tilde{\Gamma}_R^{(N)}(\xi, u, \mu, \tilde{a}, d) = \tilde{\Gamma}_R^{(N)}(\xi, u(\ell), \ell\mu, \tilde{a}, d) \exp \frac{N}{2} \int_1^\ell \zeta_\varphi(\ell') \frac{d\ell'}{\ell'} \quad (39)$$

where $\zeta_\varphi(\ell) \equiv \zeta_\varphi(u(\ell), \ell\mu\tilde{a}, d)$ and where $u(\ell)$ is the solution of the flow equation

$$\ell \frac{du(\ell)}{d\ell} = \beta_u[u(\ell), \ell\mu\tilde{a}, d] \quad (40)$$

with $u(1) = u$. In the present context the most convenient choice of the flow parameter ℓ is

$$\ell\mu = \xi^{-1}. \quad (41)$$

We rewrite the renormalized vertex functions as

$$\tilde{\Gamma}_R^{(N)}(\xi, u, \mu, \tilde{a}, d) = \xi^{-\delta_N} f^{(N)}(\mu\xi, u, \mu\tilde{a}, d) \quad (42)$$

where the amplitude functions $f^{(N)}$ are dimensionless and

$$\delta_N = d - (d-2)N/2. \quad (43)$$

The renormalizability of the φ^4 lattice model for $d \leq 4$ guarantees that the limit $\tilde{a} \rightarrow 0$ of $\tilde{\Gamma}_R^{(N)}$ at fixed u, μ and ξ exists, *i.e.*, that the function $f^{(N)}(\mu\xi, u, 0, d)$ is finite for finite $\mu\xi$ and $u > 0$ for $d \leq 4$. From (39), (41) and (42) we obtain

$$f^{(N)}(\mu\xi, u, \mu\tilde{a}, d) = f^{(N)}(1, u(\ell), \tilde{a}/\xi, d) \times \exp \frac{N}{2} \int_1^\ell \zeta_\varphi(\ell') \frac{d\ell'}{\ell'} \quad (44)$$

which provides the mapping of the amplitude function $f^{(N)}(y, u, \mu\tilde{a}, d)$ from the critical region $y \gg 1$ (where perturbation theory breaks down) to the noncritical value $y = 1$ (where perturbation theory is applicable). The temperature dependence of the amplitude function $f^{(N)}(1, u(\ell), \tilde{a}/\xi, d)$ in (44) is affected by the finite lattice constant \tilde{a} not only through the explicit dependence on \tilde{a}/ξ but also through the effective coupling $u(\ell)$ that is determined by the \tilde{a} dependent RG flow equation (40). Furthermore the lattice constant enters the form of the temperature dependence of $\xi(\ell)$ according to (A.11) of Appendix A.

2.3 Asymptotic behavior

Asymptotically ($\ell \rightarrow 0, \xi \rightarrow \infty$) the effective coupling $u(\ell)$ approaches the fixed point $u^* = u(0)$ as determined by

$$0 = \beta_u(u^*, 0, d) \quad (45)$$

which is independent of the lattice constant \tilde{a} and of the initial value u . For $\xi \rightarrow \infty$, equation (44) approaches the asymptotic form

$$f^{(N)}(\mu\xi, u, \mu\tilde{a}, d) \sim A^{(N)} f^{(N)}(1, u^*, 0, d) (\mu\xi)^{N\eta/2} \quad (46)$$

with the critical exponent

$$\eta = -\zeta_\varphi(u^*, 0, d) \quad (47)$$

and the nonuniversal amplitude (which depends on u and $\mu\tilde{a}$)

$$A^{(N)} = \exp \left\{ \frac{N}{2} \int_1^0 [\zeta_\varphi(\ell') - \zeta_\varphi(0)] \frac{d\ell'}{\ell'} \right\}. \quad (48)$$

The amplitude function $f^{(N)}(1, u, 0, d)$ is finite and non-singular at $u = u^* > 0$ for $d < 4$ (compare the above statement after (43) regarding the renormalizability of $\tilde{\Gamma}_R^{(N)}$). We see that the dependence on the lattice constant \tilde{a} has disappeared asymptotically ($\tilde{a}/\xi \rightarrow 0$) in the amplitude function on the right-hand side of (46). Thus \tilde{a} enters the asymptotic bulk critical behavior of $\tilde{\Gamma}_R^{(N)}$ only *via* $A^{(N)}$

(beyond one-loop order) which is independent of ξ , and *via* the amplitude ξ_0 of ξ (see (A.17)). Therefore, taking the limit $\tilde{a} \rightarrow 0$ in the renormalized quantity $\tilde{\Gamma}_R^{(N)}$ (as is usually done) is indeed justified in the asymptotic bulk theory since this limit does not change the asymptotic *temperature* dependence. For the asymptotic *size* dependence of the confined system, however, a corresponding property is not generally valid, as we shall see in the subsequent Sections.

Application of the results to $N = 2$ yields, according to (8), the bare (physical) bulk susceptibility at $\mathbf{k} = \mathbf{0}$

$$\chi_b = Z_\varphi(u, \tilde{a}/\xi_0, d)\xi^2 \left[f^{(2)}(1, u(\ell), \tilde{a}/\xi, d) \right]^{-1} \times \exp \int_\ell^1 \zeta_\varphi(\ell') \frac{d\ell'}{\ell'}. \quad (49)$$

The asymptotic ($\ell \rightarrow 0, \xi \rightarrow \infty$) critical behavior above T_c is

$$\chi_b = \tilde{A}_\chi \xi^{2-\eta} = A_\chi^+ t^{-\gamma}. \quad (50)$$

The amplitudes depend on \tilde{a} according to

$$\tilde{A}_\chi = Z_\varphi(u, \tilde{a}/\xi_0, d)\xi_0^\eta \left[A^{(2)} f^{(2)}(1, u^*, 0, d) \right]^{-1}, \quad (51)$$

$$A_\chi^+ = \xi_0^{2-\eta} \tilde{A}_\chi, \quad (52)$$

where we have used $\mu = \xi_0^{-1}$ and the asymptotic form

$$\xi = \xi_0 t^{-\gamma} \quad (53)$$

with $\gamma = \nu(2 - \eta)$. The dependence of ξ_0 on \tilde{a} is given in (A.17) of Appendix A.

2.4 Continuum approximation

For comparison we shall also consider the more standard version of the φ^4 theory that is based on the continuum Hamiltonian [3, 13, 51]

$$H = \int_V d^d x \left[\frac{1}{2} r_0 \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 + u_0 (\varphi^2)^2 \right] \quad (54)$$

for the n -component field $\varphi(\mathbf{x})$. Here the $(\nabla \varphi)^2$ term approximates the $(\varphi_i - \varphi_j)^2$ term of the lattice Hamiltonian (7). The fluctuations of $\varphi(\mathbf{x})$ are confined to wavenumbers less than a finite cutoff Λ corresponding to π/\tilde{a} . The bulk susceptibility corresponding to (9) is now defined by

$$\chi_b(\mathbf{k}) = \lim_{L \rightarrow \infty} \int_V d^d x \langle \varphi(\mathbf{x}) \varphi(0) \rangle e^{-i\mathbf{k} \cdot \mathbf{x}}. \quad (55)$$

In the bulk limit, most expressions of the φ^4 lattice theory at finite \tilde{a} remain applicable also to the φ^4 field theory at finite Λ after the replacements $\hat{J}_\mathbf{k} \rightarrow \mathbf{k}^2$, $J_0 \rightarrow 1$ and $\tilde{a} \rightarrow \pi/\Lambda$ have been made. This implies that the asymptotic

critical *temperature* dependence of the φ^4 field and lattice theory for bulk systems is identical (apart from different nonuniversal amplitudes). For confined systems, however, a corresponding statement regarding the *size* dependence is not generally valid as we shall see in the subsequent Sections.

3 Renormalization group and finite-size scaling

We are now in the position to discuss the size dependence of physical quantities within a renormalization-group treatment of the lattice model (7) with a finite volume $V = L^d$. (For different geometries see below.) We focus our analysis on the example of the susceptibility above T_c

$$\chi = \frac{\tilde{a}^{2d}}{L^d} \sum_{i,j} \langle \varphi_i \varphi_j \rangle \quad (56)$$

$$= \chi(\xi, u_0, L, \tilde{a}, d). \quad (57)$$

Here we consider χ as a function of the bulk correlation length ξ (rather than of r_0) as explained in Section 2.

The basic assumption in the following is that, for periodic boundary conditions, the ultraviolet divergences of χ in the limit $\tilde{a} \rightarrow 0$ for the confined system are the same as those of the bulk susceptibility χ_b . This plausible assumption is in accord with the argument of Brézin [4] regarding the decomposition of Fourier sums into bulk integrals (which carry the ultraviolet divergent part) and finite-size contributions (which are finite in the limit $\tilde{a} \rightarrow 0$). It is also in accord with one-loop results (Sect. 4) and with exact results in the large- n limit (Sect. 5). Although this assumption has far-reaching consequences regarding the validity of finite-size scaling for fixed finite L/ξ we shall show that it does not rule out the possibility of a violation of finite-size scaling in the limit $L \gg \xi$.

