Finite-Size Effects in the $\varphi^4$ Field Theory Above the Upper Critical Dimension

X.S. Chen$^{1,2}$ and V. Dolm$^1$

$^1$ Institut für Theoretische Physik, Technische Hochschule Aachen, D-52056 Aachen, Germany
$^2$ Institute of Particle Physics, Hua-Zhong Normal University, Wuhan 430070, China

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We demonstrate that the standard $O(n)$ symmetric $\varphi^4$ field theory does not correctly describe the leading finite-size effects near the critical point of spin systems on a $d$-dimensional lattice with $d > 4$. We show that these finite-size effects require a description in terms of a lattice Hamiltonian.

For $n \to \infty$ and $n = 1$ explicit results are given for the susceptibility and for the Binder cumulant. They imply that recent analyses of Monte-Carlo results for the five-dimensional Ising model are not conclusive.

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The effect of a finite geometry on systems near phase transitions is of basic interest to statistical physics and elementary particle physics. In both areas the $\varphi^4$ Hamiltonian

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

for an $n$-component field $\varphi(x)$ in a finite volume $V$ plays a fundamental role. For simplicity we consider a $d$-dimensional cube, $V = L^d$, with periodic boundary conditions, $\varphi(x) = L^{-d} \sum_k \varphi_k e^{i k \cdot x}$. The summation runs over discrete $k$ vectors with components $k_j = 2 \pi n_j / L$, $n_j = 0, \pm 1, \pm 2, ..., j = 1, 2, ..., d$, in the range $-\Lambda \leq k_j < \Lambda$ with a finite cutoff $\Lambda$.

It is generally believed that the leading finite-size effects near the critical point of $d$-dimensional systems can be described by $H$ both for $d \leq d_u$ and for $d > d_u$ where $d_u = 4$ is the upper critical dimension. Since for $d > 4$ the bulk critical behavior is mean-field like, it is plausible that the leading finite-size effects for $d > 4$ appear to be describable in terms of a simplified Hamiltonian

$$H_0(\Phi) = L^d \left[ \frac{1}{2} r_0 \Phi^2 + u_0 (\Phi^2)^2 \right]$$

involving only the homogeneous fluctuations of the lowest $(k = 0)$ mode $\varphi_0 = L^d \Phi$, $\Phi = L^{-d} \int_V d^d x \varphi(x)$. Based on the statistical weight $\exp[-H_0(\Phi)]$, universal results have been predicted for systems above $d_u$. For the case $n = 1$, the lowest-mode predictions have been compared with Monte-Carlo (MC) data for the five-dimensional Ising model [4-7]. Although disagreements were noted and doubts were raised in Ref.4, subsequent analyses [5-7] based on the Hamiltonian $H$ appeared to reconcile the MC data with the lowest-mode predictions.

In this Letter we shall demonstrate that the lowest-mode approach fails for the Hamiltonian $H$ in Eq.(1) for $d > 4$ and that the leading finite-size effects of spin systems on a $d$-dimensional lattice with $d > 4$ are not correctly described by $H$. We show that this defect of $H$ is due to the $(\nabla \varphi)^2$ term. These unexpected findings shed new light on the role of lattice effects for $d > d_u$ and imply that recent analyses of the MC data [4-7] in terms of the continuum $\varphi^4$ theory are not conclusive.

We shall prove our claims first in the large-$n$ limit where a saddle point approach [4] can be employed. Our proof is not based on the renormalization group. We have extended the saddle point approach to the finite system to derive the order-parameter correlation function

$$\chi = \frac{1}{n} \int_V d^d x < \varphi(x) \varphi(0) >$$

with the statistical weight $\exp(-H)$. In the limit $n \to \infty$ at fixed $u_0 n$ we have found the exact result

$$\chi^{-1} = r_0 + 4 u_0 n L^{-d} \sum_k (\chi^{-1} + k^2)^{-1}.$$ (4)

