Critical behavior at the extraordinary transition: Temperature singularity of surface magnetization and order-parameter profile to one-loop order

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The surface critical behavior of semi-infinite systems belonging to the Ising universality class with short-range interactions is investigated for supercritical surface enhancement $-c > 0$ and vanishing surface field h_1; Renormalization-group improved perturbation theory is applied to the standard semi-infinite scalar ϕ^4 model in $d = 4 - \epsilon$ dimensions to compute the order-parameter profile to one-loop order both for temperatures T with $\tau \equiv (T - T_{cb})/T_{cb} \gtrsim 0$ and $\tau \lesssim 0$. The associated scaling functions are found to cross smoothly over from their short-distance behavior for distances $z \ll \xi_b$ (= bulk correlation length) to their long-distance behavior for $z \gg \xi_b$ without showing the peculiar nonmonotonic behavior asserted by Peliti and Leibler [J. Phys. C **16**, 2635 (1983)]. Furthermore, the short-distance behavior of the profiles is shown to be fully consistent with a $|\tau|^{2-\alpha}$ singularity of the surface magnetization m_1 plus a regular background term; that is, in contrast to results published recently by other authors, the amplitudes A_+ and A_- of the contributions $A_\pm \tau$ to m_1 linear in $\tau > 0$ or $\tau < 0$ agree to one-loop order. Finally, we confirm that the universal profiles for the critical adsorption of fluids (governed by the critical-adsorption fixed point at $c = +\infty$ and $h_1 = \infty$) agree with the previous ones pertaining to the extraordinary-transition fixed point at $c = -\infty$ and $h_1 = 0$.

I. INTRODUCTION

It has been known for more than 15 years that several classes of surface transitions can be distinguished for macroscopic systems undergoing a continuous phase transition.[1,2] For surface transitions taking place at the bulk critical point of a semi-infinite Ising ferromagnet with short-range interactions, there are three distinct transitions.[3] Which one of these surface transitions occurs at the bulk critical temperature $T = T_{cb}$ (and in the absence of bulk and surface magnetic fields) depends on the value of a surface interaction constant c, called surface enhancement, whose negative is a measure of how much the surface bonds have been enhanced beyond a certain critical value above which the surface orders spontaneously at a higher temperature than the bulk. The ordinary, special, and extraordinary transitions correspond to the cases of subcritical ($c > 0$), critical ($c = 0$), and supercritical surface enhancement ($c < 0$), respectively.

These surface transitions have been studied theoretically in great detail in the past years. Experimental results are still scarce.[4] However, the recent experimental work by Mailänder *et al.*,[5] who investigated the surface critical behavior of Fe_3Al using scattering of synchrotron produced x rays under conditions of grazing incidence, gave surface exponents in excellent agreement with the theoretically predicted exponent values for the positive-c transition of the three-dimensional Ising model and indicates that this technique may be a very promising tool for future experimental work (cf. Ref. 6).

From a theoretical point of view, the ordinary and special transitions are fairly well understood.[1,2] By contrast, the extraordinary transition has been investigated to a much lesser degree. As far as analytical approaches such as the field-theoretical renormalization-group (RG) approach are concerned, this is partly due to technical difficulties: In the space of even thermodynamic fields $\tau = (T - T_{cb})/T_{cb}$ and c, the extraordinary transitions are located on a line $\tau = 0$, $c < 0$, separating a surface-ordered, bulk-disordered phase from a surface-ordered, bulk-ordered phase. The symmetry $\phi \to -\phi$ of the order parameter ϕ is spontaneously broken in both surface phases. Thus, irrespective of whether the transition is approached from the high-temperature ($\tau > 0$) or low-temperature side ($\tau < 0$), one has to deal with a spatially varying order-parameter profile $m_\pm(z) \equiv \langle \phi(\mathbf{x}) \rangle$, a fact which makes RG-improved perturbative calculations rather cumbersome. Here a standard semi-infinite geometry was adopted, for which the volume V of the system extends throughout the d-dimensional half-space $\mathbb{R}^d_+ \equiv \{\mathbf{x} = (\mathbf{x}_\parallel, z) | \mathbf{x}_\parallel \in \mathbb{R}^{d-1}, z \geq 0\}$ bounded by the $z = 0$ plane, its surface ∂V. The subscripts + and − on $m_\pm$ refer to the cases $\tau > 0$ and $\tau < 0$, respectively.

