# Universality and $\varphi^4$ theory of finite-size effects above the upper critical dimension

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We analyze finite-size effects in a $L^d$ geometry above the upper critical dimension $d=4$ within the $O(n)$ symmetric $\varphi^4$ theory on the basis of exact results for $n\rightarrow\infty$ and one-loop results for $n=1$. We show that finite-size effects of the $\varphi^4$ continuum theory with a smooth (rather than sharp) cutoff belong to the same universality class as those of the $\varphi^4$ lattice theory. Our analysis predicts both universal and nonuniversal features of finite-size effects and resolves long-standing discrepancies in earlier analyses of Monte Carlo (MC) data for the $d=5$ Ising model. Our estimates of two fundamental length scales $\xi_0$ and $l_0$ are confirmed by very recent MC data.

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The concept of universality plays a fundamental role in statistical and elementary particle physics [1,2]. It implies that a unifying description of various physically different lattice and continuum systems near criticality can be given within the $\varphi^4$ field theory with the Hamiltonian

$$H=\int d^dx\left[\frac{r_0}{2}\varphi^2+\frac{1}{2}(\nabla\varphi)^2+u_0(\varphi^2)^2\right]. \tag{1}$$

The wide applicability of this theory is well established below the upper critical dimension $d^*=4$ [1,2]. Particular accuracy has been achieved in testing the universal predictions of the $\varphi^4$ theory by means of numerical data for the universality class of the $d=3$ Ising model not only for bulk properties but also for finite-size effects with periodic boundary conditions (pbc) [3–5].

Less well established, however, is the range of applicability of the $\varphi^4$ theory for confined systems *above* the upper critical dimension where the critical exponents are mean-field-like [1,2]. Early disagreements between Monte Carlo (MC) data for the finite $d=5$ Ising model [6] and universal predictions based on $H$ [4] have led to a long-standing debate [7]. New discrepancies between accurate MC data [8] and recent quantitative finite-size scaling predictions [9] based on the $\varphi^4$ lattice Hamiltonian

$$\hat{H}=\sum_i\left[\frac{r_0}{2}\varphi_i^2+u_0(\varphi_i^2)^2\right]+\sum_{\langle ij\rangle}\frac{J}{2}(\varphi_i-\varphi_j)^2 \tag{2}$$

have raised the question of to what extent the $\varphi^4$ theory is capable of describing finite-size effects of the Ising model for $d>4$. In particular, the recently discovered [9,10] nonequivalence of $H$ and $\hat{H}$ for finite systems is in striking contrast to the situation for $d<4$. This nonequivalence may be relevant not only for higher-dimensional finite systems, but also for three-dimensional physical systems for which mean-field theory provides a good description, such as systems with long but finite range interactions [11], polymer mixtures near their critical point of unmixing [12], and systems with a tricritical point [13].

In this paper we resolve the existing discrepancies for $d>4$ on the basis of exact results for the $O(n)$ symmetric $\varphi^4$ theory in the limit $n\rightarrow\infty$ and of one-loop results for $n=1$. Our analysis of both $\hat{H}$ and $H$ with a smooth and a sharp cutoff allows us to specify the range of validity of universal finite-size scaling for pbc in a $L^d$ geometry. We find, for pbc, that $H$ with a smooth cutoff belongs to the same universality class as $\hat{H}$, whereas $H$ with a sharp cutoff exhibits different finite-size effects. This implies that the lowest-mode prediction [4] of universal ratios at $T_c$ for $d>4$ is indeed valid asymptotically for both the lattice $\varphi^4$ theory and the continuum $\varphi^4$ theory with a smooth cutoff but not with a sharp cutoff. We also demonstrate that our one-loop results based on $\hat{H}$ are in quantitative agreement with the MC data [8] for the $d=5$ Ising model with $4\leqslant L\leqslant 22$ and that the universal two-variable scaling results [9,14] are well applicable to $L\gtrsim 12$, contrary to earlier conclusions [8,15]. Significant lattice effects are identified for $L<12$ which imply weak maxima of the $L$ dependence of the scaled susceptibility and magnetization at $T_c$. The new strategy of our finite-size analysis also succeeds in determining the *two* fundamental length scales $\xi_0$ and $l_0$ of the $d>4$ theory. Very recent MC data [16] confirm the validity of our strategy.