Our assumption implies that the renormalized susceptibility χ_R at finite L and at finite \tilde{a} can be introduced for $d \leq 4$ as

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) = Z_\varphi^{-1} \chi(\xi, \mu^\epsilon J_0^2 Z_u u, L, \tilde{a}, d) \quad (58)$$

where $Z_\varphi(u, \mu\tilde{a}, d)$ and $Z_u(u, \mu\tilde{a}, d)$ are the *bulk* Z factors defined in Section 2 and that χ_R remains finite in the limit $\tilde{a} \rightarrow 0$ at fixed ξ, u, L and μ for $d \leq 4$. We note that there exists no justification *a priori*, however, to actually perform this limit $\tilde{a} \rightarrow 0$ in the final results of the φ^4 theory if they are to be compared with those of model systems on lattices with a finite lattice constant, *e.g.*, with Monte-Carlo data for Ising models. Therefore we shall keep \tilde{a} finite in the following analysis of the size dependence of χ_R and of χ .

We derive a renormalization-group equation for χ_R by taking the derivative of (58) with respect to μ at fixed u_0, \tilde{a}, L and $r_0 - r_{0c}$, *i.e.*, at fixed ξ . Since L is not renormalized [4] this yields

$$\left[\mu \partial_\mu + \beta_u \partial_u - \zeta_\varphi \right] \chi_R(\xi, u, L, \mu, \tilde{a}, d) = 0 \quad (59)$$

where $\beta_u(u, \mu\tilde{a}, d)$ and $\zeta_\varphi(u, \mu\tilde{a}, d)$ are defined by (37) and (38) of the bulk theory. The solution reads for $d \leq 4$

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) = \chi_R(\xi, u(\ell), L, \ell\mu, \tilde{a}, d) \times \exp \int_{\ell}^1 \zeta_\varphi(\ell') \frac{d\ell'}{\ell'} \quad (60)$$

where ℓ can be chosen arbitrarily in an exact theory. For the purpose of an application to perturbative results a natural choice is

$$\xi^{-2} + L^{-2} = \mu^2 \ell^2. \quad (61)$$

Although the RGE (59) has the same form as the bulk RGE (36) the simultaneous appearance of the *three* lengths ξ, L and \tilde{a} in the arguments of χ_R in (59) and (60) complicates the situation and requires a careful consideration of different limiting cases. To answer the question about the possible relevance of the dependence on \tilde{a} we distinguish the following three cases (i)-(iii).

(i) At $T = T_c$ or $\xi = \infty$ and at finite L , we introduce a dimensionless function \tilde{f}_χ according to

$$\chi_R(\infty, u, L, \mu, \tilde{a}, d) = L^2 \tilde{f}_\chi(\infty, u, \mu L, \tilde{a}/L, d). \quad (62)$$

In the large- L limit we obtain from (60)-(62) with $\ell = \mu^{-1}L^{-1}$

$$\chi_R(\infty, u, L, \mu, \tilde{a}, d) \sim L^2 (\mu L)^{-\eta} [A^{(2)}]^{-1} \times \tilde{f}_\chi(\infty, u^*, 1, \tilde{a}/L, d) \quad (63)$$

where η and $A^{(2)}$ are given in (47, 48). The remaining dependence of \tilde{f}_χ on \tilde{a}/L in (63) yields only a subleading correction to the leading power law $\sim L^{2-\eta}$ provided that the function $f_\chi(\infty, u^*, 1, 0, d)$ is finite. The latter property is valid for $d < 4$ (where $u^* > 0$) provided that the φ^4 theory is renormalizable at finite L and \tilde{f}_χ is non-singular at T_c for finite μL , *i.e.*, provided that the limit (at fixed u and L)

$$\lim_{\tilde{a} \rightarrow 0} \tilde{f}_\chi(\infty, u, 1, \tilde{a}/L, d) = \tilde{f}_\chi(\infty, u, 1, 0, d) \quad (64)$$

exists and is finite for $u > 0$ at $d \leq 4$.

(ii) For $0 < \xi < \infty$ at finite L , *i.e.*, at finite ratio $0 < \xi/L < \infty$, we introduce the dimensionless amplitude function f_χ according to

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) = \xi^2 f_\chi(\mu\xi, u, \mu L, \tilde{a}/L, d). \quad (65)$$

In the asymptotic region $\xi \gg \tilde{a}, L \gg \tilde{a}$ corresponding to $\ell \ll 1$ we obtain from (60)

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) \sim \xi^{2\ell\eta} [A^{(2)}]^{-1} \times f_\chi(\ell\mu\xi, u^*, \ell\mu L, \tilde{a}/L, d), \quad (66)$$

Renormalizability of the φ^4 theory at finite L guarantees that the limit

$$\lim_{\tilde{a} \rightarrow 0} f_\chi(\mu\xi, u, \mu L, \tilde{a}/L, d) = f_\chi(\mu\xi, u, \mu L, 0, d) \quad (67)$$

exists and is finite for finite arguments and $d \leq 4$. Therefore, taking the limit $L \rightarrow \infty$ in (66) at fixed finite ratio $0 < L/\xi < \infty$, *i.e.*, at fixed values of $\ell\mu\xi$ and $\ell\mu L$, yields a finite amplitude function for $d < 4$ ($u^* > 0$)

$$f_\chi(\ell\mu\xi, u^*, \ell\mu L, 0, d) = Y(L/\xi) \quad (68)$$

on the right-hand side of (66). Here we have used the fact that $\ell\mu\xi$ and $\ell\mu L$ depend only on L/ξ according to (61). Thus the dependence on \tilde{a}/L in (66) represents only a subleading correction to the leading size-dependence (68) provided that L/ξ is finite. This implies that both $\chi = Z_\varphi(u, \mu\tilde{a}, d)\chi_R$ and χ_R attain the finite-size scaling form

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) \sim \xi^{2-\eta} \mu^{-\eta} (1 + \xi^2/L^2)^{\eta/2} \times [A^{(2)}]^{-1} Y(L/\xi) \quad (69)$$

in the asymptotic region $L \gg \tilde{a}$ and $\xi \gg \tilde{a}$ for any finite ratio $0 < L/\xi < \infty$. This is in agreement with Brézin's conclusion [4] who performed the limit $\tilde{a} \rightarrow 0$ at the outset.

(iii) There exist, however, significant paths in the asymptotic $L^{-1} - \xi^{-1}$ plane (Fig. 1) along which the ratio L/ξ does not remain finite but diverges. These paths include the approach towards asymptotic bulk critical behavior at fixed $\tilde{a}/\xi > 0$ (arrow in Fig. 1). This case is not covered by the discussion of case (ii) above and was not considered in Brézin's analysis [4]. In this regime ($L/\xi \gg 1, \tilde{a}/\xi > 0$) we make the choice

$$\ell = \mu^{-1}\xi^{-1} \quad (70)$$

instead of (61). From (60), (66) and (70) we then obtain asymptotically

$$\chi_R(\xi, u, L, \mu, \tilde{a}, d) \sim \xi^{2-\eta} \mu^{-\eta} [A^{(2)}]^{-1} \times f_\chi(1, u^*, L/\xi, \tilde{a}/L, d). \quad (71)$$

In the bulk limit $L \rightarrow \infty$ at fixed $\xi < \infty$, equations (58) and (71) agree with (50) and (51) where

$$f_\chi(1, u^*, \infty, 0, d) = [f^{(2)}(1, u^*, 0, d)]^{-1} \equiv f_b^*. \quad (72)$$

Similar to the case (ii), the renormalizability of the φ^4 theory at finite L guarantees that in the limit $\tilde{a} \rightarrow 0$ the function

$$\lim_{\tilde{a} \rightarrow 0} f_\chi(1, u^*, L/\xi, \tilde{a}/L, d) = f_\chi(1, u^*, L/\xi, 0, d) \equiv f_b^* - f_1(L/\xi) \quad (73)$$

exists and is finite for finite arguments (with $u^* > 0$ for $d < 4$ dimensions). Thus, at first sight, the dependence of f_χ on \tilde{a}/L on the right-hand side of (71) appears to be a subleading correction that can be neglected in the asymptotic region $\tilde{a}/L \ll 1$, similar to the case (ii). A closer inspection shows, however, that this reasoning is not compelling in the present case (iii) where L/ξ may become arbitrarily large at fixed finite ξ .