Using simple scaling considerations, Bray and Moore[7] suggested that the surface shift exponent Δ_1 of the extraordinary transition should vanish, so that the surface magnetization $m_{1,\pm} \equiv m_\pm(z = 0)$ should have a temperature singularity $\sim |\tau|^{\beta_1}$ with $\beta_1 = 2 - \alpha - \Delta_1 = 2 - \alpha$, up to terms analytic in τ. In other words, m_1 should behave for $\tau \to 0\pm$ as

$$m_{1,\pm} - m_{1c} \approx A\,\tau + A'\,\tau^2 + B_\pm\,|\tau|^{2-\alpha}\,, \tag{1}$$

where m_{1c} is the value of m_1 at $T = T_{cb}$. As usual, the nonuniversal amplitudes B_+ and B_- of the singular term need not be equal, but their ratio B_+/B_- should be a universal number. On the other hand, the amplitudes A and A' necessarily *must be independent of the* *sign of* τ, if the terms linear and quadratic in τ are to be analytic. This prediction was recently challenged by Ohno and Okabe,[8] who presented a one-loop calculation of $m_\pm(z)$ for distances $z \ll \xi_b$, from which they inferred that A takes different values A_+ and A_- on the high and low-temperature side of the transition. If this were true, m_1 would have a cusplike temperature singularity — in marked contrast to the much weaker singularities of both mean-field theory, where the leading singularity occurs in the curvature, as well as the Bray and Moore prediction (1). Furthermore, following Ohno and Okabe, one would be led to conclude that the surface exponent β_1 would be 1 up to corrections of order $\epsilon = 4 - d$.

The purpose of the present paper is, in part, a reanalysis of the results of Ohno and Okabe.[8] We shall present a RG-improved one-loop calculation of the profiles $m_\pm(z,\tau)$, with the enhancement c set to its RG fixed-point value $c^*_{\text{ex}} = -\infty$ describing the extraordinary transition. From the short-distance behavior of these profiles and their scaling form we can extract the asymptotic behavior of the surface magnetization m_1. In contrast to Ohno and Okabe, we find this to be in complete accord with the Bray and Moore prediction (1), obtaining $A_+ = A_- \equiv A$ and $A'_+ = A'_- \equiv A'$ to the order of our calculation. This is also in conformity with a recent Monte Carlo simulation,[9] which gave no detectable difference between A_+ and A_-.

Our analytic results yield the profiles $m_\pm(z)$ in terms of integrals that can be computed numerically. Evaluating these we obtained the scaling functions of $m_\pm$ shown in Figs. 1 and 2 below. These show a smooth crossover from the behavior at short distance $z \ll \xi_b$ to the long-distance behavior ($z \gg \xi_b$).

Let us emphasize that our results for $m_+(z,\tau)$ also apply to the problem of *critical adsorption*.[10–13] As discussed by a number of authors,[8,14–19] this phenomenon can be described by the same kind of semi-infinite ϕ^4 model utilized in our analysis of the extraordinary transition, with the surface enhancement taken to be subcritical ($c > 0$) and an additional surface magnetic field h_1 included. The asymptotic behavior for $\tau \to 0$ is described by a RG fixed point with $h_1^* = \infty$ and $c \to +\infty$, which we term *critical adsorption fixed point* $\mathcal{P}^*_{\text{ca}}$, to distinguish it from the ($h_1 = 0$, $c = -\infty$) fixed point $\mathcal{P}^*_{\text{ex}}$ pertaining to the extraordinary transition. Central to the phenomenological picture of the extraordinary transition developed by Bray and Moore[7] is the idea that the order at the surface need not be due to a spontaneous symmetry breaking but could alternatively be generated by a symmetry-breaking surface field h_1. Accordingly they argued that the surface critical behavior observed for $c > 0$ and h_1 (and described by $\mathcal{P}^*_{\text{ca}}$) should asymptotically be the same as at the extraordinary transition. In conformity with this we find that the corresponding fixed-point profiles $m_\pm(z,\tau; c = -\infty, h_1 = 0)$ and $m_\pm(z,\tau; c \to +\infty, h_1 = \infty)$ agree, indeed. In a previous investigation of critical adsorption by Peliti and Leibler[16] the profile $m_+(z,\tau; c \to +\infty, h_1 = \infty)$, calculated to one-loop order in $4-\epsilon$ dimensions, was claimed to have a strange and unphysical nonmonotonous dependence on z/ξ_b. Figure 1 shows that this is not the case.

