Rapid Note

Cutoff and lattice effects in the φ^4 theory of confined systems

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Abstract. We study cutoff and lattice effects in the $O(n)$ symmetric φ^4 theory for a d-dimensional cubic geometry of size L with periodic boundary conditions. In the large-n limit above T_c, we show that φ^4 field theory at finite cutoff Λ predicts the nonuniversal deviation $\sim (\Lambda L)^{-2}$ from asymptotic bulk critical behavior that violates finite-size scaling and disagrees with the deviation $\sim e^{-cL}$ that we find in the φ^4 lattice model. The exponential size dependence requires a non-perturbative treatment of the φ^4 model. Our arguments indicate that these results should be valid for general n and $d > 2$.

The concept of finite-size scaling [1] plays a fundamental role in the theory of finite-size effects near phase transitions [1–4] and is indispensable for the analysis of numerical studies of critical phenomena in small systems [5]. Consider, for example, the susceptibility $\chi(T, L)$ of a ferromagnetic system for $T \geq T_c$ in a finite geometry of size L. Finite-size scaling is expected to be valid for large L and large correlation length $\xi \sim (T - T_c)^{-\nu}$, with a scaling form $\chi(T, L) = L^{\gamma/\nu} f(L/\xi)$ where γ and ν are bulk critical exponents and where the scaling function f depends on the geometry and boundary conditions but not on any other length scale. In this paper we shall consider only periodic boundary conditions and cubic geometry, $V = L^d$.

Finite-size scaling functions have been calculated within the $O(n)$ symmetric φ^4 field theory in $2 < d < 4$ dimensions [6–9] and quantitative agreement with Monte-Carlo (MC) data has been found [8–10]. It is the purpose of the present Rapid Note to call attention to a remarkable feature that has not been explained by the field-theoretic calculations. This is the exponential (rather than power-law) approach

$$\Delta \chi \equiv \chi(T, \infty) - \chi(T, L) \sim \exp[-\Gamma(T)L] \qquad (1)$$

towards the asymptotic bulk critical behavior $\chi(T, \infty) \sim \xi^{\gamma/\nu}$ above T_c, as has been found in several exactly solvable model systems [1, 2, 11–14]. By contrast, field theory [6–9] implies a non-exponential behavior $\Delta \chi \sim O((L/\xi)^{-d})$ in one-loop order above T_c for $d < 4$. We are not aware of numerical tests of this property, *e.g.*, by MC simulations.

We shall analyze this problem on the basis of the exact result [15] for χ in the large-n limit of the φ^4 model. In

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particular we shall study the effect of a finite cutoff Λ and of a finite lattice spacing in the field-theoretic and lattice version of the φ^4 theory. We find that field theory at finite cutoff predicts the leading nonuniversal deviation $\Delta \chi \sim (\Lambda L)^{-2}$ from bulk critical behavior that violates finite-size scaling for $d > 2$ and differs from equation (1). This is in contrast to the general belief [3–10, 15–23] (and corrects our recent statement [15, 23]) that the finite-size scaling functions of the φ^4 field theory are universal for $2 < d < 4$ (for cubic geometry and periodic boundary conditions). We shall show that the φ^4 *lattice* theory with a finite lattice spacing accounts for the exponential size-dependence of equation (1). We shall argue that a loop expansion destroys this exponential form and that a non-perturbative treatment [21] of the φ^4 theory is required.

The φ^4 field theory is based on the statistical weight $\exp(-H)$ with the Landau-Ginzburg-Wilson continuum Hamiltonian

$$H = \int_V d^d x \left[\frac{r_0}{2} \varphi_0^2 + \frac{1}{2}(\nabla \varphi_0)^2 + u_0(\varphi_0^2)^2 \right], \qquad (2)$$

with $r_0 = r_{0c} + a_0 t$, $t = (T - T_c)/T_c$ where the n-component field $\varphi_0(x)$ has spatial variations on length scales larger than a microscopic length $\tilde{a}$ corresponding to a finite cutoff $\Lambda = \pi/\tilde{a}$. Since we wish to perform a convincing comparison with the finite-size effects of lattice systems which have a finite lattice constant $\tilde{a}$ we must keep Λ finite even if a well defined limit $\Lambda \to \infty$ can formally be performed at fixed $r_0 - r_{0c}$ for $2 < d < 4$ [6, 16, 17]. It is well-known that this limit is justified for bulk systems [17] where finite-cutoff effects are only subleading corrections to the leading bulk critical temperature dependence.