On a formal level this is seen by rewriting the dimensionless function f_χ as

$$f_\chi(1, u^*, L/\xi, \tilde{a}/L, d) = F_\chi(L/\xi, \tilde{a}/\xi) \quad (74)$$

where the dependence of F_χ on \tilde{a} appears in the form \tilde{a}/ξ rather than \tilde{a}/L . Now there exists no argument why the dependence on \tilde{a}/ξ should be negligible in the limit $L/\xi \gg 1$ at fixed $\tilde{a}/\xi > 0$. More specifically, consider the decomposition

$$F_\chi(L/\xi, \tilde{a}/\xi) = f_b^* - f_1(L/\xi) - f_2(L/\xi, \tilde{a}/\xi) \quad (75)$$

where f_b^* and f_1 are independent of \tilde{a} as defined in (72) and (73). The last term f_2 contains the complete \tilde{a} dependence of f_χ and vanishes for $\tilde{a} \rightarrow 0$.

Clearly only the term $f_1(L/\xi)$ in (75) is in agreement with finite-size scaling in contrast to the term $f_2(L/\xi, \tilde{a}/\xi)$. Thus the fundamental question arises whether the size dependence of f_2 at finite \tilde{a}/ξ and for large L/ξ is asymptotically negligible compared to that of f_1 . Only if the ratio

$$R(L/\xi, \tilde{a}/\xi) = \frac{f_2(L/\xi, \tilde{a}/\xi)}{f_1(L/\xi)} \quad (76)$$

of equations (3)-(6) would vanish as $L/\xi \rightarrow \infty$ at fixed $0 < \tilde{a}/\xi < \infty$ there would be no violation of finite-size scaling. Renormalizability guarantees the existence of the function $f_1(L/\xi)$ but does not say anything about the magnitude and sign of the ratio $R(L/\xi, \tilde{a}/\xi)$ in the regime $L/\xi \gg 1$. Although it is clear that the *total* finite-size deviation from asymptotic bulk critical behavior (compare (2))

$$\Delta\chi \equiv \frac{\chi_b - \chi}{\chi_b} = \frac{f_b^* - f_\chi(1, u^*, L/\xi, \tilde{a}/L, d)}{f_b^*} \quad (77)$$

$$= \frac{f_1(L/\xi)}{f_b^*} \left[1 + R(L/\xi, \tilde{a}/\xi) \right] \quad (78)$$

must approach zero as L/ξ increases, renormalizability does not rule out the possibility that the *relative* contribution described by $|R|$ increases and becomes large compared to 1 with increasing L at fixed $\xi < \infty$ and $\tilde{a} > 0$ in the region $L \gg \xi$. In fact it does not even rule out the possibility that $R(L/\xi, \tilde{a}/\xi)$ *diverges* as $L/\xi \rightarrow \infty$ at fixed $0 < \tilde{a}/\xi < \infty$. If this is the case then f_2 becomes dominant compared to f_1 in (75) and finite-size scaling is violated in the lower part of the $L^{-1} - \xi^{-1}$ plane close to the bulk limit (Fig. 1).

We illustrate these considerations by a simple example: if $f_2(x, y)$ would be xy for small y and for general (arbitrarily large) x , then one should not dismiss $f_2(x, y)$ as a correction that is negligible (compared to $f_1(x)$) for small $y > 0$ since f_2 can become large for $x \gg 1/y$. Actually we shall specify $f_2(x, y)$ essentially as an exponential function of xy^2 (see Eqs. (103) and (104)).

No general arguments but only explicit calculations can answer our question about the magnitude and sign of the *nonuniversal* quantity R . In Section 4 we shall calculate R for general n in one-loop order. In Section 5 the

exact form of R will be derived in the large- n limit. We shall indeed show that R diverges,

$$\lim_{x \rightarrow \infty} R(x, \tilde{a}/\xi) = \infty, \quad \tilde{a}/\xi \text{ fixed}, \quad \tilde{a}/\xi > 0 \quad (79)$$

at any finite \tilde{a}/ξ for the φ^4 lattice model below four dimensions. Corresponding properties remain valid also in the cases $d = 4$ and $d > 4$ whose consequences will be studied elsewhere [58].

The analysis of this Section can be repeated for the field-theoretic φ^4 model at finite cutoff Λ . The reasoning remains of course parallel to that given above and leads to the question about the magnitude and sign of the ratio $R_{\text{field}}(L/\xi, \Lambda\xi)$. We shall show in Sections 4 and 5 that R_{field} differs fundamentally from R and that in both cases finite-size scaling is violated for $L/\xi \gg 1$.

Finally we note that the analysis of this Section did not make explicit use of periodic boundary conditions except that the renormalizability in terms of bulk Z factors was assumed according to (58). Therefore our line of thoughts should remain applicable more generally to those cases where the bulk renormalizations suffice to renormalize the physical quantities of the confined system. Our analysis should also be extended to the important case where additional (surface) renormalizations come into play which, for confined systems, have been studied so far only in the continuum approximation (54) (with surface terms) and only in the limit $\Lambda \rightarrow \infty$.

4 Perturbation theory above T_c

As is well known a calculation of finite-size effects within the φ^4 theory including the size-dependence at T_c requires a decomposition into modes where the lowest mode is separated and only the higher modes are treated perturbatively [16,17]. As noted recently [52], however, this perturbative calculation does not correctly capture the exponential size dependence of the approach towards bulk critical behavior within the φ^4 lattice model. Covering the size dependence in the entire $L^{-1} - \xi^{-1}$ plane, *i.e.*, both at $T = T_c$ as well as for $L/\xi \gg 1$ at fixed $\xi < \infty$, would require a non-perturbative treatment [52] within the mode expansion mentioned above. Such a treatment could be given on the basis of the order-parameter distribution function [47] that includes the higher modes in a non-perturbative way.

Here we point out, however, that such a non-perturbative treatment can be avoided because the exponential size dependence of the φ^4 lattice model above T_c is not of a truly non-perturbative nature, unlike the effects due to the Goldstone modes below T_c [47]. We shall show that an ordinary renormalized perturbation approach is sufficient if one restricts oneself to the region $L > \xi$ above T_c . This is just the region where the nonuniversal finite-size effects due to a finite lattice constant become significant. In this region a separation between the lowest mode and the higher modes is unnecessary since the lowest mode does not become dangerous in the bulk limit $L \rightarrow \infty$ at fixed

$\xi < \infty$. It does not even become dangerous in the limit $L \rightarrow \infty, \xi \rightarrow \infty$ at fixed finite ratio $L/\xi > 0$. Therefore we do not separate the lowest mode but instead shall present an ordinary perturbation approach, similar to bulk perturbation theory, where all modes are treated in the same way. Although this approach deteriorates with increasing ξ/L and breaks down in the region $\xi \gg L$ due to the dangerous lowest mode, it is well applicable for $L > \xi$.

4.1 Lattice model at finite lattice constant

We start out from the φ^4 lattice Hamiltonian (7) (for a d dimensional cube with $V = L^d$ and periodic boundary conditions) in the Fourier representation

$$H = L^{-d} \sum_{\mathbf{k}} \frac{1}{2} [r_0 + \hat{J}_{\mathbf{k}}] \varphi_{\mathbf{k}} \varphi_{-\mathbf{k}} + u_0 L^{-3d} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{k}''} (\varphi_{\mathbf{k}} \varphi_{\mathbf{k}'})(\varphi_{\mathbf{k}''} \varphi_{-\mathbf{k}-\mathbf{k}'-\mathbf{k}''}), \quad (80)$$

$$\varphi_{\mathbf{k}} = \tilde{a}^d \sum_j e^{-i\mathbf{k} \cdot \mathbf{x}_j} \varphi_j \quad (81)$$

where $\hat{J}_{\mathbf{k}}$ is defined by (22) and (23) but now for the finite lattice. The summations in (80) run over discrete \mathbf{k} vectors with components $k_j = 2\pi m_j/L, m_j = 0, \pm 1, \pm 2, \dots, j = 1, 2, \dots, d$ in the range $-\pi/\tilde{a} \leq k_j < \pi/\tilde{a}$ with a finite lattice spacing \tilde{a} .

