Surface critical behavior in fixed dimensions $d < 4$: Nonanalyticity of critical surface enhancement and massive field theory approach

H. W. Diehl and M. Shpot

Fachbereich Physik, Universität - Gesamthochschule - Essen, D-45117 Essen, Federal Republic of Germany

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The critical behavior of semi-infinite systems in fixed dimensions $d < 4$ is investigated theoretically. The appropriate extension of Parisi’s massive field theory approach is presented. Two-loop calculations and subsequent Padé-Borel analyses of surface critical exponents of the special and ordinary phase transitions yield estimates in reasonable agreement with recent Monte Carlo results. This includes the crossover exponent $\Phi(d = 3)$, for which we obtain the values $\Phi(n = 1) \approx 0.54$ and $\Phi(n = 0) \approx 0.52$, considerably lower than the previous $c$-expansion estimates.

Methods of field theory have become an essential ingredient of the modern theory of critical phenomena, providing both a conceptually appealing theoretical framework as well as powerful tools for quantitative analyses. Many important field-theoretical techniques, developed and tested originally in the study of bulk critical behavior, have been extended to systems with boundaries and utilized with considerable success in the analysis of surface critical phenomena at bulk critical points.

One important method that, to our knowledge, has not yet been employed in the study of surface critical phenomena is the field-theoretic renormalization group (RG) approach in a fixed space dimension $d$ below the upper critical dimension $d^*$.

In the present Letter we show how this approach can be generalized to systems with surfaces. Aside from the fundamental importance of such an extension, we have been motivated by the discrepancies existing between the results of recent Monte Carlo analyses for the crossover surface exponent $\Phi$ in three-dimensional systems and previous numerical estimates of $\Phi$ obtained by extrapolation of its second-order $c = 4 - d$ expansion to $c = 1$. In particular, the most recent Monte Carlo values for $\Phi$ of both the Ising and polymer universality classes are substantially lower than the original $c$-expansion estimates, and also significantly lower than previous results of computer simulations. The annoyingly large discrepancy with the $c$-expansion results calls for clarification and improvement of field-theoretic analyses. With this in mind, we have extended the massive field theory approach to the study of surface critical behavior. Using this approach, we have performed two-loop calculations for the semi-infinite $\phi^4$ model. Subsequent Padé-Borel analyses of the resulting series expansions yield the estimates for surface critical exponents shown in Table 1.

The Hamiltonian of the model is

$$\mathcal{H} = \int_V d^4x \left( \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} \tau_0 \phi^2 + \frac{1}{2} u_0 |\phi|^4 \right) \hspace{1cm} (1)$$

where $\phi = (\phi_\alpha(x))$ is an $n$-component field on the half-space $V = \{ x = (x_j, z) \mid x_j \in \mathbb{R}^{d-1}, z \geq 0 \}$ bounded by $\partial V$, the $z = 0$ plane. For the time being we assume the regularization of parallel-momentum integrations by a large-momentum cutoff $\Lambda$.

In wishing to study critical systems in fixed dimensions $d < d^*$ by means of perturbative methods, one is faced with the familiar occurrence of infrared (ir) singularities. Feynman integrals involving massless propagators become ill-defined. This is a problem typical of massless superrenormalizable field theories. Nevertheless such theories exist, owing to the appearance of a non-perturbative critical bare mass shift. In the dimensionally regularized theory, this shift corresponds to a critical value of $\tau_0$ of the form $\tau_{0c} = u_0^{2/\epsilon} \mathcal{T}(\epsilon)$, where $\mathcal{T}(\epsilon)$ has simple poles at $\epsilon = \epsilon_k \equiv 2/k$, $k \in \mathbb{N}$.

In the case of our semi-infinite model, an independent mass scale is provided by $c_0$, the bare surface enhancement. Its physical significance is well-known: depending on whether $c_0$ is smaller, equal, or larger than a certain critical value $c_{sp} = c_{sp}(\epsilon, u_0, \Lambda)$, distinct types of surface transitions occur at the bulk critical point, called ordinary, special, and extraordinary transitions, respectively. Finite values of $c_{sp}$ exist, of course, only if $d$ exceeds the lower critical dimension $d_0(n) = 3 - \delta_{n1}$ for the occurrence of surface ordering.

The quantity $c_{sp}$ has a number of properties analogous to $\tau_{0c}$. First, in the cut-off regularized theory, it diverges as $\Lambda \to \infty$. Its leading uv singularity for $d < 4$ is of the form $u_0 \Lambda^{d-3}$, similar as $\tau_{0c}$ has one $\sim u_0 \Lambda^{d-2}$. 

