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

\[ H = \int d^d x \left[ \frac{\tau_0}{2} \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 + u_0 (\varphi^2)^2 \right]. \tag{1} \]

The wide applicability of this theory is well established below the upper critical dimension d^* = 4 [12]. Particularly accurate has been achieved in testing the universal predictions of the φ^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 (p.b.c.) [3–5].

Less well established, however, is the range of applicability of the φ^4 theory for confined systems above the upper critical dimension d = 4 [12]. Early disagreements between Monte Carlo (MC) data for the finite d = 5 Ising model [3] and universal predictions based on H [12] have led to a longstanding debate [4]. New discrepancies between accurate MC data [3] and recent quantitative finite-size scaling predictions [13] based on the φ^4 lattice Hamiltonian

\[ \hat{H} = \sum_i \left[ \frac{\tau_0}{2} \varphi_i^2 + u_0 (\varphi_i^2)^2 \right] + \sum_{<ij>} \frac{J}{2} (\varphi_i - \varphi_j)^2 \tag{2} \]

have raised the question to what extent the φ^4 theory is capable of describing finite-size effects of the Ising model for d > 4. In particular the recently discovered non-equivalence of H and \( \hat{H} \) for finite systems is in striking contrast to the situation for d < 4. This non-equivalence 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 Letter we resolve the existing discrepancies for d > 4 on the basis of exact results for the O(n) symmetric φ^4 theory in the limit n → ∞ and of one-loop results for n = 1. Our analysis of both H and \( \hat{H} \) with a smooth and a sharp cutoff is not restricted to large L and allows us to specify the range of validity of universal finite-size scaling for p.b.c. in a L^d geometry. We find, for p.b.c., that \( \hat{H} \) with a smooth cutoff belongs to the same universality class as H whereas H with a sharp cutoff exhibits different nonuniversal 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 φ^4 theory and the continuum φ^4 theory with a smooth cutoff. We demonstrate, however, that the existing MC data for the d = 5 Ising model of small size [12,14] are outside the asymptotic scaling regime and cannot be explained by H because of significant lattice effects. We also demonstrate that our one-loop results based on H are in quantitative agreement with the MC data [12] for 4 ≤ L ≤ 22 and that the one-loop two-variable scaling results [14] are well applicable to L ≥ 12, contrary to earlier conclusions [3,12]. We predict a weak maximum of the L-dependence of the scaled susceptibility \( \chi L^{-d/2} \) at \( T_c \), which has not yet been detected in the MC data [12].

Our analysis implies \( \xi_0 = 0.396 \) for the bulk correlation-length amplitude of the d = 5 Ising model, in disagreement with \( \xi_0 = 0.549 \) found in Ref. [14]. We start from \( \hat{H} \), Eq. (3), for the n-component variables \( \varphi_i \) on a finite square 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

\[ H_s = -K \sum_{<ij>} s_i s_j \]

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 \( -\infty \leq \varphi_{i\alpha} \leq \infty \). 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 \( u_0 \to \infty \), \( \tau_0 \to -\infty \) at fixed \( u_0/(\tau_0 J) \) for general \( L \), \( n \) and \( d \). Choosing \( u_0/(\tau_0 J) \) such that \( K = -\tau_0 J/(4u_0 n) \) we obtain by means of a saddle-point integration

\[
\lim_{u_0 \to \infty} \lim_{\tau_0 \to -\infty} \chi = \frac{K}{J} \chi_s \tag{3}
\]
The weights in Eqs. (4) and (5) are \( e^{-\mathcal{H}} \) and \( e^{-\mathcal{H}_p} \), respectively. For \( n = 1 \), this exact equivalence is of limited relevance since all calculations within the \( \varphi^d \) 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 quantitative 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 \( \varphi \) 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. [10]). An adjustment of \( A \) was not taken into account in the analysis of Ref. [10].