Here we raise the question what kind of finite-size effects exist at finite Λ. This question was left unanswered in the renormalization-group arguments of Brézin [16] and in the explicit field-theoretic calculations of references [6–10,17–22] which were performed only in the limit $\Lambda \to \infty$ and where it was tacitly assumed that finite-cutoff effects are negligible for $d < 4$. We shall prove for $d > 2$ and $n \to \infty$ that this assumption is not generally justified for the field-theoretic φ^4 model for finite systems.

We shall first examine the susceptibility of the field-theoretic model

$$\chi = (1/n) \int_V d^d x \langle \varphi_0(x) \varphi_0(0) \rangle \qquad (3)$$

in the large-n limit at fixed $u_0 n$. For cubic geometry, $V = L^d$, the exact result for $d > 2$ is determined by the implicit equation [15]

$$\chi^{-1} = r_0 - r_{0c} - 4u_0 n \tilde{\Delta}_1$$
$$+ 4u_0 n \left\{ \chi L^{-d} - \chi^{-1} \int_{\mathbf{k}} \left[\mathbf{k^2}(\chi^{-1} + \mathbf{k^2}) \right]^{-1} \right\}, \quad (4)$$

$$\tilde{\Delta}_1 = \int_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-1} - L^{-d} \sum_{\mathbf{k} \neq \mathbf{0}} (\chi^{-1} + \mathbf{k}^2)^{-1}, \quad (5)$$

where $r_{0c} = -4u_0 n \int_{\mathbf{k}} \mathbf{k}^{-2}$. Here $\int_{\mathbf{k}}$ stands for $(2\pi)^{-d} \int d^d k$ with $|k_j| \leq \Lambda$, and the summation $\sum_{\mathbf{k} \neq \mathbf{0}}$ runs over discrete $\mathbf{k}$ vectors with components $k_j = 2\pi m_j / L, m_j = \pm 1, \pm 2, \ldots, j = 1, 2, \ldots, d$, in the range $-\Lambda \leq k_j < \Lambda$. For large L at finite Λ we have found for $d > 2$

$$\tilde{\Delta}_1 = I_1(\chi^{-1} L^2) L^{2-d}$$
$$+ \Lambda^{d-2} \left\{ a_1(d, \chi^{-1} \Lambda^{-2})(\Lambda L)^{-2} + O\left[(\Lambda L)^{-4}\right] \right\}, \quad (6)$$

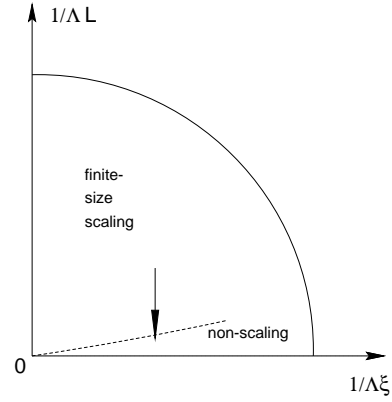$$I_1(x) = -(2\pi)^{-2} \int_0^\infty dy \, e^{-(xy/4\pi^2)} \left[K(y)^d - (\pi/y)^{d/2} - 1 \right], \quad (7)$$

$$a_1(d, \chi^{-1} \Lambda^{-2}) = \frac{d}{3(2\pi)^{d-2}} \int_0^\infty dx \, x \left[\int_{-1}^1 dy e^{-y^2 x} \right]^{d-1}$$
$$\times \exp\left[-(1 + \chi^{-1} \Lambda^{-2}) x \right] \qquad (8)$$

with $K(y) = \sum_{m=-\infty}^\infty e^{-ym^2}$. Near T_c, i.e., for small $\chi^{-1} \Lambda^{-2}$ at finite Λ, the bulk integral in equation (4) yields for $2 < d < 4$

$$\int_{\mathbf{k}} \left[\mathbf{k}^2(\chi^{-1} + \mathbf{k}^2) \right]^{-1} = A_d \chi^{\epsilon/2} \epsilon^{-1} \left\{ 1 + O\left[(\chi^{-1} \Lambda^{-2})^{\epsilon/2} \right] \right\} \quad (9)$$

with $\epsilon = 4 - d$ and $A_d = 2^{2-d} \pi^{-d/2}(d-2)^{-1} \Gamma(3 - d/2)$. This leads to the large-L and small-t representation at finite Λ