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A second analogy becomes apparent if we consider the uv behavior of correlation functions. In the case of the $\phi^4_4$ bulk theory (with $V = R^4$), a mass shift $\tau_0 = \tau_0 + \delta\tau_0$ is known to be sufficient to absorb the uv singularities of the $N$-point vertex and correlation functions. In our semi-infinite case we must keep track in correlation functions of which points are taken on or off the surface. Let $G^{(N,M)}(\{x_i\}, \{r_j\}; \tau_0, u_0, c_0, \Lambda)$ be the (regularized) connected $(N + M)$-point correlation functions involving $N$ fields $\phi(x_i)$ at distinct points $x_i$, $1 \leq i \leq N$, off the surface and $M$ fields $\phi(r_j, z = 0) \equiv \phi_s(r_j)$ at distinct surface points with parallel coordinates $r_j$, $1 \leq j \leq M$. To absorb the uv singularities of these functions for $d < 4$ both a mass shift and a surface-enhancement shift $c_0 = c_{sp} + \delta c_0$ is required; i.e., the limits $\Lambda \rightarrow \infty$ of the $G^{(N,M)}$ with fixed $\delta\tau_0 > 0$ and $\delta c_0 > 0$ exist.

A further analogy is the form of $c_{sp}$ in the dimensionally regularized theory. On dimensional grounds one expects it to read

$$c_{sp} = \delta_0^{1/\epsilon} C(\epsilon),$$

(2)

where $C(\epsilon)$ has poles at the above values $\epsilon_k$. The value of $c_{sp}$ is fixed by the requirement that the layer susceptibility $\chi_{11} = G^{(0,2)}(\{0\}; \phi = 0)$ diverges at the special point $(\tau_0, c_{sp})$. Here $G^{(0,2)}(\{0\}; \phi = 0)$ is the parallel Fourier transform of $G^{(0,2)}(r - r')$. Hence $c_{sp}$ is the solution to $\chi_{11} = G^{(0,2)}(\{0\}; \tau_0, u_0, z = c_{sp}) = 0$. By explicit computation of the $O(\tau_0)$ term in the expansion of $\chi_{11}$ one may verify that it has indeed a pole at $d = 3$, which must be eliminated by a surface-enhancement shift. Thus, just as in the bulk theory, one encounters the following situation: although, by making appropriate shifts of $\tau_0$ and $c_0$, the theory can be made uv-finite for $d < 4$, the critical values $\tau_{0c}$ and $c_{sp}$ cannot be determined by perturbation theory owing to their nonanalytic dependence on $u_0$. In order to obtain meaningful results in spatial dimensions $d$ with $d_* < d < d^*$ one should employ an appropriate extended version of the massive field theory RG approach, avoiding direct computations of both $\tau_{0c}$ and $c_{sp}$.

To explain our method, we start by recalling from Ref. [I] that the field $\phi(x)$ and the surface field $\phi_s(r)$ should be reparametrized by distinct renormalization factors. Accordingly we introduce the renormalized correlation functions through

$$G^{(N,M)}_{\text{ren}}(\{x\}, \{r\}; m, u, c) = Z^{-N+M/2}_0 Z^{-M/2}_1 G^{(N,M)}. $$

(3)

Unlike the renormalized surface enhancement constant $c$ and the renormalization factor $Z_1$ (which are specific to our surface-bounded system), the renormalized mass $m$, renormalized coupling constant $u$, and $Z_0$ are bulk quantities. We fix the latter ones by standard normalization conditions for the renormalized bulk vertex functions $\Gamma^{(N)}_{\text{b,ren}}$. In terms of their Fourier transforms $\hat{\Gamma}^{(N)}_{\text{b,ren}}(\{q\})$ these conditions read [J]

$$\hat{\Gamma}^{(2)}_{\text{b,ren}}(0; m, u) = m^2,$$

(4)

$$\frac{\partial}{\partial q^2} \hat{\Gamma}^{(2)}_{\text{b,ren}}(q; m, u)\big|_{q^2=0} = 1,$$

(5)

$$\hat{\Gamma}^{(4)}_{\text{b,ren}}(\{0\}; m, u) = m^4 u.$$  (6)

In order to specify $c$ and $Z_1$, we require that

$$\hat{\Gamma}^{(0,2)}_{\text{ren}}(p; m, u, c) \big|_{p=0} = \frac{1}{m + c}$$

(7)

and

$$\frac{\partial}{\partial p^2} \hat{\Gamma}^{(0,2)}_{\text{ren}}(p; m, u, c) \big|_{p^2=0} = -\frac{1}{2m(m+c)^2}.$$  (8)

These normalization conditions are suggested by the familiar zero-loop expression $\frac{1}{\epsilon} Z_c(1 + (p^2 + m^2 + \tau_0)^{1/2} - 1)$ for $\hat{\Gamma}^{(0,2)}_{\text{b,ren}}(p)$. Together with (2), the first one, (4), ensures that the special point is located at $m = c = 0$. Equation (6) fixes $Z_1$ in much the same way as (4) determines $Z_0$.