Of particular interest is the case \( n \to \infty \) since it provides the opportunity of studying 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 \( u_0n \) the susceptibility \( \chi = 2J\chi \) for p.b.c. is determined implicitly by Eq. (10)

\[
\chi = \frac{L^d}{(2J) + J^2u_0n L^{-d} \sum_k G_k(\chi^{-1})},
\]

with \( G_k(\chi^{-1}) = (\chi^{-1} + J_k)^{-1} \) and \( J_k = 2\sum_{j=1}^d (1 - \cos k_j) \) where \( \sum_k \) runs over \( k \) vectors with components \( k_j = 2\pi m_j/L, \ m_j = 0, \pm 1, \pm 2, ..., j = 1, 2, ..., d \) in the range \(-\pi < k_j < \pi \). At \( T = T_c \) we derive from Eq. (6) the exact implicit equation for \( d > 4 \)

\[
\chi^2 = \frac{L^d}{\lambda_0(u_0) - \chi^{(d-1)/2} f_b(\chi^{-1})} \frac{\chi^{-1}}{1 - L^d \Delta_1(\chi^{-1}, L)},
\]

with \( \lambda_0(u_0) = (J^2 + u_0n \int J_k^2)(u_0n)^{-1} \) and

\[
f_b(\chi^{-1}) = \chi^{(d-6)/2} \int J_k^2(\chi^{-1} + J_k)^{-1},
\]

\[
\Delta_m(\chi^{-1}, L) = \int G_k(\chi^{-1})^m - L^{-d} \sum_{k \neq 0} G_k(\chi^{-1})^m,
\]

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

In Fig. 1a we show the exact result of \( \chi L^{-5/2} \) for \( n \to \infty \) and \( d = 5 \) at \( T_c \) by solving Eq. (7) numerically with \( \lambda_0 = \int_k J_k^{-2} = 0.01935 \). We find that \( \chi L^{-5/2} \) has a weak maximum at \( L = 9 \) which is not contained in the (large \( L \)) scaling form \( \chi_{scal} = L^{d/2} P(L^{-d}/\lambda_0) \) of Ref. [10] (dashed curve). In \( \chi_{scal} \) the nonasymptotic Wegner correction \( f_b \) was neglected and \( \Delta_1 \) was approximated only by the leading term \( \Delta_1 = I_1(\chi^{-1} L^2) L^{-d} \) with

\[
I_m(x) = \int_0^\infty dt \frac{t^{m-1}[K_b(t)d - K(t)d + 1]}{(2\pi)^2 m \exp(-j^2 t)},
\]

where \( K_b(t) = (\pi/t)^{1/2} \) and \( K(t) = \sum_{j=-\infty}^{\infty} \exp(-j^2 t) \).

Both \( \chi \) and \( \chi_{scal} \) show the predicted slow approach to the large-\( L \) limit \( \chi_0 L^{-d/2} = \lambda_0^{1/2} \) corresponding to the lowest-mode approximation (horizontal line in Fig. 1a). Note that both \( \chi \) and \( \chi_{scal} \) approach \( \chi_0 \) from above.

The small difference between \( \chi \) and \( \chi_{scal} \) in Fig. 1a for \( L \gtrsim 15 \) arises from the negative Wegner correction term \( -\chi^{(d-1)/2} f_b(\chi^{-1}) \) \( \sim -L^{(d-1)/2} d^d f_b(0) \) in the numerator of Eq. (8). The pronounced departure of \( \chi \) from \( \chi_{scal} \) for \( L \lesssim 10 \), however, is a lattice effect that is dominated by the subleading term \( -\hat{M}_1 L^{-d} \) in

\[
\hat{M}_1(\chi^{-1}, L) = I_1(x)L^{2-d} - \hat{M}_1(x)L^{-d} + O(L^{-d-2}),
\]
\[ M_1(x) = \int_0^\infty dt \frac{K(t)^{d-1}K''(t) - K_b(t)^{d-1}K''_b(t)}{e^{(x^2/4t^2)}} \]  