We start from $\hat{H}$, Eq. (2), for the $n$-component variables $\varphi_i$ on a sc lattice of volume $L^d$ with a nearest-neighbor coupling $J>0$. The basic question is to what extent $\hat{H}$ is equivalent to the spin Hamiltonian $H_s=-K\Sigma_{\langle ij\rangle}s_is_j$ where the $n$-component spin variables have a fixed length $s_i^2=n$, in contrast to $\varphi_i$, whose components $\varphi_{i\alpha}$ vary in the range $-\infty\leqslant\varphi_{i\alpha}\leqslant\infty$. For $n=1$, $H_s$ is the Ising Hamiltonian with $s_i=\pm 1$ and $K>0$.

An exact equivalence between $\hat{H}$ and $H_s$ exists in the limit $u_0\rightarrow\infty$, $r_0\rightarrow-\infty$ at fixed $u_0/(Jr_0)$ for general $L$, $n$, and $d$. Choosing $u_0/(Jr_0)$ such that $K=-Jr_0/(4u_0n)$ we obtain by means of a saddle-point integration

$$\lim_{\substack{u_0\rightarrow\infty\\ -r_0\rightarrow\infty}}\chi=\frac{K}{J}\chi_s, \tag{3}$$

where $\chi$ and $\chi_s$ are the susceptibilities

 

$$\chi=(nL^d)^{-1}\sum_{i,j}\langle\varphi_i\varphi_j\rangle, \tag{4}$$

$$\chi_s=(nL^d)^{-1}\sum_{i,j}\langle s_i s_j\rangle. \tag{5}$$

The weights in Eqs. (4) and (5) are $e^{-\hat{H}}$ and $e^{-H_s}$, respectively. For $n=1$, this exact equivalence is of limited relevance, since all calculations within the $\varphi^4$ model are performed at *finite* $u_0$. Hence, even in an exact theory, we have $\chi_s \neq J\chi/K$ at finite $u_0$. Therefore, in a comparison of $\chi$ with MC data for $\chi_s$, one must allow for a ($T$- and $L$-independent) overall amplitude $A$ which is adjusted such that $\chi_s = AJ\chi/K$. For finite $u_0$, the constant $A$ accounts for an appropriate normalization of the variables $\varphi_i$ relative to the discrete variables $s_i=\pm 1$. In an approximate theory, the value of $A$ depends on the approximations made for $\chi$. This corresponds to an adjustment merely of the *nonuniversal bulk* amplitude and not of the $L$ dependence of $\chi$ (for $d=3$ see, e.g., Ref. [5]). An adjustment of $A$ was not taken into account in the analysis of Ref. [8].

Of particular interest is the case $n\to\infty$, since it provides the opportunity to study the *exact* $u_0$ dependence including $u_0\to\infty$. This reveals the structural similarity between $\chi$ at finite $u_0$ and at $u_0=\infty$. This is most informative for $d>4$ where the leading and subleading powers of $L$ are independent of $n$ and should apply also to the Ising universality class with $n=1$.

For $n\to\infty$ at fixed $u_0 n$ the susceptibility $\hat{\chi}=2J\chi$ for pbc is determined implicitly by [10]

$$\hat{\chi}^{-1}=r_0/(2J)+J^{-2}u_0 nL^{-d}\sum_{\mathbf{k}} G_{\mathbf{k}}(\hat{\chi}^{-1}), \tag{6}$$

with $G_{\mathbf{k}}(\hat{\chi}^{-1})=(\hat{\chi}^{-1}+J_{\mathbf{k}})^{-1}$ and $J_{\mathbf{k}}=2\Sigma_{j=1}^{d}(1-\cos k_j)$ where $\Sigma_{\mathbf{k}}$ runs over $\mathbf{k}$ vectors with components $k_j = 2\pi m_j/L$, $m_j=0,\pm1,\pm2\ldots$, $j=1,2,\ldots,d$ in the range $-\pi\leq k_j<\pi$. At $T=T_c$ we derive from Eq. (6) the exact implicit equation for $d>4$,