The standard one-loop expression for the (inverse) susceptibility (56) above T_c reads for the finite system

$$\chi^{-1} = r_0 + 4(n+2)u_0 L^{-d} \sum_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} + O(u_0^2) \quad (82)$$

and

$$\chi_b^{-1} = r_0 + 4(n+2)u_0 \int_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} + O(u_0^2) \quad (83)$$

for the bulk system. Since $\hat{J}_{\mathbf{k}}$ is a periodic function of each component k_j the one-loop sum in (82) satisfies the Poisson identity at finite \tilde{a} [4,83]

$$L^{-d} \sum_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} = \sum_{\mathbf{n}} \int_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} e^{i\mathbf{k} \cdot \mathbf{n}L} \quad (84)$$

where $\mathbf{k} \cdot \mathbf{n} = \sum_j k_j n_j$. The sum $\sum_{\mathbf{n}}$ runs over all integers $n_j, j = 1, 2, \dots, d$ in the range $-\infty \leq n_j \leq \infty$ (whereas $\sum_{\mathbf{k}}$ and $\int_{\mathbf{k}}$ have finite cutoffs $\pm\pi/\tilde{a}$). The crucial quantity that contains all finite-size effects is the function

$$D(r_0, L, \tilde{a}) = L^{-d} \sum_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} - \int_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} \quad (85)$$

$$= \sum_{\mathbf{n} \neq \mathbf{0}} \int_{\mathbf{k}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} e^{i\mathbf{k} \cdot \mathbf{n}L}. \quad (86)$$

The sum $\sum_{\mathbf{k}}$ in (85) includes the lowest-mode ($\mathbf{k} = \mathbf{0}$) term $L^{-d} r_0^{-1}$. It is only this lowest-mode term that diverges for $r_0 \rightarrow 0$ at finite L whereas the $\mathbf{k} \neq \mathbf{0}$ contributions remain finite in this limit. For finite $r_0 L^2 > 0, D(r_0, L, \tilde{a})$ is of $O(L^{2-d})$ whereas for $r_0 L^2 \gg 1$ it is of $O(\exp -Lr_0^{1/2})$ (see below). A simple rearrangement yields

$$\chi(\xi, u_0, L, \tilde{a}, d)^{-1} = J_0 \xi^{-2} \times \left[1 + 4(n+2)u_0 J_0^{-2} \xi^2 \tilde{D} + O(u_0^2) \right] \quad (87)$$

with $\tilde{D} = J_0 D(J_0 \xi^{-2}, L, \tilde{a})$, *i.e.*,

$$\tilde{D}(\xi, L, \tilde{a}) = L^{-d} \sum_{\mathbf{k}} (\xi^{-2} + \hat{J}_{\mathbf{k}}/J_0)^{-1} - \int_{\mathbf{k}} (\xi^{-2} + \hat{J}_{\mathbf{k}}/J_0)^{-1} \quad (88)$$

where we have used $\chi_b^{-1} = J_0 \xi^{-2} + O(u_0^2)$ on the level of bare perturbation theory according to (8) and (20).

The quantity \tilde{D} remains finite in the limit $\tilde{a} \rightarrow 0$ for finite ξ in arbitrary dimensions. This means that the ultraviolet divergence of χ at finite L in one-loop order is absorbed by the *bulk* correlation length ξ , in accord with the assumption in Section 3. For $\tilde{a} \rightarrow 0$ and $L/\xi > 0$, the function \tilde{D} can be represented as [16,17]

$$\tilde{D}(\xi, L, 0) = L^{2-d} I(L^2/\xi^2) \quad (89)$$

where

$$I(x) = (4\pi^2)^{-1} \int_0^\infty dz e^{-xz/4\pi^2} \left[K(z)^d - \left(\frac{\pi}{z}\right)^{d/2} \right] \quad (90)$$

with

$$K(z) = \sum_{m=-\infty}^\infty \exp(-zm^2). \quad (91)$$

$I(x)$ diverges for $x \rightarrow 0$ due to the lowest-mode term but is exponentially small for $x \gg 1$. For $\tilde{a} > 0$ we decompose \tilde{D} as

$$\tilde{D}(\xi, L, a) = L^{2-d} f_D(L/\xi, \tilde{a}/\xi), \quad (92)$$

$$f_D(L/\xi, \tilde{a}/\xi) = I(L^2/\xi^2) + M(L/\xi, \tilde{a}/\xi), \quad (93)$$

where $M(L/\xi, \tilde{a}/\xi)$ contains the \tilde{a} dependence of \tilde{D} and vanishes for $\tilde{a} \rightarrow 0$. The explicit form of $M(L/\xi, \tilde{a}/\xi)$ will be determined by equations (98), (101), (103) and (104) below.

We note that \tilde{D} does not require a renormalization as it depends only on L, ξ and \tilde{a} . Application of the RG analysis of the preceding Section to (87) yields

$$\chi = Z_\varphi(u, \mu \tilde{a}, d) f_\chi[\ell \mu \xi, u(\ell), \ell \mu L, \tilde{a}/L, d] \xi^2 \times \exp \int_\ell^1 \zeta_\varphi(\ell') \frac{d\ell'}{\ell'} \quad (94)$$

where in one-loop order

$$f_\chi(\mu\xi, u, \mu L, \tilde{a}/L, d) = J_0^{-1} \left\{ 1 - 4(n+2)u\mu^\epsilon \xi^\epsilon (\xi/L)^{d-2} \times f_D(L/\xi, \tilde{a}/\xi) + O(u^2) \right\}. \quad (95)$$

For the application to $L/\xi \gg 1$ at $\tilde{a}/\xi > 0$ we choose the flow parameter as $\ell = \mu^{-1}\xi^{-1}$. Then the finite-size deviation $\Delta\chi$ from the bulk susceptibility

$$\chi_b = Z_\varphi(u, \mu\tilde{a}, d) \left\{ J_0^{-1} + O[u(\ell)^2] \right\} \xi^2 \exp \int_\ell^1 \zeta_\varphi(\ell') \frac{d\ell'}{\ell'} \quad (96)$$

becomes in one-loop order

$$\frac{\chi_b - \chi}{\chi_b} = 4(n+2)u(\ell)(\xi/L)^{d-2} I(L^2/\xi^2) \times \left[1 + R(L/\xi, \tilde{a}/\xi) \right] + O[u(\ell)^2] \quad (97)$$

with

$$R(L/\xi, \tilde{a}/\xi) = \frac{M(L/\xi, \tilde{a}/\xi)}{I(L^2/\xi^2)}. \quad (98)$$

These results are valid at finite \tilde{a} for both $d < 4$ and $d = 4$ dimensions and still contain all non-asymptotic contributions (Wegner corrections [82]) within the φ^4 model. These contributions enter through $u(\ell)$ as well as through the non-asymptotic form of ξ as a function of t as determined by (A.11) of Appendix A. Sufficiently close to T_c such non-asymptotic contributions become negligible. By contrast, the nonuniversal term $R(L/\xi, \tilde{a}/\xi)$ *cannot be considered as a non-asymptotic contribution* since it is nonnegligible at any $T > T_c$ for sufficiently large L as we shall see below.

Neglecting the deviation of $u(\ell)$ from the fixed point value u^* we obtain for $d < 4$

$$\Delta\chi \equiv \frac{\chi_b - \chi}{\chi_b} = g(L/\xi) \left[1 + R(L/\xi, \tilde{a}/\xi) \right] \quad (99)$$

with the universal part

$$g(L/\xi) = 4(n+2)u^*(\xi/L)^{d-2} I(L^2/\xi^2) + O(u^{*2}). \quad (100)$$

For $L/\xi \gg 1$ the function $I(L^2/\xi^2)$ becomes

$$I(L^2/\xi^2) = d(2\pi)^{(1-d)/2} (L/\xi)^{(d-3)/2} \exp(-L/\xi). \quad (101)$$

The nonuniversal part $R(L/\xi, \tilde{a}/\xi)$ depends on the detailed form of $\hat{J}_{\mathbf{k}}$. For simplicity we assume a simple-cubic lattice with nearest-neighbor coupling J ,

$$\hat{J}_{\mathbf{k}} = \frac{4J}{\tilde{a}^2} \sum_{j=1}^d [1 - \cos(\tilde{a}k_j)], \quad (102)$$

which implies $J_0 = 2J$. A calculation parallel to that in Appendix A of reference [66] yields for $L \gg \xi \gg \tilde{a}$

$$R(L/\xi, \tilde{a}/\xi) = \exp \left[\Gamma(\tilde{a}/\xi) \frac{L}{\xi} \right] - 1 \quad (103)$$

with the function

$$\Gamma(\tilde{a}/\xi) = \frac{1}{24} (\tilde{a}/\xi)^2 + O[(\tilde{a}/\xi)^3]. \quad (104)$$

We see that, at any fixed $\tilde{a}/\xi > 0$, R diverges for $L/\xi \rightarrow \infty$. Thus the term $R(L/\xi, \tilde{a}/\xi)$ is nonnegligible for sufficiently large L , even arbitrarily close to T_c , unlike the Wegner corrections [82] arising from the deviation of the effective coupling $u(\ell)$ in (97) from its fixed point value u^* . The resulting asymptotic size dependence of $\Delta\chi$ for large L/ξ and fixed $\tilde{a}/\xi > 0$ is determined by

$$\frac{\chi_b - \chi}{\chi_b} \sim g(L/\xi) R(L/\xi, \tilde{a}/\xi) = 4(n+2)u^* d(2\pi)^{(1-d)/2} (L/\xi)^{(1-d)/2} \quad (105)$$

$$\times \exp \left[\frac{1}{24} (\tilde{a}/\xi)^2 \frac{L}{\xi} \right] \exp(-L/\xi) \quad (106)$$

with $u^* > 0$ for $d < 4$. This behavior is nonuniversal and depends on the *two* ratios L/ξ and \tilde{a}/ξ in an essential way, rather than only on L/ξ . A dominant influence of \tilde{a}/ξ exists in the non-scaling region where $R > 1$ corresponding to the region below the dashed line in the $L^{-1} - \xi^{-1}$ plane in Figure 1. This line is determined by $R = 1$, *i.e.*,

$$\tilde{a}/L = [24 \ln 2]^{-1} (\tilde{a}/\xi)^3. \quad (107)$$

Non-negligible effects arising from R exist already above this line.