(12)

where \( x = \tilde{\chi}^{-1}L^2 \). Unlike the leading term \( I_1 L^{2-d} \), the lattice term \(-M_1 L^{-d}\) cannot be incorporated in the universal finite-size scaling function \( \tilde{P}(y) \) which depends on \( y = (L/L_0)^{d-d} \) with \( L_0^{d-d} = \lambda_0 \). In summary, the leading \( L \) dependence of \( \tilde{\chi} \) is represented as

\[ \tilde{\chi} = \left( \lambda_0 L^d \frac{1 - q_2 L^{d-d}/4}{1 - q_1 L^{d-d}/2 + q_3 L^{d-d}} \right)^{1/2} \]  

(13)

with \( q_1 = \lambda_0^{1/2}I_1(x), q_2 = \lambda_0^{d-d}/4 f_0(0), \) and \( q_3 = \lambda_0^{1/2}M_1(x) \). The functions \( I_1(x) \) and \( M_1(x) \) have a weak \( x \) dependence with \( I_1(0) = 0.107 \) and \( M_1(0) = 0.676 \) for \( d = 5 \). Eq. (13) is shown in Fig. 1a as dot-dashed line which approximates the exact result, Eq. (3), with very good accuracy down to \( L = 3 \).

Now we turn to the question to what extent \( H \), Eq. (4), is equivalent to \( \tilde{H} \). From our result of \( \tilde{\chi} \), Eqs. (6) - (9), we obtain the corresponding result of \( \chi_{\text{field}} \) 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 \( A \) which restricts the \( \mathbf{k} \) vector to \( |\mathbf{k}| \leq \Lambda \), (b) a smooth cutoff \( A \) where \( -\infty \leq k_x, k_y \leq \infty \) but where \( (\tilde{\chi}^{-1} + k^2)^{-m} \) is replaced by the (Schwinger type) regularized form \( (\tilde{\chi}^{-1} + k^2)^{-m} = \int_{\Lambda^2} ds \, s^{-m-1} \exp[-(\tilde{\chi}^{-1} + k^2)s] \). The former case (a) implies \( \chi_{\text{field}} \propto L^{-2} \) and \( \chi_{\text{field}} \propto L^{-2} \) at \( T_c \) which differs fundamentally from the lattice result \( \chi \propto L^{d/2} \). In the latter case (b), however, Eqs. (6) and (7) are replaced by

\[ \Delta_1(\tilde{\chi}^{-1}, L) = I_1(x)L^{2-d} - M_1(\tilde{\chi}^{-1})L^{-d} + O(e^{-L^2/2}), \]  

(14)

\[ M_1(\tilde{\chi}^{-1}) = \tilde{\chi}[1 - \exp(-\tilde{\chi}^{-1}L^2)], \]  

(15)

with the same leading term \( I_1 L^{2-d} \). This implies that \( \chi_{\text{field}} \) with a smooth cutoff has the same asymptotic (large \( L \)) finite-size scaling behavior as \( \tilde{\chi}_{\text{scale}} \). Adjustment of the leading amplitude \( \lambda_{\text{field}}^{d-2} = \int_{k} (k^2)^{-2} \) to the lattice counterpart \( \lambda_0 = \int_{k} J_k \) fixes the cutoff as \( \Lambda = 0.185 \) and \( M_1(0) = \Lambda^{-2} = 0.034 \) for \( d = 5 \) which is smaller than \( M_1(0) \) by a factor of 20. This difference between \( M_1 \) and \( M_1 \) constitutes a significant lattice effect for small \( L \) that is exhibited in Fig. 1a, with \( \chi_{\text{field}} L^{-5/2} \) represented by the dotted line. We conclude that \( H \) with a smooth cutoff yields the same (large \( L \)) finite-size scaling behavior as \( \tilde{H} \) (for cubic geometry and p.b.c.) but does not account for the strong \( L \)-dependence of \( \tilde{\chi} L^{-d/2} \) for small \( L \). We expect this conclusion to hold for general \( n \).