$$\hat{\chi}^2=L^d\frac{\lambda_0(u_0)-\hat{\chi}^{(4-d)/2}f_b(\hat{\chi}^{-1})}{1-L^d\hat{\chi}^{-1}\hat{\Delta}_1(\hat{\chi}^{-1},L)}, \tag{7}$$

with $\lambda_0(u_0)=(J^2+u_0 n\int_{\mathbf{k}}J_{\mathbf{k}}^{-2})(u_0 n)^{-1}$ and

$$f_b(\hat{\chi}^{-1})=\hat{\chi}^{(d-6)/2}\int_{\mathbf{k}}[J_{\mathbf{k}}^2(\hat{\chi}^{-1}+J_{\mathbf{k}})]^{-1}, \tag{8}$$

$$\hat{\Delta}_m(\hat{\chi}^{-1},L)=\int_{\mathbf{k}}G_{\mathbf{k}}(\hat{\chi}^{-1})^m-L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}G_{\mathbf{k}}(\hat{\chi}^{-1})^m, \tag{9}$$

where $\int_{\mathbf{k}}\equiv(2\pi)^{-d}\int d^dk$ with $|k_j|\leq\pi$. We see that the structure of the $L$ dependence of $\hat{\chi}$ for finite $u_0>0$ is the same as for $u_0\to\infty$, where $\lambda_0(u_0)$ is reduced to $\lambda_0=\int_{\mathbf{k}}J_{\mathbf{k}}^{-2}$. It is reasonable to expect that also for $n=1$ the calculation of $\hat{\chi}$ at finite $u_0$ yields essentially the correct structure of $\chi_s$.

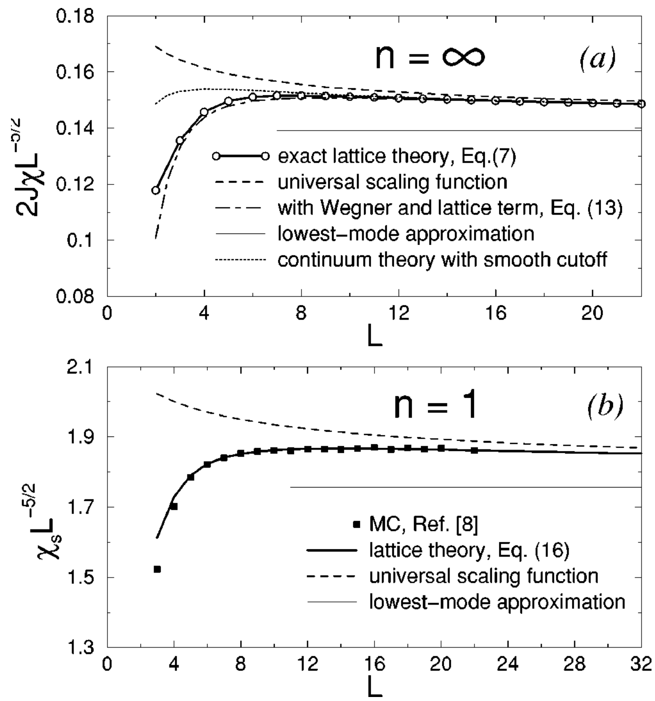


FIG. 1. Scaled susceptibilities for $d=5$ at $T_c$. Solid and dashed lines approach the lowest-mode lines for $L\to\infty$.