Since we are also interested in the crossover exponent $\phi$, we should also consider correlation functions with insertions of the surface operator $\phi^2$. Let $G^{(N,M';1,1)}(\{r\}; \phi = 0)$ denote the connected correlation function with $N$ fields $\phi$ off the surface, $M$ surface fields $\phi_s$, $1$ insertions of $\phi^2$ at points off the surface, and $1$ insertions of $\phi^2_s$. We write the renormalized operators as $(\phi^2)_{\text{ren}} = Z_0^2 \phi^2$ and $(\phi^2_s)_{\text{ren}} = Z_c \phi^2_s$. The bulk factor $Z_{\phi^2}$ we fix through the usual normalization condition $\hat{\Gamma}^{(2,1)}_{\text{b,ren}}(\{0\}) = 1$ for the Fourier transform of the bulk two-point vertex function with an insertion of $\phi^2$. To specify $Z_c$ we require that

$$\hat{\Gamma}^{(0,2,0,1)}_{\text{ren}}(p; m, u, c) \big|_{p=0} = (m + c)^{-2}.$$  (9)

Again, this condition is suggested by the zero-loop result for $\hat{\Gamma}^{(0,2)}_{\text{b,ren}}$, as can be seen by comparison with (2), noting that the bare analog of the left-hand side of (2) may be written as $(-\partial/\partial c_0) \hat{\Gamma}^{(0,2)}_{\text{b,ren}}(0) = 1$.

The above normalization conditions determine $\tau_0$, $u_0$, $Z_{\phi^2}$, $Z_{\phi^2_s}$, $c_0$, $Z_1$, and $Z_c$ as functions of $u$, $c$, and $\Lambda$. All $Z$-factors have a finite $\Lambda \rightarrow \infty$ limit in the $d < 4$ case considered here. Let us set $\Lambda = \infty$ in the sequel. (In our calculations we actually took $\Lambda = \infty$ from the outset, employing dimensional regularization.) Then the bulk $Z$-factors $Z_{\phi^2}$ and $Z_{\phi^2_s}$ become functions of the single dimensionless variable $u$. However, with our choice of normalization conditions, the surface $Z$-factors $Z_1$ and $Z_c$ depend on both $u$ and the dimensionless ratio $c/m$.

By varying $m$ at fixed $u_0$, $c_0$, and $\Lambda$, the analogs of the Callan-Symanzik equations (CSE) can be derived in a straightforward fashion. Let us define the functions $\beta(u) = m\partial m_0|u, B_s(u, c/m) \equiv m\partial m_0|\ln c, \eta_0(u) \equiv m\partial m_0|\ln Z_0$, and $\eta_1(u, c/m) \equiv m\partial m_0|\ln Z_1$, where $|_0$ indicates that the derivatives are taken at fixed $u_0$, $c_0$, and $\Lambda$. Upon introducing the differential operator
\[ D_m = m \partial_m + \beta \partial_u + B \partial_c + \frac{N + M}{2} \eta + \frac{M}{2} \eta_1 , \]

the CSE of the \( G_{\text{ren}}^{(N,M)} \) can be written as

\[ D_m G_{\text{ren}}^{(N,M)} = -(2 - \eta_c) m^2 \int \frac{d^4 X}{V} G_{\text{ren}}^{(N,M;1,0)} , \]

where the integration is over the position \( X \) of the inserted \( \phi^2 \) operator.

Just as in the bulk case, and as could be corroborated by means of a short-distance expansion, the inhomogeneity on the right-hand side should be negligible in the critical regime. The resulting homogeneous CSE differs from its standard bulk analog in that it involves functions \( \beta_c \) and \( \eta_1 \) of two variables, \( u \) and \( c/m \). In a study of the crossover from the critical behavior characteristic of the inserted \( \phi^2 \) operator.