We shall denote the bulk critical temperature by $T_c$. For $T \geq T_c$, $\chi$ can be interpreted as the susceptibility (per component) of the finite system. In the bulk limit the standard equation [8] for the bulk susceptibility $\chi_b$ for $T \geq T_c$ is recovered from Eq.(4) as

$$\chi_b^{-1} = r_0 + 4 u_0 n \int_k (\chi_b^{-1} + k^2)^{-1}.$$ (5)

where $\int_k$ stands for $(2\pi)^{-d} \int d^d k$ with a finite cutoff $|k| \leq \Lambda$. It is convenient to rewrite Eq.(4) in terms of $r_0 - r_{0c} = a_0 t$ where $r_{0c} = -4 u_0 n \int_k k^{-2}$ is the bulk critical value of $r_0$ as determined from Eq.(4) (with $\chi_b^{-1} = 0$), and $t = (T-T_c)/T_c$. Furthermore it is important to separate the $k = 0$ part $4 u_0 n L^{-d} \chi$ from the sum in Eq.(4). After a simple rearrangement we obtain

$$\chi^{-1} = \frac{\delta r_0 + \sqrt{(\delta r_0)^2 + 16 u_0 n L^{-d} (1 + S)}}{2(1 + S)},$$ (6)

$$\delta r_0 = a_0 t - \Delta,$$ (7)

$$S = 4 u_0 n L^{-d} \sum_{k \neq 0} [k^2 (\chi^{-1} + k^2)]^{-1},$$ (8)

$$\Delta = 4 u_0 n \left[ \int_k k^{-2} - L^{-d} \sum_{k \neq 0} k^{-2} \right].$$ (9)
These equations are the starting point of our analysis. They are exact in the limit $n \to \infty$ at fixed $u_0$ and are valid, at finite cutoff $\Lambda$, for $d > 2$, for arbitrary $L$ and for arbitrary $r_0$. They are written in a form that separates the $k = 0$ contribution $16u_0nL^{-d}$ from the effect of the $k \neq 0$ modes. The latter is contained in $S$ and $\Delta$.

In addition to the finite-size effect of the $k = 0$ mode, the $k \neq 0$ modes cause two different finite-size effects: (i) a finite renormalization of the coupling $u_0n$ due to $S$ which for $d > 4$ attains the finite bulk value $S_0 = 4u_0n \int [k^2(\chi_{k-1}^2 + k^2)]^{-1}$, and (ii) a shift of the temperature scale due to $\Delta$ which vanishes in the bulk limit. These two kinds of finite-size effects were also identified by Brézin and Zinn-Justin [8] who argued that for $d > 4$ these effects do not change the leading $L$ dependence obtained within the lowest-mode approximation. These arguments do not depend on $n$ and, if correct, should remain valid also in the large-$n$ limit.

The finite-size effect (ii) comes from $\Delta$ which, for $d > 2$ and finite $\Lambda$, has the nontrivial large-$L$ behavior

$$\Delta \sim 4u_0n\Lambda^{d-2}\left[a_1(d)(1\Lambda)^{-2} + a_2(d)\Lambda L^{2-d}\right]$$

(10)
apart from more rapidly vanishing terms. For the coefficients $a_1(d)$ and $a_2(d)$ we have found

$$a_1(d) = \frac{d}{3(2\pi)^{d-2}} \int_0^\infty dx e^{-x} \left[\int_1^0 dy e^{-y^2}x\right]^{d-1},$$

(11)

and

$$a_2(d) = -\frac{1}{4\pi^2} \int_0^\infty dy \left[\sum_{m=-\infty}^\infty e^{-ym^2}y - \left(\frac{\pi}{y}\right)^{d/2} - 1\right].$$

(12)
as confirmed in Fig.1 by numerical evaluation of Eq.(10) for $d = 3, 4, 5$. Thus, for $d > 4$, $\Delta$ vanishes as $L^{-2}$, and not as $L^{-2-d}[2, 5-7]$ or as $L^{-d/2}$ [8]. This implies that in Eq.(8) the zero-mode term proportional to $L^{-d}$ does no longer constitute the dominant finite-size term.