In Fig. 1(a) we show the exact result of $\hat{\chi}L^{-5/2}$ for $n\to\infty$ and $d=5$ at $T_c$ by solving Eq. (7) numerically with $\lambda_0=\int_{\mathbf{k}}J_{\mathbf{k}}^{-2}=0.019\,35$. We find that $\hat{\chi}L^{-5/2}$ has a weak maximum at $L=9$ which is not contained in the universal scaling form $\hat{\chi}_{scal}=L^{d/2}P(L^{4-d}/\lambda_0)$ of Ref. [10] (dashed curve). In $\hat{\chi}_{scal}$ the nonasymptotic Wegner correction $\propto f_b$ was neglected and $\hat{\Delta}_1$ was approximated only by the leading term $\hat{\Delta}_1=I_1(\hat{\chi}^{-1}L^2)L^{2-d}$ with

$$I_m(x)=\int_0^\infty dt\frac{t^{m-1}[K_b(t)^d-K(t)^d+1]}{(2\pi)^{2m}e^{(xt/4\pi^2)}}, \tag{10}$$

where $K_b(t)=(\pi/t)^{1/2}$ and $K(t)=\Sigma_{j=-\infty}^{\infty}\exp(-j^2t)$. Both $\hat{\chi}$ and $\hat{\chi}_{scal}$ show the predicted [9] slow $O(L^{(4-d)/2})$ approach to the large-$L$ limit $\hat{\chi}_0 L^{-d/2}=\lambda_0^{1/2}$ corresponding to the lowest-mode approximation [horizontal line in Fig. 1(a)]. Note that $\hat{\chi}_0$ is approached from *above*.

The small difference between $\hat{\chi}$ and $\hat{\chi}_{scal}$ in Fig. 1(a) for $L\gtrsim 15$ arises from the negative Wegner correction term $\propto -L^{(4-d)d/4}f_b(0)$ in Eq. (7). The pronounced departure of $\hat{\chi}$ from $\hat{\chi}_{scal}$ for $L\lesssim 10$, however, is a lattice effect that is dominated by the second term in

$$\hat{\Delta}_1(\hat{\chi}^{-1},L)=I_1(x)L^{2-d}-\hat{M}_1(x)L^{-d}+O(L^{-d-2}), \tag{11}$$

$$\hat{M}_1(x)=\int_0^\infty dt\frac{[K(t)^{d-1}K''(t)-K_b(t)^{d-1}K_b''(t)]}{e^{(xt/4\pi^2)}}, \tag{12}$$

with $x=\hat{\chi}^{-1}L^2$. Unlike the universal term $I_1L^{2-d}$, the lattice term $-\hat{M}_1L^{-d}$ cannot be incorporated into the universal finite-size scaling function $P(y)$, which depends on $y=(L/l_0)^{4-d}$ with $l_0^{4-d}=\lambda_0$. In summary, the leading $L$ dependence of $\hat{\chi}$ is represented as

$$\hat{\chi}=\left(\lambda_0L^d\frac{1-q_2L^{(4-d)d/4}}{1-q_1L^{(4-d)/2}+q_3L^{-d/2}}\right)^{1/2}, \tag{13}$$

where $q_1=\lambda_0^{-1/2}I_1(x)$, $q_2=\lambda_0^{-d/4}f_b(0)$, and $q_3=\lambda_0^{-1/2}\hat{M}_1(x)$. The functions $I_1(x)$ and $\hat{M}_1(x)$ have a weak $x$ dependence with $I_1(0)=0.107$ and $\hat{M}_1(0)=0.676$ for $d=5$. Equation (13) is shown in Fig. 1(a) as a dot-dashed line which approximates the exact result, Eq. (7), with very good accuracy down to $L=3$.

Now we turn to the question of to what extent $H$, Eq. (1), is equivalent to $\hat{H}$. From our result of $\hat{\chi}$, Eqs. (6)–(9), we obtain the corresponding result of $\chi_{field}=n^{-1}\int d^dx\langle\varphi(x)\varphi(0)\rangle$ after replacing $J_{\mathbf{k}}$ by $k^2$ and setting $2J=1$. A novel feature for $d>4$ is the fact that $\Delta_1$ depends significantly on the cutoff procedure. We need to distinguish two cases: (a) a *sharp* cutoff $\Lambda$ which restricts the $\mathbf{k}$ vector to $|k_j|\leqslant\Lambda$, and (b) a *smooth* cutoff $\Lambda$ where $-\infty\leqslant k_j\leqslant\infty$ but where $(\hat{\chi}^{-1}+k^2)^{-m}$ is replaced by the (Schwinger type) regularized form [2]

$$(\hat{\chi}^{-1}+k^2)^{-m}_{reg}=\int_{\Lambda^{-2}}^{\infty}ds\, s^{m-1}\exp[-(\hat{\chi}^{-1}+k^2)s].$$