The exponential part of (106) could be written in the form $\exp(-L/\xi_{\text{eff}})$ with $\xi_{\text{eff}} = \xi/[1 - (\tilde{a}/\xi)^2/24 + \dots]$ which then would hide the violation of finite-size scaling (whereas the violation is quite explicit in the form of (103)-(106)). But the true bulk correlation length ξ (including all non-asymptotic bulk corrections) is already precisely defined by (10) and cannot be arbitrarily redefined here to comply with scaling.

As a remarkable feature we note that, in one-loop order, the nonuniversal function R and the condition (107) are independent of the dimension d , of the number of components n and of the fixed point value u^* of the four-point coupling. Therefore the same function $R(L/\xi, \tilde{a}/\xi)$ causes a violation of the two-variable finite-size scaling form [59,60,63,66-68] above four dimensions as will be further discussed elsewhere [58].

These results can be easily generalized to a d dimensional system with a partially finite geometry that is confined in \tilde{d} dimensions (size L) and is infinite in $d - \tilde{d}$ dimensions. This includes the cubic, film and cylindrical geometries as special cases $\tilde{d} = d$, $\tilde{d} = 1$ and $\tilde{d} = d - 1$, respectively. Instead of (82) we then have

$$\chi^{-1} = r_0 + 4(n+2)u_0 L^{-\tilde{d}} \sum_{\mathbf{q}, \mathbf{p}} (r_0 + \hat{J}_{\mathbf{k}})^{-1} + O(u_0^2) \quad (108)$$

where the d -dimensional vector $\mathbf{k} = (\mathbf{q}, \mathbf{p})$ has \tilde{d} components $\mathbf{q} = (q_1, \dots, q_{\tilde{d}})$ and $d - \tilde{d}$ components

$\mathbf{p} = (p_{\tilde{d}+1}, \dots, p_d)$. Equation (88) is modified accordingly. The integral representation of $I(L^2/\xi^2)$, (90), is replaced by

$$I(x) = (4\pi^2)^{-1} \int_0^\infty dz e^{-xz/4\pi^2} \times \left[K(z)^{\tilde{d}} \left(\frac{\pi}{z} \right)^{(d-\tilde{d})/2} - \left(\frac{\pi}{z} \right)^{d/2} \right]. \quad (109)$$

For $L/\xi \gg 1$ this yields, instead of (101),

$$I(L^2/\xi) = \tilde{d}(2\pi)^{(1-d)/2} (L/\xi)^{(d-3)/2} \exp(-L/\xi). \quad (110)$$

The function $R(L/\xi, \tilde{a}/\xi)$, however, remains unchanged, *i.e.*, it is independent of the geometry (in one-loop order). Thus the leading finite-size deviation $\Delta\chi$ for large L/ξ and fixed $\tilde{a}/\xi > 0$ for general $\tilde{d} \leq d < 4$ is given by

$$\frac{\chi_b - \chi}{\chi_b} \sim 4(n+2)u^* \tilde{d}(2\pi)^{(1-d)/2} (L/\xi)^{(1-d)/2} \times \exp \left[\frac{1}{24} (\tilde{a}/\xi)^2 \frac{L}{\xi} \right] \exp(-L/\xi). \quad (111)$$

This differs from (106) only by the replacement $d \rightarrow \tilde{d}$ in the prefactor.

We conclude that finite-size scaling is violated below four dimensions in the φ^4 lattice model with periodic boundary conditions above T_c in one-loop order for general n in the region $L/\xi \gg 1$ at any finite $\xi < \infty$ even arbitrarily close to T_c . Clearly higher-loop contributions cannot remedy this violation.

Although one should trust the perturbative results of the φ^4 theory primarily for $2 < d \leq 4$ one cannot exclude the possibility that an extrapolation to $d = 2$ yields sensible results, possibly for general n above T_c and for $n = 1$ below T_c . This appears to be suggestive for the structure of our results (97), (106) and (111). This could be of particular relevance for the case $n = 1$ for which exact results of the two-dimensional Ising model in a confined geometry are available [53, 84]. In all cases, contributions with an exponential size dependence were found above T_c for $L \gg \xi$. It would be interesting to reanalyze these results [53, 84] including all exponential and non-exponential prefactors which so far have not been worked out explicitly (see, *e.g.*, Eq. (6.8) of Ref. [6]) and to compare the structure of these results with that of our equations (106) and (111). Our results suggest that these prefactors may contain *nonuniversal* contributions (such as our \tilde{a} dependent exponential factor) that cannot be neglected in the limit $L/\xi \gg 1$ at fixed $\tilde{a}/\xi > 0$.

4.2 Field-theoretic model at finite sharp cutoff

The susceptibility above T_c of the field-theoretic model (54) is defined as

$$\chi = \int_V d^d x \langle \varphi(\mathbf{x}) \varphi(\mathbf{0}) \rangle. \quad (112)$$

The one-loop expression of the susceptibility for a cubic geometry, $V = L^d$, reads (compare (87) and (88))

$$\chi(\xi, u_0, L, \Lambda, d)^{-1} = \xi^{-2} \left[1 + 4(n+2)u_0 \xi^2 \tilde{D}_{\text{field}} + O(u_0^2) \right] \quad (113)$$

where now

$$\tilde{D}_{\text{field}}(\xi, L, \Lambda) = L^{-d} \sum_{\mathbf{k}} (\xi^{-2} + \mathbf{k}^2)^{-1} - \int_{\mathbf{k}} (\xi^{-2} + \mathbf{k}^2)^{-1}. \quad (114)$$

Here the range of \mathbf{k} is limited by a sharp cutoff Λ according to $|k_j| \leq \Lambda$ for the bulk integral $\int_{\mathbf{k}}$ and $-A \leq k_j < A$ for

the sum $\sum_{\mathbf{k}}$. For $\Lambda \rightarrow \infty$ the function \tilde{D}_{field} becomes identical with \tilde{D} for $\tilde{a} \rightarrow 0$. Thus we decompose

$$\tilde{D}_{\text{field}} = L^{2-d} [I(L^2/\xi^2) + M_{\text{field}}(\Lambda L, \Lambda \xi)] \quad (115)$$

with $M_{\text{field}}(\infty, \infty) = 0$ where the function $I(L^2/\xi^2)$ is the same as for the lattice model for $\tilde{a} \rightarrow 0$, (90) and (91), but the cutoff dependent part M_{field} of \tilde{D}_{field} differs fundamentally from the \tilde{a} dependent part M of \tilde{D} , as we shall see.

Application of the RG analysis of Section 3 to the field-theoretic model leads to

$$\frac{\chi_b - \chi}{\chi_b} = 4(n+2)u(\ell)(\xi/L)^{d-2} I(L^2/\xi^2) \times \left[1 + R_{\text{field}}(L/\xi, \Lambda \xi) \right] + O[u(\ell)^2] \quad (116)$$

with

$$R_{\text{field}}(L/\xi, \Lambda L) = \frac{M_{\text{field}}(\Lambda L, \Lambda \xi)}{I(L^2/\xi^2)}. \quad (117)$$

Equation (116) is valid for $d \leq 4$. For $\Lambda L \gg 1$ and $\Lambda \xi \gg 1$ we have found [52, 63, 66]

$$M_{\text{field}}(\Lambda L, \Lambda \xi) = -da_0(d)(\Lambda L)^{d-4} + O[(\Lambda L)^{d-6}, \exp(-\Lambda^{-2}\xi^{-2})] \quad (118)$$

where

$$a_0(d) = \frac{2\pi}{3} \int_0^\infty dx x e^{-x} \left[\frac{1}{2\pi} \int_{-1}^1 dy \exp(-y^2 x) \right]^{d-1}. \quad (119)$$

Together with $I(L^2/\xi^2)$, (101), this yields the large ΛL behavior of R_{field} at fixed $\Lambda \xi \gg 1$

$$R_{\text{field}}(L/\xi, \Lambda L) = -(2\pi)^{(d-1)/2} a_0(d) (L/\xi)^{(3-d)/2} \times (\Lambda L)^{d-4} e^{L/\xi}. \quad (120)$$

We see that, at fixed $\Lambda \xi \gg 1$, R_{field} diverges exponentially towards $-\infty$ for $L/\xi \rightarrow \infty$ and $\Delta\chi$ has the asymptotic size dependence in this limit (for cubic geometry and $d < 4$)

$$\frac{\chi_b - \chi}{\chi_b} \sim g(L/\xi) R_{\text{field}}(L/\xi, \Lambda L) \quad (121)$$

$$= -4(n+2)u^* da_0(d) (\Lambda \xi)^{d-2} (\Lambda L)^{-2}. \quad (122)$$

For the non-cubic geometries defined in Section 4.1 the corresponding results are obtained by substituting $I(L^2/\xi^2)$ in the form of (110) instead of (101) and by the replacement $d \rightarrow \tilde{d}$ in the prefactor of (122). R_{field} remains unchanged.