Now we consider \( \tilde{H} \) for the relevant case \( n = 1 \). We start from the one-loop result for \( \tilde{\chi} = 2J \chi \) and for the ratio \( Q = \tilde{\Phi}^2 > 2 / < \Phi^4 > \) of moments \(< \Phi^m > \) for the order parameter distribution where \( \Phi = L^{-d} \Sigma_j \varphi_j \).

The analytic result reads for arbitrary \( L \)

\[ \tilde{\chi} = L^{d/2} \frac{(\tilde{u}_0)^{-1/2}}{2} \varphi \frac{(Y_{\text{eff}})}{2}, \]  

(16)

\[ Q = \omega (\varphi_0^2) / \varphi (Y_{\text{eff}}), \]  

(17)

\[ Y_{\text{eff}} = L^{d/2} \frac{\tilde{u}_0}{2} \frac{(\varphi_0^2)^{-1/2}}{2}, \]  

(18)

\[ \varphi (m) = \int_0^\infty ds d \exp \left(-\frac{1}{2} \frac{1}{Y} s^2 - s^4 \right) \]  

(19)

with the effective parameters

\[ \tilde{u}_0 = \tilde{u}_0 + t \tilde{u}_0 \frac{(S_0 - 1)}{2} + 144 \tilde{u}_0 M_2 S_2, \]  

(20)

\[ \tilde{u}_0^2 = \tilde{u}_0 - 36 \tilde{u}_0 S_2, \]  

(21)

\[ S_m = L^{-d} \sum_{k \neq 0} \frac{a_k + 12 \tilde{u}_0 M_0 + j_k}{2^{m}}, \]  

(22)

\[ M_0^2 = L^{-d} \tilde{u}_0^{-1/2} \frac{\varphi_0^2}{2} \tilde{u}_0 \tilde{u}_0^{-1/2}. \]  

(23)

The r.h.s. of Eqs. (20) - (23) depend only on the parameters \( \tilde{u}_0 = \tilde{u}_0 / (4^{d/2}) \) and \( \tilde{u}_0 = \tilde{u}_0 / (2J) \) where \( \tilde{u}_0 = (r_0 - r_0) / t \) with \( t = (T - T_c) / T_c \). Eqs. (20) - (23) were evaluated previously only for large \( L \). Here we present the numerical evaluation of Eqs. (20) - (23) for arbitrary \( L \leq 32 \) 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 \( Q = T / T_c \) depends only on \( \tilde{u}_0 \) and that no overall adjustment for \( Q \) is required since \( \lim_{T_c} Q = 0 \) is universal. Thus we adjust \( \tilde{u}_0 = 0.93 \) to the MC data \( \tilde{Q} \) of \( T_c \) (Fig. 2), then we use the same \( \tilde{u}_0 \) for \( \tilde{\chi} \) at \( T_c \). For the comparison of \( \tilde{\chi} \) with the MC data for \( \chi_s \) at \( T_c \) we introduce the ampliude \( A \) according to \( \chi_s = A J / K = A / (2K) \). Using \( \tilde{K} = 0.1139155 \) and adjusting \( A = 0.678 \) yields the solid line in Fig. 1b. At \( T \neq T_c \) we determine \( \tilde{u}_0 = 2.87 \) from the bulk susceptibility \( \tilde{\chi} = 1.322^{-1} \) of series expansion results.