Case (a) implies [9,10] $\Delta_1\propto L^{-2}$ and $\chi_{field}\propto L^{d-2}$ at $T_c$, which differs fundamentally from the lattice result $\hat{\Delta}_1\propto L^{2-d}$ and $\hat{\chi}\propto L^{d/2}$. In case (b), however, Eqs. (11) and (12) are replaced by

$$\Delta_1(\hat{\chi}^{-1},L)=I_1(x)L^{2-d}-M_1(\hat{\chi}^{-1})L^{-d}+O(e^{-\Lambda^2L^2}), \tag{14}$$

$$M_1(\hat{\chi}^{-1})=\hat{\chi}[1-\exp(-\hat{\chi}^{-1}\Lambda^{-2})], \tag{15}$$

with the same universal term $I_1L^{2-d}$. This implies that $\chi_{field}$ with a smooth cutoff has the same finite-size scaling behavior as $\hat{\chi}_{scal}$. Adjustment of the leading amplitude $\lambda_0^{field}=\int_{\mathbf{k}}(k^{-2})^{-2}_{reg}$ to the lattice counterpart $\lambda_0=\int_{\mathbf{k}}J_{\mathbf{k}}^{-2}$ fixes the cutoff as $\Lambda=0.185$ and $M_1(0)=\Lambda^{-2}=0.034$ for $d=5$, which is smaller than $\hat{M}_1(0)$ by a factor of 20. This difference between $\hat{M}_1$ and $M_1$ constitutes a significant lattice effect for small $L$ that is exhibited in Fig. 1(a), with $\chi_{field}L^{-5/2}$ represented by the dotted line. We conclude that $H$ with a *smooth* cutoff yields the same universal finite-size scaling behavior as $\hat{H}$ (for cubic geometry and pbc) but does not account for the strong $L$ dependence of $\hat{\chi}L^{-d/2}$ for small $L$. We expect this conclusion to hold for general $n$.

Now we consider $\hat{H}$ for the relevant case $n=1$. We start from the one-loop result for $\hat{\chi}=2J\chi$ and for the ratio $Q$

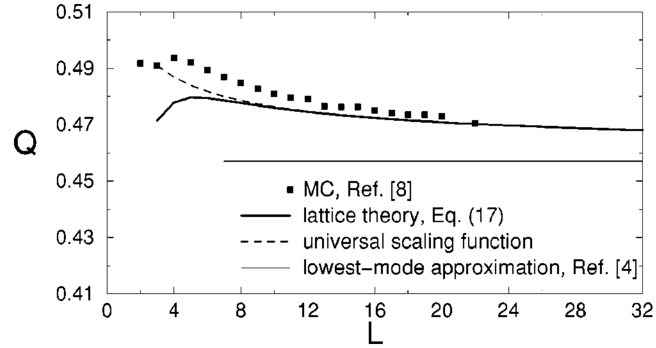


FIG. 2. Moment ratio $Q$ at $T_c$ for $d=5$ and $n=1$. Solid and dashed lines approach the lowest-mode line for $L\to\infty$.