Like the result (106) for the lattice model, the behavior (122) is nonuniversal and violates finite-size scaling, as pointed out recently [52]. The non-scaling effect becomes significant in the region below the dashed line in Figure 1 which, for the field-theoretic model, is determined by $|R_{\text{field}}| = 1$ [52],

$$(2\pi)^{(1-d)/2} (L/\xi)^{(d-3)/2} \exp(-L/\xi) = a_0(d)(\Lambda L)^{d-4}, \quad (123)$$

for both cubic and non-cubic geometries.

The structure of (122) differs fundamentally from that of (106) for the lattice model in three respects: (i) the size-dependence of (122) is non-exponential, (ii) the dependence on Λ is non-exponential, and (iii) the sign of (122) is negative. Since for $\xi \gg L$ we must have $\chi_b - \chi > 0$ this sign implies the existence of a crossing point of the bulk curve for χ_b and the curve for χ at some $T > T_c$, in contrast to (106) where χ does not cross the bulk curve for $T \geq T_c$. We conclude that the φ^4 field theory with a sharp cutoff does not correctly describe the leading finite-size deviations from the bulk critical behavior of lattice systems below four dimensions. This is true also at $d \geq 4$; for $d = 4$ this follows from (97), (103) and (116), (120). The case $d > 4$ will be discussed elsewhere [58].

In Section 3 we have employed renormalization conditions in order to define the renormalized theory at finite \tilde{a} and finite Λ for $d \leq 4$. For a calculation of the universal part $g(L/\xi)$ of the finite-size effect, however, it is possible to employ a more convenient RG approach using dimensional regularization and minimal subtraction at fixed $2 < d < 4$ [81,85], as has been done in the finite-size calculations of references [39–41,46,47,50]. In this case the fixed point value u^* in (106) and (122) is replaced by $A_d^{-1} u_{\text{min}}^*$ where now u_{min}^* can be taken from the accurate Borel-resummed results of the minimally renormalized bulk theory [81,86,87]. For $d = 3$ the corresponding values are $A_3^{-1} = 4\pi$ and $u_{\text{min}}^* = 0.0404, 0.0362, 0.0327$ for $n = 1, 2, 3$, respectively [87]. In the large n -limit (at fixed un) the exact fixed point value is $u_{\text{min}}^* n = (4-d)/4$ for $2 < d < 4$.

5 Exact results in the large- n limit

In the following we perform the analysis of finite-size effects in the φ^4 model above T_c in the large- n limit at finite lattice constant and finite cutoff for $d < 4$ without using the renormalization group. The exact results in this limit will confirm the perturbative RG results of the preceding Section, in particular the existence of a non-scaling region for both the field-theoretic and the lattice φ^4 model in the range $L \gg \xi$. The existence of this region was overlooked in our recent work [66].

5.1 Lattice model at finite lattice constant for $n \rightarrow \infty$

We start from the exact result for the susceptibility $\chi/n = \hat{\chi}$ per component of the φ^4 lattice model above T_c in the limit $n \rightarrow \infty$ at fixed $u_0 n$ in a cubic geometry as determined by the implicit equation [66]

$$\hat{\chi}^{-1} = r_0 + 4u_0 n L^{-d} \sum_{\mathbf{k}} (\hat{J}_{\mathbf{k}} + \hat{\chi}^{-1})^{-1}. \quad (124)$$

For $d > 2$ this can be rewritten as

$$\hat{\chi}^{-1} = r_0 - r_{0c} + 4u_0 n D(\hat{\chi}^{-1}, L, \tilde{a}) - 4u_0 n \hat{\chi}^{-1} \times \int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}} (\hat{J}_{\mathbf{k}} + \hat{\chi}^{-1}) \right]^{-1} \quad (125)$$

where $D(\hat{\chi}^{-1}, L, \tilde{a})$ is defined by (85) and

$$r_{0c} = -4u_0 n \int_{\mathbf{k}} \hat{J}_{\mathbf{k}}^{-2}. \quad (126)$$

The bulk susceptibility $\hat{\chi}_b$ and the bulk correlation length ξ are determined by

$$\hat{\chi}_b^{-1} = r_0 - r_{0c} - 4u_0 n \hat{\chi}_b^{-1} \int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}} (\hat{J}_{\mathbf{k}} + \hat{\chi}_b^{-1}) \right]^{-1}, \quad (127)$$

$$\xi^2 = J_0 \hat{\chi}_b. \quad (128)$$

Although RG arguments will not be needed in the following we note that the ultraviolet ($\tilde{a} \rightarrow 0$) behavior of $\hat{\chi}$, (125), is the same as that of $\hat{\chi}_b$ because the function D has no ultraviolet ($\tilde{a} \rightarrow 0$) divergence. This supports the assumption made in Section 3. In the following we keep \tilde{a} finite.

For $L \gg \tilde{a}$ and $\xi \gg \tilde{a}$, *i.e.*, for small $\hat{\chi}^{-1} \tilde{a}^2$ at finite \tilde{a} , the bulk integral in (125) yields for $2 < d < 4$

$$\int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}} (\hat{J}_{\mathbf{k}} + \hat{\chi}^{-1}) \right]^{-1} = J_0^{-d/2} A_d \hat{\chi}^{\epsilon/2} \times \epsilon^{-1} \left\{ 1 + O \left[(\hat{\chi}^{-1} \tilde{a}^2)^{\epsilon/2} \right] \right\} \quad (129)$$

with $\epsilon = 4 - d$ and

$$A_d = 2^{2-d} \pi^{-d/2} (d-2)^{-1} \Gamma(3-d/2). \quad (130)$$

For $u_0 n J_0^{-d/2} A_d \epsilon^{-1} \hat{\chi}^{\epsilon/2} \gg 1$ this leads to

$$\hat{\chi} = \hat{\chi}_b \left[1 + \epsilon A_d^{-1} \xi^{d-2} \tilde{D}(J_0^{1/2} \hat{\chi}^{1/2}, L, \tilde{a}) \right]^{2/(2-d)} \quad (131)$$

where the function \tilde{D} is defined by (88). For $L \gg \xi$ we may replace $J_0^{1/2} \hat{\chi}^{1/2}$ by $J_0^{1/2} \hat{\chi}_b^{1/2} = \xi$ in \tilde{D} . Using the decomposition (93) we arrive at

$$\Delta \hat{\chi} \equiv \frac{\hat{\chi}_b - \hat{\chi}}{\hat{\chi}_b} = \hat{g}(L/\xi) \left[1 + \hat{R}(L/\xi, \tilde{a}/\xi) \right] \quad (132)$$

where

$$\hat{g}(L/\xi) = 2\epsilon A_d^{-1} (d-2)^{-1} (\xi/L)^{d-2} I(L^2/\xi^2) \quad (133)$$

with $I(L^2/\xi^2)$ given by (101), and

$$\hat{R}(L/\xi, \tilde{a}/\xi) = \exp \left[\Gamma(\tilde{a}/\xi) \frac{L}{\xi} \right] - 1 \quad (134)$$

with $\Gamma(\tilde{a}/\xi)$ given by (104). The structure of \hat{g} agrees with that of g , (100). (We note that the factor ϵA_d^{-1} in (133) can be interpreted as $4u^*n$ where u^* is the fixed point value in the large- n limit, see the last paragraph of Sect. 4.) The function \hat{R} turns out to be same as R , (103) and (104), which was to be expected because R is independent of n (in one-loop order).

For non-cubic geometries defined in Section 4.1 the result is only modified by the replacement $d \rightarrow \tilde{d}$ in the prefactor of the expression for $I(L^2/\xi^2)$ as given by (110), thus \hat{g} reads explicitly

$$\hat{g}(L/\xi) = 2\tilde{d}\pi^{1/2} [\Gamma(\epsilon/2)]^{-1} (2\xi/L)^{(d-1)/2} e^{-L/\xi}. \quad (135)$$

Equations (132)-(135) prove that finite-size scaling is violated for $2 < d < 4$ in the large- n limit for $L/\xi \gg$ at fixed $\tilde{a}/\xi > 0$ above T_c . This exact result supports the correctness of our conclusions in the preceding Section based on one-loop results. We note that the results (133)-(135) have finite limits for $d \rightarrow 2$ at fixed ξ .