$$\chi = L^{\gamma/\nu} P(t(L/\xi_0)^{1/\nu}, \Lambda L) \qquad (10)$$

Fig. 1. Asymptotic $L^{-1} - \xi^{-1}$ plane (schematic plot) above T_c for the φ^4 field-theoretic model at finite cutoff Λ in the large-n limit in three dimensions where L is the system size and ξ is the bulk correlation length. Finite-cutoff effects become non-negligible in the non-scaling region below the dotted line. This crossover line has a vanishing slope at the origin and is determined by equation (15) with $\gamma/\nu = 2, \gamma = 2$ and $a_1(3,0) = 0.226$ for $d = 3$. Well above this line the cutoff dependence is negligible in equation (11). The arrow indicates an approach towards bulk critical behavior at constant $0 < t \ll 1$ through the non-scaling region where equation (14) is valid.

where the function P is determined implicitly by

$$P^{-1/\gamma} = t(L/\xi_0)^{1/\nu}$$
$$+ \epsilon A_d^{-1} \left[P - I_1(P^{-1}) + a_1(d,0)(\Lambda L)^{d-4} \right], \quad (11)$$

apart from $O\left[(\Lambda L)^{d-6}\right]$ corrections, with the critical exponents $\nu = (d-2)^{-1}$ and $\gamma = 2/(d-2)$, and with the bulk correlation-length amplitude ξ_0 [15]. We note that the term $I_1(P^{-1})$ is a $\mathbf{k} \neq \mathbf{0}$ contribution whereas the term $\sim P$ on the r.h.s. of equation (11) comes from the $\mathbf{k} = \mathbf{0}$ mode.

At first sight, the Λ dependent term in equation (11) seems to be a subleading correction and appears to be negligible for large L. This is asymptotically correct as long as $P - I_1(P^{-1}) > 0$ does not vanish in the large-L limit. This is indeed the case for $t(L/\xi_0)^{1/\nu} < \infty$, i.e., as long as the critical point is approached at finite ratio L/ξ. This corresponds to paths in the $L^{-1} - \xi^{-1}$ plane (Fig. 1) that approach the origin $L^{-1} = 0, \xi^{-1} = 0$ along curves with a non-vanishing asymptotic slope $\xi/L > 0$. Along these paths the function P remains finite and hence $P - I_1(P^{-1})$ remains non-zero (positive) which was tacitly assumed previously [15] where the Λ-dependent terms in equation (11) were dropped (see Eq. (62) of Ref. [15]).

There exist, however, significant paths in the $L^{-1} - \xi^{-1}$ plane where $t(L/\xi_0)^{1/\nu}$ becomes arbitrarily large. This includes paths at constant $t > 0$ or $\xi < \infty$ with increasing L corresponding to an approach towards the asymptotic bulk value χ_b (arrow in Fig. 1). We emphasize that these paths lie entirely in the asymptotic region $\xi \gg \Lambda^{-1}, L \gg \Lambda^{-1}, \chi_b = \xi^2 \gg \Lambda^{-2}$. In such limits the quantity $P \sim (\xi/L)^{\gamma/\nu}$ approaches zero. As a remarkable feature we find that in equation (11) the function $I_1(P^{-1})$

(which originates from the $\mathbf{k} \neq \mathbf{0}$ modes) completely cancels the term P (which comes from the $\mathbf{k} = \mathbf{0}$ mode) according to the small-P representation

$$I_1(P^{-1}) = P + O\left[P^{(3-d)/4}\exp(-P^{-1/2})\right]. \qquad (12)$$

In other words, the higher-mode contribution $\sim I_1(P^{-1})$ does not represent a "correction" to the lowest-mode term P but becomes as large as the lowest-mode term itself. This result is quite plausible because above T_c, at fixed temperature $T - T_c > 0$, the lowest mode does not play a significant role and does not become dangerous in the bulk limit, unlike the case $T \leq T_c$ where the separation of the lowest mode is an important concept [6,7].