$=\langle\Phi^2\rangle^2/\langle\Phi^4\rangle$ of moments $\langle\Phi^m\rangle$ for the order parameter distribution where $\Phi=L^{-d}\Sigma_j\varphi_j$. The analytic result reads for arbitrary $L$ [9]

$$\hat{\chi}=L^{d/2}(u_0^{eff})^{-1/2}\vartheta_2(Y^{eff}), \tag{16}$$

$$Q=\vartheta_2(Y^{eff})^2/\vartheta_4(Y^{eff}), \tag{17}$$

$$Y^{eff}=L^{d/2}r_0^{eff}(u_0^{eff})^{-1/2}, \tag{18}$$

$$\vartheta_m(Y)=\frac{\int_0^\infty ds\, s^m\exp\left(-\frac{1}{2}Ys^2-s^4\right)}{\int_0^\infty ds\exp\left(-\frac{1}{2}Ys^2-s^4\right)}, \tag{19}$$

with the effective parameters

$$r_0^{eff}=\tilde{a}_0t+12\tilde{u}_0(S_1-\lambda_0)+144\tilde{u}_0^2M_0^2S_2, \tag{20}$$

$$u_0^{eff}=\tilde{u}_0-36\tilde{u}_0^2S_2, \tag{21}$$

$$S_m=L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}(\tilde{a}_0t+12\tilde{u}_0M_0^2+J_{\mathbf{k}})^{-m}, \tag{22}$$

$$M_0^2=(L^d\tilde{u}_0)^{-1/2}\vartheta_2(L^{d/2}\tilde{a}_0t\tilde{u}_0^{-1/2}). \tag{23}$$

The right-hand side of Eqs. (16)–(23) depend only on the parameters $\tilde{u}_0=u_0/(4J^2)$ and $\tilde{a}_0=a_0/(2J)$, where $a_0=(r_0-r_{0c})/t$ with $t=(T-T_c)/T_c$. Equations (16)–(23) were evaluated previously [9] only for large $L$. Here we present the numerical evaluation of Eqs. (16)–(23) for arbitrary $L\leqslant32$ *without further approximation* for $d=5$ including Wegner corrections and lattice terms. Our strategy of adjusting $\tilde{u}_0$ is based on the fact that $Q$ at $T=T_c$ depends only on $\tilde{u}_0$ and that no overall adjustment for $Q$ is required, since $\lim_{L\to\infty}Q=Q_0$ is universal. Thus we adjust $\tilde{u}_0=0.93$ to the MC data [8] of $Q$ at $T_c$ (Fig. 2), then we use the same $\tilde{u}_0$ for $\hat{\chi}$ at $T_c$. For a comparison of $\hat{\chi}$ with the MC data for $\chi_s$ at $T_c$, we introduce the amplitude $A$ according to $\chi_s=AJ\chi/K=A\hat{\chi}/(2K_c)$. Using [8] $K_c=0.1139155$ and adjusting $A=0.678$ yields the solid line in Fig. 1(b). At $T\neq T_c$ we de-

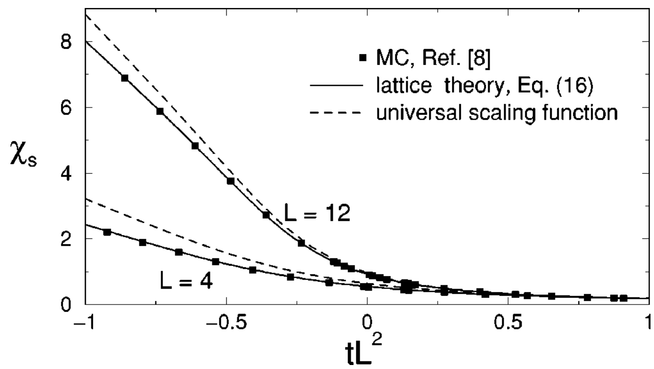


FIG. 3. Temperature dependence of susceptibilities for $d=5$ and $n=1$: $10^{-2}\chi_s$ for $L=4$ and $10^{-3}\chi_s$ for $L=12$.

termine $\tilde{a}_0=2.87$ from the *bulk* susceptibility $\chi_s=1.322t^{-1}$ of series expansion results [17].