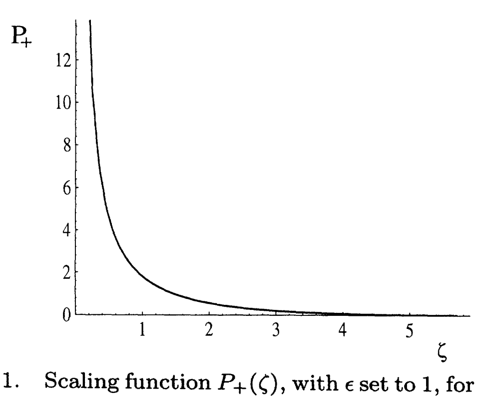

FIG. 1. Scaling function $P_+(\zeta)$, with ϵ set to 1, for reduced temperature $\tau > 0$.

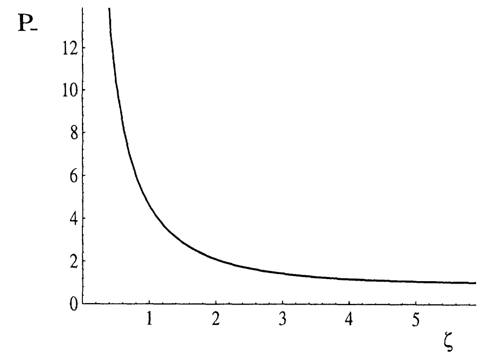

FIG. 2. Scaling function $P_-(\zeta)$, with ϵ set to 1, for reduced temperature $\tau < 0$.

In the next section we explain the calculation of the profiles. In Sec. III the short-distance behavior of these profiles is analyzed in order to determine the temperature singularity of $m(z \ll \xi_b)$. Our conclusions are briefly summarized in Sec. IV. There are three appendixes describing technical details.

II. CALCULATION OF ORDER-PARAMETER PROFILES

We consider a semi-infinite scalar ϕ^4 model described by the Hamiltonian

$$\mathcal{H} = \int d^{d-1}x_\parallel \int_0^\infty dz \left[\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}\tau_0\,\phi^2 + \tfrac{1}{4!}u_0\,\phi^4 + \delta(z)\left(\tfrac{1}{2}c_0\,\phi^2 - h_{1,0}\,\phi\right)\right], \qquad (2)$$

where the z integral over $\delta(z)$ is understood to capture the entire δ peak, so that the volume integral $\int_V \delta(z)\,[\cdots]$ over $V = \mathbb{R}^d_+$ reduces to an integral $\int_{\partial V}[\cdots]$ over the surface ∂V. For background on this model and its RG analysis the reader is referred to Ref. 2, whose conventions and notation we shall adopt as far as possible and convenient. In particular, we shall utilize its method of dimensional regularization and minimal subtraction of poles in $\epsilon = 4 - d$ in our RG calculation. Thus the bare interaction constants of the Hamiltonian (2) are related to their renormalized counterparts via

$$\tau_0 = \left[1 + \tfrac{u}{\epsilon} + O(u^2)\right] \mu^2 \tau \,, \tag{3a}$$

$$u_0\, s_d = \left[1 + \tfrac{3u}{\epsilon} + O(u^2)\right] \mu^\epsilon u \,, \qquad s_d \equiv \left(2\sqrt{\pi}\right)^{-d} , \tag{3b}$$