The crucial consequence of equation (12) is that the term $P - I_1(P^{-1})$ in equation (11) is reduced to the exponentially small contribution $\sim \exp(-P^{-1/2}) \sim \exp(-L/\xi)$. This implies that the leading finite-size deviation from bulk critical behavior is now governed by the cutoff-dependent power-law term $(\Lambda L)^{d-4}$ in equation (11) which was dropped in reference [15]. This leads to the explicitly Λ dependent result, at finite $t \ll 1$ and finite $\Lambda L \gg 1$,

$$P(t(\tfrac{L}{\xi_0})^{1/\nu}, \Lambda L) = \left[t(\tfrac{L}{\xi_0})^{1/\nu} + \epsilon A_d^{-1} a_1(d,0)(\Lambda L)^{d-4}\right]^{-\gamma}, \qquad (13)$$

$$\chi = \chi_b\left[1 - \frac{\epsilon 2^{d-1}\pi^{d/2}}{\Gamma(3-d/2)}a_1(d,0)(\Lambda\xi)^{d-2}(\Lambda L)^{-2}\right], \qquad (14)$$

apart from $O\left[(\Lambda L)^{-4}, e^{-L/\xi}\right]$ corrections. Equation (14) is valid for $2 < d < 4$ and is applicable to the region below the dotted line in Figure 1. This line is a representative of a smooth crossover region and may be defined by requiring that the cutoff dependent term in equation (11) is as large as the term $P - I_1(P^{-1})$. In the latter term, P can be approximated by $(L/\xi)^{-\gamma/\nu}$, i.e., the dotted line is determined by

$$(L/\xi)^{-\gamma/\nu} - I_1((L/\xi)^{\gamma/\nu}) = a_1(d,0)(\Lambda L)^{d-4}. \qquad (15)$$

Equation (15) represents a line in a crossover region separating the scaling region (where cutoff effects can be considered as small corrections) from the nonscaling region (where cutoff effects are dominant) close the bulk limit.

The power law $\sim (\Lambda L)^{-2}$ in equation (14) disagrees with the exact result for the spherical model on a lattice where an exponential L dependence, analogous to equation (1), has been found [12,14] for general $d > 2$. This proves that φ^4 field theory at finite cutoff does not correctly describe the leading finite-size deviations from bulk critical behavior of spin systems on a lattice above T_c, not only for $d > 4$, as stated in reference [23], but more generally for $d > 2$, at least in the large-n limit. Furthermore, the result in equation (14) violates finite-size scaling *in the asymptotic region* where $L^{-\gamma/\nu}\chi$ should only depend on L/ξ, not on ΛL. Thus φ^4 field theory at finite cutoff is inconsistent with usual finite-size scaling not only for $d > 4$, but more generally for $d > 2$,

at least in the large-n limit. This is not in conflict with the renormalization-group arguments of Brézin [16] who considered only the limit of infinite cutoff in which the non-scaling region (Fig. 1) shrinks to zero. The existence of the non-scaling region for the field-theoretic φ^4 model below four dimensions has been overlooked in Section 4.1 of our recent work [15].

In the following we briefly analyze the corresponding properties in the φ^4 lattice model for $d > 2$. The φ^4 lattice Hamiltonian reads

$$\hat{H}(\varphi_i) = \tilde{a}^d\left\{\sum_i\left[\tfrac{\hat{r}_0}{2}\varphi_i^2 + \hat{u}_0(\varphi_i^2)^2\right] + \sum_{ij}\frac{1}{2\tilde{a}^2}J_{ij}(\varphi_i - \varphi_j)^2\right\} \quad (16)$$

where $\tilde{a}$ is the lattice constant. As noted recently [15], the susceptibility $\hat{\chi}$ of the lattice model is obtained from χ of the field-theoretic model by the replacement $\mathbf{k}^2 \to \hat{J}_{\mathbf{k}}$ in the sums and integrals in equations (4, 5), where

$$\hat{J}_{\mathbf{k}} = \frac{2}{\tilde{a}^2}[J(0) - J(\mathbf{k})] = J_0\mathbf{k}^2 + O(k_i^2 k_j^2), \qquad (17)$$

$$J(\mathbf{k}) = (\tilde{a}/L)^d\sum_{ij}J_{ij}e^{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}, \qquad (18)$$

$$J_0 = \frac{1}{d}(\tilde{a}/L)^d\sum_{ij}(J_{ij}/\tilde{a}^2)(\mathbf{x}_i - \mathbf{x}_j)^2. \qquad (19)$$