Our claims are most convincingly examined at bulk $T_c$. Then Eq.(8) is reduced to

$$\chi_c^{-1} = -\Delta + \sqrt{\Delta^2 + 16u_0nL^{-d}(1 + S_c)}$$

(13)

where $S_c$ is given by the r.h.s. of Eq.(8) with $\chi^{-1}$ replaced by $\chi_c^{-1}$. We see that the large-$L$ behavior is significantly affected by the $\Delta^2$ term. For large $L$ and $d > 4$ we obtain from Eqs.(10) and (11)

$$\chi_c \sim \frac{L^d\Delta}{4u_0n} \sim a_1(d)\Lambda L^{d-4}L^{-d-2}.$$  

(14)

By contrast, the lowest-mode approximation with $\Delta = 0$ and $S_c = 0$ yields $\chi_{0c} = (4u_0n)^{-1/2}L^{d/2}$. This proves that the lowest-mode approach fails in the present case. We note that the arguments in Ref.2 regarding the finite-size effect (ii) are not compelling since they are focused on the contributions of individual terms at lowest non-zero $k$ rather than on an analysis of the summed effect of these contributions.

Furthermore we see that the $L^{d-2}$ power law in Eq.(14) differs from the $L^{d/2}$ power law obtained from the exact solution of the $n$-vector model on a lattice for $n \to \infty$ [8] and of the mean spherical model on a lattice [10]. This proves that the field-theoretic Hamiltonian $\hat{H}$ in Eq.(1) does not correctly describe the leading finite-size effects of spin models on a $d$-dimensional lattice with $d > 4$, at least in the large-$n$ limit.

In the following we show that this defect is due to the $(\nabla\varphi)^2$ or $k^2\varphi_k\varphi_{-k}$ term of

$$H = L^{-d} \sum_k \frac{1}{2}(r_0 + k^2)\varphi_k\varphi_{-k}$$

$$+ u_0 L^{-3d} \sum_{kk'k''}
\begin{cases}
(\varphi_k\varphi_{k'})((\varphi_{k''}\varphi_{-k-k'-k''})
\end{cases}$$

(15)

with $\varphi_k = \int d^d x e^{-ikx}x$. Instead we consider a lattice Hamiltonian $\hat{H}(\varphi_i)$ for $n$-component vectors $\varphi_i$ with components $\varphi_{i\alpha}$, $-\infty \leq \varphi_{i\alpha} \leq \infty$, $\alpha = 1, ..., n$, on lattice points $x_i$ of a simple cubic lattice with volume $V = L^d$ and with periodic boundary conditions. We assume

$$\hat{H}(\varphi_i) = \hat{a}^d \left\{ \sum_i \frac{r_0}{2} \varphi_i^2 + \hat{u}_0 (\varphi_i^2)^2 \right\} + \sum_{ij} \frac{J_{ij}^2 (\varphi_i - \varphi_j)^2}{2\hat{a}^2}$$

(16)

where $J_{ij}$ is a pair interaction and $\hat{a}$ is the lattice spacing. In terms of $\hat{\varphi}_k = \hat{a}^d \sum \hat{e}^{-ikx}x_i x_j \varphi$ the Hamiltonian $\hat{H}$ has the same form as Eq.(14) but with $r_0 + k^2$ replaced by $\hat{r}_0 + 2\delta J(k)$ where $\delta J(k) = \hat{J}(0) - J(k)$ and

![FIG. 1. $\Lambda$-dependence of $\Delta_0 = \Delta/(4u_0n\Lambda^{d-2})$ with $\Delta$ from Eq.(1) for $d = 3, 4, 5$ (solid curves). The dashed lines represent Eq.(10) with $a_1(3) = 0.27706$, $a_1(4) = 0.08333$, $a_1(5) = 0.02443$, and $a_2(3) = 0.22578$, $a_2(4) = 0.14046$, $a_2(5) = 0.10712$. The arrows indicate the large-$\Lambda$ limits.