In Figs. 1(b)–3 our analytic results (solid lines) are compared with the MC data of Ref. [8]. We conclude that our theory based on $\hat{H}$ satisfactorily describes the existing MC data for $4\leqslant L\leqslant 22$, both at $T_c$ and away from $T_c$ (Fig. 3), including lattice effects for small $L$. We attribute the remaining deviations of $Q$ for small $L$ to the inaccuracy of our one-loop approximation. At $T_c$ our results approach the lowest-mode results $\lim_{L\to\infty}\chi_s L^{-5/2}=p_0=1.757$ and $Q_0=0.4569$ [horizontal lines in Figs. 1(b) and 2] from *above*. Thus we predict a nonmonotonic $L$ dependence of $\chi_s L^{-5/2}$, of $Q$ (Fig. 2) and of the scaled magnetization $\langle|\Phi|\rangle L^{5/4}$ at $T_c$.

The important question that remains to be answered is whether or not the MC data in Figs. 1(b)–3 can be described by the universal finite-size scaling forms of $\hat{\chi}_{scal}=2J\chi_{scal}$ and $Q_{scal}$ derived previously [Eqs. (76)–(88) of Ref. [9]] on the basis of $\hat{H}$. These scaling forms neglect Wegner corrections and lattice effects. We have found that the same scaling functions can be derived on the basis of $H$ provided that a smooth cutoff is used. A crucial issue is to identify the fundamental reference lengths $\xi_0$ and $l_0$ of the two scaling variables $x=t(L/\xi_0)^2$ and $y=(L/l_0)^{4-d}$ where $\xi_0\propto\tilde{a}_0^{-1/2}$ is the amplitude of the bulk correlation length above $T_c$ and $l_0\propto\tilde{u}_0^{1/(d-4)}$ [10]. Since the one-loop results for $\hat{\chi}$ and $\hat{\chi}_{scal}$ differ at $O(\tilde{u}_0^2)$, one must allow for a different amplitude $A_{scal}\neq A$ in the adjustment of $\hat{\chi}_{scal}$ to $\chi_s=A_{scal}\hat{\chi}_{scal}/(2K_c)$. Using the same strategy of adjustment as described above, we find $A_{scal}=1.925$ and

$$l_0=2.641,\quad \xi_0=0.396. \tag{24}$$

The corresponding scaling results are shown in Figs. 1(b)–3 as dashed lines. They disagree with the MC data for *small L*, as noted already by Luijten *et al.* [8]. As a significant achievement of our present analysis, we now see, however, that there is satisfactory agreement between our universal scaling results and the MC data for $L\gtrsim 12$, contrary to the disagreement found in Ref. [8]. The latter disagreement is due to the (unjustified) identification [8] $J=K,\chi_s=\chi$ corresponding to $A_{scal}=1$ which, together with the fitting formula Eq. (32) of Ref. [8], implied $l_0=0.603$ and $\xi_0=0.549$. This formula omits the leading Wegner correction $\propto L^{(4-d)d/4}$ and a negative lattice term $\propto L^{-d/2}$ [compare our Eq. (13)] and therefore implies an *increasing* $\chi_s L^{-5/2}$ (Fig. 9 of Ref. [8]) towards [15] $\lim_{L\to\infty}\chi_s L^{-5/2}=p_0=1.87$, in contrast to the *decreasing* $\chi_s L^{-5/2}$ with $p_0=1.76$ of our one-loop theory [Fig. 1(b)]. We emphasize that this decrease is a *universal* feature of the scaling function $P(y)$. The validity of our strategy can be tested by calculating the amplitudes $A_M$ and $B_M$ of the bulk magnetization $M_b=A_M(-t)^{1/2}$ at zero external field $h=0$ below $T_c$ and $M_b=B_M h^{1/3}$ at $T_c$ for small $h>0$ as functions of $\xi_0$ and $l_0$ within the $\varphi^4$ theory at $d=5$. Substituting our parameter values, Eq. (24), we find in one-loop order $A_M=2.26$ and $B_M=1.89$. Very recent MC simulations [16] for the $d=5$ Ising model confirm these predictions (and exclude those implied by the parameter values of Ref. [8]), thus supporting the correctness of the strategy of our finite-size analysis.

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