$$c_0 = \left[1 + \tfrac{u}{\epsilon} + O(u^2)\right] \mu\, c \,, \tag{3c}$$

and

$$h_{1,0} = \left[1 - \tfrac{u}{2\epsilon} + O(u^2)\right] \mu^{d/2}\, h_1 \,, \tag{3d}$$

where μ is an arbitrary momentum scale. At the order of one loop, to which we will restrict ourselves, no wave-function renormalization of ϕ is needed, so that no distinction between the bare field ϕ with $z > 0$ and its renormalized counterpart is needed. (We shall not consider the renormalization of the surface operator $\phi_s \equiv \phi|_{z=0}$, which would need a renormalization factor even at one-loop order.[2])

Let us start with the loop expansion

$$m(z) = m^{[0]}(z) + m^{[1]}(z) + O(\text{two loops}) \tag{4}$$

for the bare profile. The zero-loop term $m^{[0]}(z)$ is the solution to

$$(-\partial_z^2 + \tau_0)\, m^{[0]}(z) + \tfrac{1}{6}\, u_0\, m^{[0]}(z)^3 = 0 \tag{5}$$

that satisfies the boundary condition

$$(\partial_z - c_0)\, m^{[0]}(z)|_{z=0} = -h_{1,0} \tag{6}$$

together with the requirement that the appropriate bulk quantity is approached in the limit $z \to \infty$, i.e.,

$$\lim_{z\to\infty} m^{[0]}(z) = m_b^{[0]} \equiv \begin{cases} 0 & \text{if } \tau_0 > 0\,. \\ \sqrt{\frac{6|\tau_0|}{u_0}} & \text{if } \tau_0 < 0\,. \end{cases} \tag{7}$$

The well-known results for $\tau_0 > 0$ and $\tau_0 < 0$ are[3,2,8]

$$m_+^{[0]}(z) = \sqrt{\tfrac{12\,\tau_0}{u_0}}\, \operatorname{csch}\left[\Xi_+\,(z + z_+)\right] \tag{8}$$

and

$$m_-^{[0]}(z) = \sqrt{\tfrac{6|\tau_0|}{u_0}}\, \coth\left[\Xi_-\,(z + z_-)\right] , \tag{9}$$

where $\Xi_\pm$ is defined by

$$\Xi_+ \equiv \sqrt{\tau_0}\,, \qquad \Xi_- \equiv \sqrt{|\tau_0|/2}\,, \tag{10}$$

while $z_\pm$ is a complicated function of c_0 and $h_{1,0}$, which is determined by Eq. (6). In our calculation we can (and will) choose values of c_0 and $h_{1,0}$ corresponding to the extraordinary and critical-adsorption fixed points $\mathcal{P}^*_{\text{ex}}$ and $\mathcal{P}^*_{\text{ca}}$, respectively. In both cases $z_\pm$ vanishes, i.e.,

$$z_\pm(c_0 = -\infty,\, h_{1,0} = 0) = z_\pm(c_0 \to +\infty,\, h_{1,0} = \infty) = 0\,. \tag{11}$$

The one-loop contribution is given by

$$m^{[1]}(z) = -\tfrac{u_0}{2} \int_0^\infty dz'\, \hat{G}(\mathbf{0}; z, z')\, m^{[0]}(z') \int_{\mathbf{p}} \hat{G}(\mathbf{p}; z', z')\,. \tag{12}$$

Here $\mathbf{p}$ is a $(d-1)$-dimensional parallel momentum, $\int_{\mathbf{p}} \equiv \int d^{d-1}(p/2\pi)$, and

$$\hat{G}(\mathbf{p}; z, z') \equiv \int G(\mathbf{x}, \mathbf{x}')\, e^{-i\mathbf{p}\cdot\mathbf{r}}\, d^{d-1}r\,, \tag{13}$$