5.2 Field-theoretic model at finite cutoff for $n \rightarrow \infty$

The analysis of the susceptibility $\hat{\chi} = \chi/n$ in the field-theoretic φ^4 model at finite Λ for $n \rightarrow \infty$ at fixed u_0n is parallel to that in Section 5.1. Equations (124)-(130) remain valid after the replacements $\hat{J}_{\mathbf{k}} \rightarrow \mathbf{k}^2$ and $J_0 \rightarrow 1$. Instead of (131) we now obtain for $L \gg \Lambda^{-1}$ and $\xi \gg \Lambda^{-1}$ (for $2 < d < 4$) [52]

$$\hat{\chi} = \hat{\chi}_b \left[1 + \epsilon A_d^{-1} \xi^{d-2} \tilde{D}_{\text{field}}(\xi, L, \Lambda) \right]^{2/(2-d)} \quad (136)$$

where \tilde{D}_{field} is defined by (114) and (115). For $L \gg \xi$ we arrive at

$$\Delta\hat{\chi} \equiv \frac{\hat{\chi}_b - \hat{\chi}}{\hat{\chi}_b} = \hat{g}(L/\xi) \left[1 + \hat{R}_{\text{field}}(L/\xi, \Lambda L) \right] \quad (137)$$

where \hat{g} is identical with (133) or (135). Furthermore \hat{R}_{field} is identical with R_{field} , (120), as expected because R_{field} is independent of n (in one-loop order). These exact results confirm the conclusions drawn in Section 4 about the violation of finite-size scaling in the φ^4 theory and about the failure of the continuum approximation with a sharp cutoff for finite lattice systems in the region $L \gg \xi$ above T_c .

5.3 Spherical model

Since the φ^4 lattice model in the large- n limit and the spherical model [88,89] are expected to yield asymptotically identical results (for the case of periodic boundary conditions) we compare our results with those by Barber and Fisher [54] and by Singh and Pathria [56]. Here we only study the approach of the susceptibility towards the bulk critical behavior above T_c .

Barber and Fisher (BF) considered the spherical model with a film geometry which should correspond to our result (132, 134, 135) with $\tilde{d} = 1$. The result of BF for the dimensionless susceptibility χ_{BF} reads for fixed $T > T_c$ and $L/\tilde{a} \rightarrow \infty$

$$\chi_{\text{BF}} \sim \chi_{\text{BF}}^b + J_0^{-1} B_d^0(T) (L/\tilde{a})^{(1-d)/2} \exp[-\Gamma_d(T)L/\tilde{a}] \quad (138)$$

where χ_{BF}^b is the dimensionless bulk susceptibility and $J_0 = 2J$. (Here we have corrected a misprint in (8.11) of Ref. [54] by replacing the exponent $(3-d)/4$ by $(1-d)/2$, compare (8.9) and (8.10) of Ref. [54].) Both functions $B_d^0(T)$ and $\Gamma_d(T)$ are expressed in terms of the dimensionless function $\Phi_0(T)$ which is given by the dimensionless inverse bulk susceptibility according to $\Phi_0(T) = J_0^{-1} (\chi_{\text{BF}}^b)^{-1} = (\tilde{a}/\xi)^2$. Calculating the small- Φ_0 behavior of the derivative of the generalized Watson function $W_d(\Phi_0)$ as

$$W'_d(\Phi_0) \sim -2^{-d} \pi^{-d/2} \Gamma(\epsilon/2) \Phi_0^{-\epsilon/2} \quad (139)$$

with $\epsilon = 4 - d$ we have found

$$B_d^{(0)}(T) \sim -2^{(d+1)/2} \pi^{1/2} [\Gamma(\epsilon/2)]^{-1} \Phi_0^{-(d+3)/4} \quad (140)$$

for $T \rightarrow T_c$. This leads to

$$\frac{\chi_{\text{BF}}^b - \chi_{\text{BF}}}{\chi_{\text{BF}}^b} \sim 2\pi^{1/2} [\Gamma(\epsilon/2)]^{-1} (2\xi/L)^{(d-1)/2} e^{-\Gamma_d(T)L/\tilde{a}}. \quad (141)$$

The non-exponential part agrees with that of our $\hat{g}(L/\xi)$, (135), for $\tilde{d} = 1$. If we expand the exponent $\Gamma_d(T) = 2\text{arcsinh}(\Phi_0^{1/2}/2)$ to *third* order in $\Phi_0^{1/2}$ and express it in terms of \tilde{a}/ξ we obtain

$$\begin{aligned} & \exp \left[-\Gamma_d(T)L/\tilde{a} \right] \\ &= \exp \left[- (2L/\tilde{a}) \text{arcsinh} \left(\frac{1}{2} \tilde{a}/\xi \right) \right] \\ &= \exp \left\{ -L/\xi + \frac{1}{24} (\tilde{a}/\xi)^2 L/\xi + O \left[(\tilde{a}/\xi)^4 L/\xi \right] \right\} \end{aligned} \quad (142)$$

$$(143)$$

which also agrees with the exponential part of our solution (132, 134, 135) of the φ^4 lattice model. The importance of the *positive* second term $\sim (\tilde{a}/\xi)^2$ in (143) for the leading finite-size deviations from bulk critical behavior (for $L/\xi \rightarrow \infty$ at fixed $\tilde{a}/\xi > 0$) was overlooked by BF [54]

(who considered the exponent in (138) only in the limit $T \rightarrow T_c$ at fixed $L/\tilde{a} < \infty$ rather than $L/\tilde{a} \rightarrow \infty$ at fixed $T > T_c$, see also equations (5.75)-(5.77) of reference [5]).

The solution of Singh and Pathria (SP) [56] for $\Delta\hat{\chi}$ (see equation (19) of Ref. [56]) in the large- L limit at fixed $T > T_c$ agrees with the universal part \hat{g} of our result, (135). Our non-universal contribution \hat{R} , (134), is not contained in the solution of SP.

6 Summary and conclusions

In the following we summarize and further comment on the results of this paper as follows.

We have studied the consequences of renormalizability (in terms of bulk renormalizations) of the φ^4 theory in a confined geometry with periodic boundary conditions below four dimensions. We have found that the consequences for the confined system are in contrast to those for the bulk system. While for the bulk system renormalizability implies that the leading critical *temperature* dependence is not significantly affected by a finite lattice constant \tilde{a} or by a finite cutoff Λ this is not generally the case for the leading *size* dependence of the confined system. Lattice and cutoff effects are asymptotically negligible as criticality is approached at fixed finite ratio L/ξ but not in the limit $L/\xi \gg 1$ above T_c . In the latter case the *leading* finite-size effect on the susceptibility χ turns out to be nonuniversal, *i.e.*, to depend explicitly on \tilde{a} and Λ (see Eqs. (106) and (122)), and to violate finite-size scaling in the region $L \gg \xi$ of the $L^{-1} - \xi^{-1}$ plane (Fig. 1).

Although lattice and continuum models yield the same asymptotic critical behavior of bulk systems we have shown that this is not the case for confined systems. While lattice systems (with periodic boundary conditions) have an exponential size dependence of $\Delta\chi$ above T_c for large L/ξ , a power-law behavior $\Delta\chi \propto (\Lambda L)^{-2}$ is obtained from the φ^4 field theory with a sharp cutoff [52].

It is expected that part of our conclusions apply also to $T < T_c$ for the case $n = 1$. For $n \geq 2$ (and for periodic boundary conditions) the power-law behavior of the Goldstone modes is expected to govern the finite-size deviations from bulk critical behavior such that nonuniversal exponential terms become subleading.

Our results for the leading finite-size deviations from bulk critical behavior have been derived for $2 < d \leq 4$ dimensions but our conclusions may be applicable to $d = 2$ dimensions. A detailed reexamination of the exponential terms in the existing exact results for the two-dimensional Ising model [53,84] would be interesting.

Part of our results remain valid also at and above four dimensions. One of the consequences is that the universal two-variable finite-size scaling form for the φ^4 lattice model for $d > 4$ [59,60,63,66–68] is violated for $L/\xi \gg 1$ above T_c for general n and below T_c for $n = 1$. A further consequence is that the predictions of the lowest-mode approach [16] and of the phenomenological scaling theory implying a single-variable scaling form [61,62] fail qualitatively in the region $\xi/L \gg 1$ where these theories predict a

universal power-law behavior $\Delta\chi \propto L^{-d}$ instead of a non-universal exponential size dependence $\Delta\chi \propto e^{-cL}$. The latter can easily be incorporated in our theory above four dimensions [63] by extending our present perturbation approach of Section 4 to $d > 4$ [58].

From a quantitative point of view, our prediction of a violation of finite-size scaling is difficult to be tested by means of Monte Carlo simulations (*e.g.*, for Ising models) because the non-scaling effect on χ occurs predominantly in the region $L \gg \xi$ where the total finite-size effects on χ are exponentially small (for periodic boundary conditions).

Our general arguments regarding the consequences of renormalizability (as presented in Sect. 3) are presumably not restricted to periodic boundary conditions but may be generalized to *non-periodic* boundary conditions. We consider this to be potentially important for applications to real systems where finite-size deviations from bulk critical behavior are not exponentially small. We do no longer see a stringent reason to believe that renormalizability implies the validity of finite-size scaling in the more complicated cases of non-periodic boundary conditions where additional renormalizations and nonuniversal length scales come into play. In particular for the important case of confined ${}^4\text{He}$ near the superfluid transition where the entire region $L > \xi$ and $L \leq \xi$ is perfectly well accessible to high-resolution experiments [69,70,72–77,79,80,90] we cannot exclude the existence of nonuniversal non-scaling effects in the φ^4 (lattice and field) theory with Dirichlet boundary conditions. This could eventually lead to a natural explanation of longstanding and recent discrepancies between experimental data [69–80] and theoretical predictions [5,11,24,29,31,32,36,37,42,49] that were based on (seemingly plausible) assumptions which imply the validity of finite-size scaling. Also for the exploration of finite-size effects on transport properties in ${}^4\text{He}$ on earth [72,74,79,90] and under microgravity conditions [91] as well as on thermodynamic properties near ordinary critical points under microgravity conditions [92], detailed knowledge on the effect of a finite atomic distance may turn out to be important.