Furthermore we see that the $L^{d-2}$ power law in Eq.(14) differs from the $L^{d/2}$ power law obtained from the exact solution of the $n$-vector model on a lattice for $n \to \infty$ [8] and of the mean spherical model on a lattice [10]. This proves that the field-theoretic Hamiltonian $\hat{H}$ in Eq.(1) does not correctly describe the leading finite-size effects of spin models on a $d$-dimensional lattice with $d > 4$, at least in the large-$n$ limit.

In the following we show that this defect is due to the $(\nabla\varphi)^2$ or $k^2\varphi_k\varphi_{-k}$ term of
\[ J(k) = (\hat{a}/L)^d \sum_{i,j} J_{ij} e^{-i k \cdot (x_i - x_j)}. \]  

The \( k \) values are restricted by \( -\pi/\hat{a} \leq k_j < \pi/\hat{a} \). In the large-\( n \) limit at fixed \( \hat{u}_0 n \) the susceptibility \( \hat{\chi} = (4\hat{\Delta}/L)^d \sum_{i,j} < \varphi_i \varphi_j > \) is determined by Eqs.(11) with \( k^2 \) replaced by \( 2\delta J(k) \). The large-\( L \) behavior of the crucial quantity \( \hat{\Delta} \) is for \( d > 2 \)

\[ \hat{\Delta} = 2\hat{u}_0 n \left( \int_k |\delta J(k)|^{-1} - L^{-d} \sum_{k \neq 0} |\delta J(k)|^{-1} \right) \]

\[ \sim 4\hat{u}_0 n J_0^{-1} a_2(d) L^{2-d} \]

which for \( d > 4 \) differs from that of the continuum version \( \Delta \), Eq.(10), where \( 2\delta J(k) \) was approximated by \( k^2 \). This approximation turns out to be the unjustified for \( d > 4 \). Eq.(14) is valid for short-range interactions where

\[ J_0 = \frac{1}{d} (\hat{a}/L)^d \sum_{i,j} (J_{ij}/\hat{a}^2) (x_i - x_j)^2 \]

is finite. As a consequence of Eq.(19), the leading \( L \) dependence of \( \hat{\chi} \) at \( T_c \) is for \( d > 4 \)

\[ \hat{\chi}_c \sim \frac{1}{2}(\hat{u}_0 n)^{-1/2} (1 + S_b)^{1/2} L^{d/2}. \]

This agrees with the \( L^{d/2} \) power law of the exact solution of the lattice models of Refs. 9 and 10 for \( d > 4 \) and with the lowest-mode result \( \hat{\chi}_0 c = \frac{1}{2}(\hat{u}_0 n)^{-1/2} L^{d/2} \). We see that at \( T_c \) for \( d > 4 \) the \( k \neq 0 \) modes of \( H \) do not change the leading exponent \( d/2 \) of the lowest-mode approximation. Nevertheless they produce a finite change of the amplitude of \( \hat{\chi}_c \) through \( S_b = \hat{u}_0 n \int_k |\delta J(k)|^{-2} \). Furthermore we conclude from Eqs.(14) and (23) that for \( d > 4 \) the lattice Hamiltonian \( H \) yields significantly different finite-size effects compared to those of \( H \).

An analysis of the temperature dependence of \( \chi(t,L) \), Eq.(11), and of \( \chi(t,L) \) shows that for \( d > 4 \) finite-size scaling in its usual form is not valid, as expected [9], but we find that it remains valid in a generalized form with two reference lengths. The asymptotic scaling structure of \( \hat{\chi} \) is

\[ \chi(t,L) = L^{\gamma/\nu} \hat{\chi}(t/L^{\zeta_0} \nu, (L/\tilde{l}_0)^{4-d}) \]