In a study of the critical behavior characteristic of the special transition (for \( c/m \ll 1 \)) to that of the ordinary transition (for \( c/m \gg 1 \)) it would be essential to carry along this dependence on \( c/m \). Such a crossover analysis is beyond the scope of this Letter. Our main aim here is the calculation of the surface critical exponents of these two surface transitions. Therefore we focus directly on the respective asymptotic behavior.

The easier case is the special transition, which we consider first. Its critical behavior can be investigated upon setting \( c = 0 \). The homogeneous CSE can then be integrated in a standard fashion. One finds that the surface correlation exponent can be written as

\[ \eta^{sp}_{||} = \eta^{sp}_{1}(u^*) + \eta , \]

where \( \eta \equiv \eta_{\phi}(u^*) \) is the standard bulk correlation exponent, \( u^* \) is the ir-stable zero of \( \beta(u) \), and \( \eta^{sp}_{1}(u) \equiv \eta_{1}(u,0) \). A similar analysis applied to the CSE for correlation functions with insertions of \( \phi^2 \) shows that the anomalous dimension of this operator is given by the fixed-point value of the function \( \eta_{1}(u,c/m) \equiv m\partial_m \ln Z_c \). Hence the surface crossover exponent can be expressed as

\[ \Phi = \nu[1 + \eta^{sp}_{1}(u^*)] \]

in terms of \( \eta^{sp}_{1}(u) \equiv \eta_{1}(u,0) \) and the bulk exponent \( \nu \).

We have computed the perturbation expansions of the functions \( \eta^{sp}_{1}(u) \equiv \eta^{sp}_{1}(u) + \eta_{\phi}(u) \) and \( \eta^{sp}_{1}(u) \) to two-loop order for \( d = 3 \). Let us make the usual change of normalization of \( u \) such that \( \beta(u) = -u + u^2 + O(u^3) \). Then our results become

\[ \eta^{sp}_{1}(u) = -\frac{n + 2}{n + 8} u + \frac{12(n + 2)}{(n + 8)^2} \left[ 2A \right. \]

\[ + \frac{n + 2}{6} \left( \frac{1}{2} - \ln 2 + \ln^2 2 \right) - \frac{n + 6}{16} \right] u^2 \]

and

\[ \eta^{sp}_{2}(u) = -\frac{n + 2}{n + 8} \left( \ln 4 - \frac{1}{2} \right) u \]

\[ -\frac{24(n + 2)}{(n + 8)^2} \left[ A - B + \frac{n + 8}{12} \left( \ln 2 - \frac{1}{4} \right) \right] + \frac{n + 2}{3} \left( \ln^2 2 - \frac{7}{4} \ln 2 + \frac{19}{32} \right) u^2 . \]

The numbers \( A \) and \( B \) are associated with contributions of two-loop diagram with three equivalent internal lines. We have determined them by numerical integration, obtaining \( A = 0.202428 \) and \( B = 0.678061 \).

From these results analogous series expansions can be derived for other surface exponents by means of scaling laws \( \Box \). The coefficients of most of the resulting series alternate in sign and decrease in absolute value \( \Box \). Exceptions are some series involving \( \eta^{sp}_{1} \), whose behavior is rather bad. We have performed Padé analyses and Padé-Borel resummations of the direct and inverse series for the indices \( \eta_{1}, \Delta_1, \eta_{2}, \beta_{1}, \gamma_{11}, \gamma_{1}, \delta_1, \delta_1, \alpha_{11}, \alpha_{1}, \alpha_{11}, \) and \( \Phi \).

In these computations we have used the fixed-point values \( u^*(n = 0) = 1.632 \) and \( u^*(n = 1) = 1.597 \) from the Padé-Borel calculations of Refs. \( [21] \) and \( [22] \).

In the group of exponents \( \eta_1, \ldots, \delta_{11} \) related to \( \eta^{sp}_{1}(u^*) \) the most reliable estimate is obtained for \( \Delta_{1} \), which appears to exhibit the best convergence properties. Padé-Borel resummations of this series yield the values \( \Delta_{1}(n = 0) = 0.921 \) and \( \Delta_{1}(n = 1) = 0.997 \). The estimates in Table 1 for the other exponents of this group have been derived from these values of \( \Delta_{1} \) via scaling relations, using the \( d = 3 \) values of \( \nu \) and \( \eta \) given in Ref. \( [6] \).

In the group of exponents \( \alpha_1, \alpha_{11}, \Phi \) related to \( \eta^{sp}_{1}(u^*) \) the series for \( \alpha_1 \) yields estimates with the least scattering. The values of \( \alpha_{11} \) and \( \Phi \) listed in Table 1 have been obtained from our results for \( \alpha_1 \) and the accepted bulk values of \( \nu \) and \( \eta \).