In Figs. 1b-3 our analytic result (solid lines) is compared with the MC data of Ref. [1]. We conclude that our one-loop finite-size theory based on \( \tilde{H} \) satisfactorily describes the existing MC data for \( 4 \leq L \leq 22 \), both at \( T_c \) and away from \( T_c \) (Fig.3). We attribute the remaining deviations of \( Q \) for small \( L \) to the (expected) inaccuracy of our one-loop approximation. At \( T = T_c \) our analytic results approach the lowest-mode results \( \lim_{L \to \infty} \chi_s L^{-5/2} = \eta \) and \( Q_0 = 0.4569 \) (horizontal lines in Figs. 1b and 2) from above, in particular our theory predicts a (weak) maximum of \( \chi_s L^{-5/2} \) at \( T_c \) (similar to that in Fig. 1a for \( n = \infty \)) that has not yet been detected in the MC data. Our theory also predicts a monotonically decreasing \( \chi_s L^{-5/2} \) at \( T_c \) and of the scaled magnetization \( < \Phi > / \Phi \) at \( T_c \).

Finally we answer the question to what extent the MC data in Figs. 1b-3 can be described by the finite-size scaling forms of \( \tilde{\chi}_{\text{scale}} = 2J \chi_{\text{scale}} \) and \( Q_{\text{scale}} \) derived previously (Eqs. (76) - (88) of Ref. [1]) on the basis of \( \tilde{H} \). These scaling forms neglect Wegner corrections and lattice effects. We have found that the same scaling functions can be derived on the basis of \( \tilde{H} \) provided that a
smooth cutoff is used. The corresponding scaling functions depend on 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 and \( l_0 \propto \tilde{u}_0^{1/(d-4)} \) is a second reference length. Thus, instead of \( \tilde{u}_0 \) and \( \tilde{a}_0 \), we now have \( l_0 \) and \( \xi_0 \) as adjustable parameters. Since the one-loop results for \( \tilde{\chi} \) and \( \tilde{\chi}_{scal} \) differ at \( O(u_0^2) \) one must allow for a different amplitude \( A_{scal} \neq A \) in the adjustment of \( \tilde{\chi}_{scal} \) to \( \chi_s \). Using the same strategy of adjustment as described above we find \( l_0 = 2.641 \) from \( Q \) at \( T_c \) and \( A_{scal} = 1.925 \) from \( \chi_s = A_{scal} \tilde{\chi}_{scal}/(2K_c) \). Finally we determine \( \xi_0 = 0.396 \) from the one-loop bulk result \( \lim_{t \to 0} \lim_{L \to \infty} \chi_s t = A_{scal} \xi_0^2/(2K_c) = 1.322 \). The corresponding scaling results are shown in Figs. 1b-3 as dashed lines. We identify the significant departure of the MC data for \( \chi_s \) at \( T_c \) from the dashed line for \( L \lesssim 12 \) as a lattice effect that is well described by our full one-loop theory (solid line in Fig. 1b) but which is not captured by the scaling form.

This failure of the scaling form for \( L \lesssim 12 \) was first observed by Luijten et al. [8]. We see, however, that there is good agreement of our scaling results with the MC data for \( L \gtrsim 12 \), contrary to the disagreement found in Ref. [8]. The latter disagreement is due to the (unjustified) identification \[ J = K, \chi_s = \chi \] corresponding to \( A_{scal} = 1 \) which, together with the fitting formula Eq. (32) of Ref. [8], implied \( \xi_0 = 0.549 \) and \( l_0 = 0.603 \). This formula omits the leading Wegner correction \( \propto L^{(4-d)/4} \) 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 \( \lim_{L \to \infty} \chi_s A_{scal} = p_0 = 1.91 \), in contrast to the decreasing \( \chi_s L^{-5/2} \) with \( p_0 = 1.76 \) of our one-loop theory. More accurate MC data would be desirable which could distinguish between our quantitative predictions in Figs. 1b and 2 and those implied by the analysis of Ref. [8]. It would also be desirable to determine \( \xi_0 \) for the \( d = 5 \) Ising model (e.g. from series expansion results) in order to resolve the disagreement between our prediction for \( \xi_0 \) and that of Ref. [8].

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