where \( \zeta_0 \) is the bulk correlation-length amplitude and \( \tilde{l}_0 = [4\hat{u}_0 n J_0^{-1} (1 + S_b)^{-1}]^{1/(d-4)} \) is a second reference length. The \( d \)-dependent scaling function reads

\[ \hat{\chi}(x,y) = 2 J_0^{-1} \left( \delta(x,y) + \sqrt{\|\delta(x,y)\|^2 + 4y} \right)^{-1} \]

where \( \delta(x,y) = x - a_2(d) y \). In the lowest-mode approximation the term \( -a_2(d) y \) is dropped which implies that the leading finite-size term for \( t > 0 \) becomes incorrect. Thus, for \( t > 0 \), the lowest-mode approach fails for the

lattice model (and also for the continuum model whose scaling function \( P_X \) turns out to be non-universal).

In the following we extend our analysis to the case \( n = 1 \) which is of relevance to the interpretation of MC data of the five-dimensional Ising model [4-7]. We shall examine the susceptibility \( \chi \) and the Binder cumulant \( U \),

\[ \chi = \int_V d^d x \varphi(x) \varphi(0) >= L^d < \Phi^2 >, \]

\[ U = 1 - \frac{1}{3} < \Phi^4 >/ < \Phi^2 >^2, \]

within the \( \varphi^4 \) model, Eq.(11), including the effect of the \( k \neq 0 \) modes in one-loop order. For \( d > 4 \) at finite cut-off, the perturbative finite-size field theory [11,12] is applicable near \( T_c \) without a renormalization-group treatment. The averages are defined as \( < \Phi^m > = \int\int\int\int P(\Phi) \Phi^m d\Phi \) where \( P(\Phi) = Z^{-1} \int \mathcal{D}\sigma e^{-\sigma} \) is the order-parameter distribution function with \( \sigma(x) = \varphi(x) - \Phi \) representing the inhomogeneous fluctuations [12]. From Refs. 11 and 12 we derive the \( L \) dependence at \( T_c \) in one-loop order

\[ \chi_c = L^{d/2} u_0^{\epsilon_{\text{eff}}-1/2} \partial_2(y_0^{\epsilon_{\text{eff}}}), \]

\[ U_c = 1 - \frac{1}{3} \partial_4(y_0^{\epsilon_{\text{eff}}})/\partial_2(y_0^{\epsilon_{\text{eff}}})^2, \]

where

\[ y_0^{\epsilon_{\text{eff}}} = r_0^{\epsilon_{\text{eff}}} L^{d/2} u_0^{\epsilon_{\text{eff}}-1/2}, \]

\[ r_0^{\epsilon_{\text{eff}}} = r_0 + 12 u_0 S_1(r_0 L) + 144 u_0^2 M_0^2 S_2(r_0 L), \]

\[ u_0^{\epsilon_{\text{eff}}} = u_0 - 36 u_0^2 S_2(r_0 L), \]

\[ r_0 L = r_0 + 12 u_0 M_0^2, \]

\[ M_0^2 = \left( L^d u_0 \right)^{-1/2} \partial_2(r_0 L^{d/2} u_0^{-1/2}), \]

\[ \partial_4(m) = \int_0^\infty ds \left( \int_0^s ds \exp\left(-\frac{m^2 s^2}{4} - \frac{4}{3} s^4 \right) \right). \]

In this order the critical value \( r_0 < 0 \) is determined implicitly by the bulk limit (\( r_0^{\epsilon_{\text{eff}}} = 0 \)) of Eq.(29),

\[ r_0 = -12 u_0 I_1(-2r_0c) + 36 u_0 r_0c I_2(-2r_0c), \]

where \( I_m(r) = \int_k (r + k^2)^{-m} \). The finite-size effect of the \( k \neq 0 \) modes enters through

\[ S_m(r) = L^{-d} \sum_{k \neq 0} (r + k^2)^{-m}. \]