In order to study the ordinary transition, we must consider the limit \( m \to 0 \) at fixed \( c > 0 \); i.e., \( c/m \to \infty \). A well-known complication is that one cannot simply set \( c = \infty \) in the functions \( G^{(N,M)} \) with \( M > 0 \) because a Dirichlet boundary condition holds for \( c = \infty \). Yet, the cumbersome calculation of \( c \)-dependent quantities can be avoided by considering correlation functions involving instead of \( \phi_a \) the normal derivative \( \partial_n \phi \) at the surface. Let \( G_{\infty}^{(N,M)} \) be the analog of \( G^{(N,M)} \) resulting by replacement of all the \( \phi_a \) by \( \partial_n \phi_a \) with \( c_0 = \infty \). Following the strategy described in Ref. \( [6] \), we have performed an independent RG analysis of these functions. The renormalized operator \( (\partial_n \phi)_R = (Z_\phi Z_{1,\infty})^{-1/2} \partial_n \phi \) involves a renormalization factor \( Z_{1,\infty}(u) \), which we fix through the condition \( (\partial/\partial \phi^2)G^{(0,2)}_{\infty,R}(p^2,0,u)|_{p^2=0} = -1/2m \).

The associated RG function \( \eta_{1,\infty}(u) \equiv m \partial_m \ln Z_{1,\infty} \) gives us the function

\[ \eta^{ord}_{||}(u) = 2 + \eta_{1,\infty}(u) + \eta_{\phi}(u) \]

needed to determine the surface exponent \( \eta^{ord}_{||} = \)
\[ \eta_1^{\text{ord}}(u^*) \]. The explicit two-loop expression of this function for \( d = 3 \) reads

\[
\eta_1^{\text{ord}}(u) = 2 - \frac{n + 2}{2(n + 8)} u - \frac{24(n + 2)}{(n + 8)^2} \left[ C + \frac{n + 14}{96} \right] u^2
\] (17)

with \( C = -0.105063 \).

Again, this result can be combined with scaling laws to obtain the corresponding expansions of the other surface critical indices of the ordinary transition. In most cases the coefficients of these series do not alternate in sign, with similar behavior of the inverse ones. Therefore, they are not adapted to Padé-Borel resummation. The numerical values of the ordinary-transition exponents arising from \([1/1]\) Padé approximants for each individual series are listed in Table 1. The exception is \( \gamma_1^{\text{ord}} \) for which this approximant does not exist. We evaluated this index using the values of \( \eta_1^{\text{ord}} \) and \( \nu \). For \( n = 2 \) and \( n = 3 \), the fixed-point values \( u^* = 1.558 \) and \( u^* = 1.521 \) were used, respectively.

Our numerical values of the surface critical exponents gathered in Table 1 generally are in reasonable agreement both with previous estimates based on the \( \epsilon \) expansion and with those obtained by other means (see Refs. [1] and [13-24] for comparisons). Note, however, that our estimates for \( \Phi \) are definitely lower than the values \( \Phi(n = 1) \approx 0.68 \) and \( \Phi(n = 0) \approx 0.67 \) quoted in Ref. [1], which were obtained by setting \( \epsilon = 1 \) in the \( \epsilon \) expansion of \( \Phi \) to order \( \epsilon^2 \). Recent Monte Carlo simulations have yielded the significantly lower estimates \( \Phi(1) = 0.461 \pm 0.015 \) [15], \( \Phi(0) = 0.530 \pm 0.007 \) [13], and \( \Phi(0) = 0.496 \pm 0.005 \) [16]. Our results \( \Phi(1) \approx 0.54 \) and \( \Phi(0) \approx 0.52 \) are fairly close to these values. This indicates that the crossover exponents \( \Phi \) for \( d = 3 \) and \( n = 0, 1 \) are indeed smaller than previously thought. Let us also note that when the \( \epsilon \) expansion to order \( \epsilon^2 \) is extrapolated to \( d = 3 \) by means of more elaborate techniques (e.g., Padé-Borel resummation), estimates for \( \Phi(0) \) and \( \Phi(1) \) as low as ours can be obtained.

A more detailed account of our work will be given elsewhere [23].

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\(*\) Permanent Address: Institute for Condensed Matter Physics, 1 Svientsitskii str, 290011 Lviv, Ukraine.

[1] For a review, see H. W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1986), Vol. X, p. 75, and Ref. [2].