The crucial difference between the field-theoretic and lattice versions of the φ^4 model comes from the large-L behavior of the lattice version of the quantity $\hat{\Delta}_1$ in equation (5). Instead of equation (6) we now obtain for $L \gg \tilde{a}$

$$\int_{\mathbf{k}}(\hat{\chi}^{-1} + \hat{J}_{\mathbf{k}})^{-1} - L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}(\hat{\chi}^{-1} + \hat{J}_{\mathbf{k}})^{-1}$$
$$= J_0^{-1}I_1(J_0^{-1}\hat{\chi}^{-1}L^2)L^{2-d}, \quad (20)$$

apart from more rapidly vanishing terms. We have found that such terms are only exponential (rather than power-law) corrections in the regime $L \gg \xi$. This implies that, for the lattice model in the regime $L \gg \xi$, equation (11) is reduced to

$$\hat{P}^{-1/\gamma} = t(L/\hat{\xi}_0)^{1/\nu} + \epsilon A_d^{-1}\left[\hat{P} - I_1(\hat{P}^{-1})\right] \qquad (21)$$

without power-law corrections. This corresponds to equation (77) of reference [15]. Here $\hat{\xi}_0$ is the bulk correlation-length amplitude of the lattice model and $\hat{P} = \hat{\chi}L^{-\gamma/\nu}J_0$ [15]. Because of the exponential behavior of $\hat{P} - I_1(\hat{P}^{-1})$ according to equation (12) and because of the exponential corrections to equation (20) we see that the lattice φ^4 model indeed predicts an exponential size dependence for $\Delta\hat{\chi}$. The detailed form of the (L-dependent) amplitude of this exponential size-dependence is nontrivial and will be analyzed elsewhere.

In the following we extend our analysis to the case $n = 1$ of the field-theoretic model for $2 < d < 4$. The bare perturbative expressions for the effective parameters given in equations (68–71) of reference [24] for the field-theoretic φ^4 model are valid for general $d > 2$. Application

to the critical region for $2 < d < 4$ requires to renormalize these expressions by the L-independent Z-factors of the *bulk* theory. We recall that the bulk renormalizations can well be performed at finite Λ [25]. This does not eliminate the cutoff dependent term $\sim (\Lambda L)^{-2}$ in r_0^{eff} for the field-theoretic model and implies that $\Delta \chi$ will exhibit the leading size dependence $\sim (\Lambda L)^{-2}$ above T_c also for $n = 1$, $2 < d < 4$.

A grave consequence of these results is that universal finite-size scaling near the critical point of a finite system with periodic boundary conditions is less generally valid than believed previously [1–24]. Finite-size scaling is not valid in the region below the dotted line of the $L^{-1} - \xi^{-1}$ plane (Fig. 1), at least in the large-n limit, for the field-theoretic φ^4 model at finite cutoff for $d > 2$. This region is of significant interest as it describes the leading finite-size deviations from asymptotic bulk critical behavior. The violation of finite-size scaling in this region originates from the $(\nabla \varphi)^2$ term in equation (2) that approximates the interaction term $J_{ij}(\varphi_i - \varphi_j)^2$ of the φ^4 lattice Hamiltonian, equation (16). The serious defect of this approximation at finite Λ becomes more and more significant as $L/\xi \gg 1$ increases (arrow in Fig. 1) whereas it is negligible for $\xi/L > 1$. This defect does not show up in the $\Lambda \to \infty$ version (or dimensionally regularized version) of renormalized field theory. For a discussion of the case $d > 4$ we refer to [26].

From the one-loop finite-size scaling functions of reference [8] we find the nonexponential behavior $\Delta \chi \sim O((L/\xi)^{-d})$ for $n = 1$ and $2 < d < 4$ above T_c. The same behavior exists already in the lowest-mode approximation. The question arises whether higher-loop calculations would change this L dependence. The corresponding question for $n \to \infty$ can be answered on the basis of our exact solution for $\hat{\chi}$ of the φ^4 lattice model [15]. Approximating this solution by a one-loop type expansion around the lowest-mode structure leads to the large-L behavior $\Delta \hat{\chi} \sim O((L/\xi)^{-d})$ above T_c rather than $\sim e^{-cL}$. Thus, at least for $n \to \infty$, the exponential size dependence is a *non-perturbative* feature. We expect, therefore, that a conclusive answer of our question requires a non-perturbative treatment of the φ^4 lattice theory. Our previous nonperturbative order-parameter distribution function [21] is an appropriate basis for analyzing this problem which will presumably lead to an exponential size dependence for $\Delta \hat{\chi}$ within the φ^4 lattice model for general n above two dimensions.

It would be interesting to test the leading finite-size deviations from bulk critical behavior by Monte-Carlo simulations. The absence of terms $\sim (\Lambda L)^{-2}$ would provide evidence for the failure of the continuum approximation $\sim (\nabla \varphi)^2$ of the φ^4 field theory at finite Λ for confined lattice systems with periodic boundary conditions.

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