For large \( L \) we have \( r_0L = -2r_0c + O(L^{-d}) \) and

\[ r_0^{\epsilon_{\text{eff}}} = -12 u_0 |I_1(-2r_0c) - S_1(-2r_0c)| \]

\[ + 36 u_0 r_0c |I_2(-2r_0c) - S_2(-2r_0c)| + O(L^{-d}). \]

Similar to \( \Delta \) in Eqs.(11) and (14), the parameter \( r_0^{\epsilon_{\text{eff}}} > 0 \) vanishes as \( L^{-2} \) (rather than as \( L^{2-d} \)) for \( d > 4 \), thus \( r_0^{\epsilon_{\text{eff}}} < 0 \) diverges as \( L^{d-2} \) (rather than vanishes as \( L^{4-d/2} \)) for \( d > 4 \). Since \( \varphi_4(y) \sim -y/4 \) and \( \varphi_4(y) \sim y^2/16 \) for large negative \( y \) this implies that \( \chi_c \) diverges as \( L^{d-2} \) and \( U_c \) attains the large-\( L \) limit 2/3. We
conclude that the $L^{d/2}$ power law for $\chi_{0c}$ and the value $U_{0c} = 1 - \frac{1}{3} \vartheta_4(0)/\vartheta_2(0)^2 = 0.2705$ predicted \[2] for $n = 1$ within the lowest-mode approach are incorrect. From Refs. 2 and 12 we infer that analogous conclusions hold for general $n > 1$.

These unexpected results show that the widely accepted arguments in support of the asymptotic correctness of the lowest-mode approximation above the upper critical dimension in statics [1,2,5-7,13-19] and dynamics [1,20-23] are not valid and that recent interpretations [4-7] of the Monte-Carlo data of the five-dimensional Ising model in terms of predictions based on the Hamiltonian $H$, Eq.(4), are not conclusive, in spite of the apparent agreement found in Refs. 5-7.

Guided by our exact results in the large-$n$ limit, we propose a solution to this puzzle by replacing the field-theoretic $\varphi^4$ Hamiltonian $H$, Eq.(4), by the lattice $\varphi^4$ Hamiltonian $H$, Eq.(10), with $n = 1$ for the comparison with the five-dimensional Ising model. This involves a reexamination of $\nu_{eff}$, Eq.(3), with $k^2$ replaced by $2[J(0) - J(k)]$. We anticipate that the resulting value for the Binder cumulant $\tilde{U}_c$ of the lattice model will be close to (or possibly identical with) that of the lowest-mode approach. This expectation is based on our result (for $n \to \infty$) that at $T_c$ the lowest-mode approach yields the correct leading finite-size exponent of $\tilde{\chi}_c$. In addition, however, a detailed analysis of non-asymptotic (finite-$L$) correction terms is required which, for the Hamiltonian $H$, are expected to be different from those employed in a recent analysis based on $H$ \[3].

We summarize our findings for the continuum and lattice versions of the $\varphi^4$ model for $d > 4$ as follows: Lattice effects manifest themselves not only in changes of nonuniversal amplitudes but also in changes of the exponents of the leading finite-size terms as compared to the exponents of the continuum $\varphi^4$ model. The lowest-mode approach fails for the continuum $\varphi^4$ model, and also for the lattice model for $t > 0$. Therefore the values for the amplitude ratios derived previously \[3] cannot be justified on the basis of the $\varphi^4$ continuum theory. For the lattice Hamiltonian, however, the lowest-mode approach is qualitatively justified at $T_c$ for $n \to \infty$, at least for $\chi_c$. We conjecture that this is the reason for a fortuitous (approximate) agreement found between MC (lattice) data [4-7] and the lowest-mode predictions \[2]. Further work is necessary in terms of the $\varphi^4$ lattice model, Eq.(16), to fully establish our conjecture.

We also anticipate lattice and cutoff effects on leading finite-size terms at $d = d_{cr}$. This is relevant to future studies of tritritical phenomena at $d = 3$, e.g., in $^3$He-$^4$He mixtures \[2] and to MC simulations for lattice models of elementary particle physics at $d = 4$.

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