Note added in proof

We have found that the finite-size effects of the continuum φ^4 model depend on the cutoff procedure. Consider, for example, the modified continuum Hamiltonian [93]

$$\tilde{H} = \int_V d^d x \left[\frac{1}{2} r_0 \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 + u_0 (\varphi^2)^2 + \frac{1}{2\Lambda^2} (\nabla^2 \varphi)^2 \right]$$

where the last term implies a smooth cutoff. The finite-size effects of \tilde{H} differ from those of the standard Landau-Ginzburg-Wilson continuum Hamiltonian (54) with a sharp cutoff. These differences affect the leading finite-size terms in the range $L \gg \xi$ for general $d > 2$ and in the entire $L^{-1} - \xi^{-1}$ plane for $d \geq 4$ (for periodic boundary conditions).

Specifically we have obtained from \tilde{H} the exponential non-scaling form of the susceptibility (for $L \gg \xi \gg \Lambda^{-1}$)

$$\Delta\chi \sim g(L/\xi) \exp \left[-\frac{1}{2} (\Lambda\xi)^{-2} \frac{L}{\xi} \right]$$

where $g(L/\xi)$ is the universal function (100). This result demonstrates that the continuum Hamiltonian \tilde{H} allows for an exponential behavior of $\Delta\chi$ and that the power-law $\Delta\chi \propto (\Lambda L)^{-2}$ in equation (122) is an artifact of the sharp cutoff associated with the $(\nabla\varphi)^2$ term of (54). Nevertheless \tilde{H} does not correctly describe the non-scaling part of $\Delta\chi$ of the lattice model as given in (106).

This means that it is the standard Landau-Ginzburg-Wilson continuum approximation (54) *with a sharp cutoff* whose finite-size effects differ fundamentally from those of the lattice φ^4 theory, whereas different continuum Hamiltonians (with a smooth cutoff) such as \tilde{H} yield finite-size effects that are similar to (but not identical with) those of the φ^4 lattice model. In retrospect, it is not primarily the continuum description but the sharp-cutoff procedure which causes the crucial term $(\Lambda L)^{d-4}$ in (118) of the φ^4 field theory.

Specifically for $T = T_c$ and $d > 4$ the Hamiltonian \tilde{H} yields $\chi_c \sim L^{d/2}$ and the same large- L limit of the Binder cumulant as for the φ^4 lattice model, at least in one-loop order and in the spherical limit. In all cases finite-size scaling is violated for $d > 2$ in the range $L \gg \xi$ but the detailed form of the violation differs in each case. These aspects will be further discussed elsewhere.

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Appendix A: Bulk correlation length at finite lattice constant

In this Appendix we determine the bulk correlation length ξ above T_c as a function of t at finite lattice spacing for $d \leq 4$. The derivation is parallel to that at infinite cutoff in reference [81]. We introduce the renormalized temperature variable

$$r = Z_r^{-1}(r_0 - r_{0c}) = Z_r^{-1}a_0 t \quad (\text{A.1})$$

where Z_r is identical with the Z factor $Z_{\varphi^2} = Z_r$ that is needed to renormalize the bare vertex function $\tilde{\Gamma}^{(1,2)}(\xi, u_0, \tilde{a}, d)$ [3, 13, 51] for $d \leq 4$

$$\tilde{\Gamma}_R^{(1,2)}(\xi, u, \mu, \tilde{a}, d) = Z_r Z_\varphi \tilde{\Gamma}^{(1,2)}(\xi, \mu^\epsilon J_0^2 Z_u u, \tilde{a}, d). \quad (\text{A.2})$$

The one-loop expression for $\tilde{\Gamma}^{(1,2)}$ is

$$\begin{aligned} \tilde{\Gamma}^{(1,2)}(\xi, u_0, \tilde{a}, d) &= 1 - 4(n+2)u_0 \\ &\times \int_{\mathbf{k}} \left[\hat{J}_{\mathbf{k}} + J_0 \xi^{-2} \right]^{-2} + O(u_0^2). \quad (\text{A.3}) \end{aligned}$$

The Z factor $Z_r(u, \mu\tilde{a}, d)$ for $d \leq 4$ is determined by the renormalization condition at $\xi = \mu^{-1}$

$$\tilde{\Gamma}_R^{(1,2)}(\mu^{-1}, u, \mu, \tilde{a}, d) = 1 \quad (\text{A.4})$$

which yields in one-loop order

$$Z_r(u, \mu\tilde{a}, d) = 1 + 4(n+2)uI(\mu\tilde{a}, d) + O(u^2) \quad (\text{A.5})$$

where $I(\mu\tilde{a}, d)$ is given in (35). Using (A.1) we rewrite the right-hand side of (17) in terms of renormalized quantities as

$$r_0 - r_{0c} = h(\xi, \mu^\epsilon J_0^2 Z_u u, \tilde{a}, d) \quad (\text{A.6})$$

$$= Z_r(u, \mu\tilde{a}, d) \mu^2 Q(\mu\xi, u, \mu\tilde{a}, d) \quad (\text{A.7})$$

with the dimensionless amplitude function Q . Taking the derivative with respect to μ at fixed u_0, \tilde{a} and $r_0 - r_{0c}$ (*i.e.* fixed ξ) yields the RGE

$$[\mu\partial_\mu + \beta_u\partial_u + (2 - \zeta_r)] Q(\mu\xi, u, \mu\tilde{a}, d) = 0, \quad (\text{A.8})$$

$$\zeta_r(u, \mu\tilde{a}, d) = (\mu\partial_\mu \ln Z_r^{-1})_0. \quad (\text{A.9})$$

The formal solution is

$$\begin{aligned} Q(\mu\xi, u, \mu\tilde{a}, d) \\ = Q(1, u(\ell), \tilde{a}/\xi, d) \exp \int_1^\ell (2 - \zeta_r(\ell')) \frac{d\ell'}{\ell'} \quad (\text{A.10}) \end{aligned}$$

with $\ell = (\mu\xi)^{-1}$ where $\zeta_r(\ell) \equiv \zeta_r(u(\ell), \ell\mu\tilde{a}, d)$. Equations (A.1, A.7, A.10) can be summarized as

$$r = at = \xi^{-2} Q(1, u(\ell), \tilde{a}/\xi, d) \exp \int_1^{1/\mu\xi} \zeta_r(\ell') \frac{d\ell'}{\ell'} \quad (\text{A.11})$$

with

$$a = Z_r(u, \mu\tilde{a}, d)^{-1} a_0 > 0 \quad (\text{A.12})$$

where the bare parameter a_0 is defined in (11). Equation (A.11) determines $t > 0$ as a function of ξ for $d \leq 4$ at finite \tilde{a} . Inverting (A.11) yields $\xi(t)$ including non-asymptotic (Wegner [82]) corrections. The asymptotic ($\xi \rightarrow \infty$) form of the correlation length follows from (A.11) as

$$\xi = \xi_0 t^{-\nu} \quad (\text{A.13})$$

with the critical exponent

$$\nu = (2 - \zeta_r^*)^{-1} \quad (\text{A.14})$$

and the amplitude

$$\xi_0 = \mu^{2\nu-1} a^{-\nu} \left\{ Q^* \exp \int_1^0 [\zeta_r^* - \zeta_r(\ell')] \frac{d\ell'}{\ell'} \right\}^\nu \quad (\text{A.15})$$

where $\zeta_r^* = \zeta_r(u^*, 0, d)$ and

$$Q^* = Q(1, u^*, 0, d). \quad (\text{A.16})$$

After the choice $\mu = \xi_0^{-1}$, the correlation-length amplitude ξ_0 is determined implicitly in terms of the bare parameter a_0 , the lattice spacing \tilde{a} and the renormalized coupling u by

$$\xi_0^2 = Z_r(u, \tilde{a}/\xi_0, d) a_0^{-1} Q^* \exp \int_1^0 [\zeta_r^* - \zeta_r(\ell')] \frac{d\ell'}{\ell'}. \quad (\text{A.17})$$

We note that the functions $h(\xi, u_0, \tilde{a}, d)$ and $Q(\mu, \xi, u, \mu\tilde{a}, d)$ do not have an expansion in integer powers of u_0 and u , respectively, beyond one-loop order [81]. The one-loop expression of $Q(\mu\xi, u, \mu\tilde{a}, d)$ and of Q^* can be derived from (19), (34), (A.5) and (A.7). An integral representation of Q in terms of expandable functions can be derived at finite \tilde{a} along the lines of Section 4.1 of reference [81].

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