with $\mathbf{x} = (\mathbf{x}_\parallel, z)$, $\mathbf{x}' = (\mathbf{x}'_\parallel, z')$, and $\mathbf{r} = \mathbf{x}_\parallel - \mathbf{x}'_\parallel$, is the Fourier transform of the zero-loop correlation function $G(\mathbf{x}, \mathbf{x}')$. In the equation for G, the profile may be replaced by its zero-loop approximation. Hence $\hat{G}$ satisfies the equation[3,8,2]

$$\left[-\partial_z^2 + p^2 + \tau_0 + \tfrac{u_0}{2}\, m^{[0]}(z)^2\right] \hat{G}(\mathbf{p}; z, z') = \delta(z - z') \tag{14}$$

with the boundary condition

$$\left[\partial_z - c_0\right] \hat{G}(\mathbf{p}; z = 0, z' > 0) = 0\,, \tag{15}$$

aside from the requirement that the appropriate bulk limit is attained for $z \to \infty$. The solution can be found by standard techniques (described, e.g., in Ref. 3). Let us introduce the scaled variables

$$y \equiv \Xi_\pm\, z \tag{16}$$

and

$$\mathbf{P} \equiv \mathbf{p}/\Xi_\pm\,, \tag{17}$$

where as before the subscript + (−) refers to the case $\tau_0 > 0$ ($\tau_0 < 0$). Then the solution can be written in the form

$$\hat{G}(\mathbf{p}; z, z') = \tfrac{1}{\Xi_\pm}\, U_P(y)\, W_P(y')\, \theta(y' - y) + (y \leftrightarrow y')\,, \tag{18}$$

where $\theta(y)$ means the usual step function. For the values of c_0 and $h_{1,0}$ corresponding to the fixed points $\mathcal{P}^*_{\text{ex}}$ and $\mathcal{P}^*_{\text{ca}}$, we have

$$W_P(y) = e^{-\omega_P y}\, (\omega_P^2 - 1 + 3\,\omega_P \coth y + 3 \coth^2 y) \tag{19a}$$

and

$$U_P(y) = \frac{1}{\omega_P\, (\omega_P^2 - 1)(\omega_P^2 - 4)} \left[\sinh(\omega_P y)\, (\omega_P^2 - 1 + 3\,\omega_P \coth^2 y) - 3\,\omega_P \cosh(\omega_P y) \coth y\right] \tag{19b}$$

with

$$\omega_P \equiv \begin{cases} \omega_P^+ = \sqrt{P^2+1} & \text{if } \tau_0 > 0\ . \\ \omega_P^- = \sqrt{P^2+4} & \text{if } \tau_0 < 0\ . \end{cases} \tag{20}$$

This result agrees with Eqs. (13a) and (13b) of Ref. 8 up to what appear to be misprints.

For the $\mathbf{p} = \mathbf{0}$ propagator appearing in the one-loop expression (12), we also need the $\mathbf{P} \to \mathbf{0}$ limits of these functions. These limits exist and are given by

$$U_0^+(y) = -\tfrac{1}{3}\,\sinh y + \tfrac{1}{2}\big(\coth y - y\,\mathrm{csch}^2 y\big)\cosh y\ , \tag{21a}$$

$$W_0^+(y) = 3\,e^{-y}\coth y\,(1+\coth y)\ , \tag{21b}$$

and

$$U_0^-(y) = -\tfrac{1}{6}\big(\tfrac{3}{4}\cosh 2y\coth y - \sinh 2y - \tfrac{3}{4}\,y\,\mathrm{csch}^2 y\big)\ , \tag{22a}$$

$$W_0^-(y) = 3\,e^{-2y}\,(1 + 2\coth y + \coth^2 y)\ , \tag{22b}$$

for $\tau_0 > 0$ and $\tau_0 < 0$, respectively.

The self-energy integral in Eq. (12) can be decomposed as

$$\int_{\mathbf{P}} \hat{G}(\mathbf{p}; z, z) = \Xi_\pm^{d-2}\,[D_\pm(y) + C_\pm(y)]\ , \tag{23}$$

where $C_\pm$ is uv convergent (regular in ϵ), while $D_\pm$ has a pole in ϵ. Explicitly we have

$$C_\pm(y) = -\tfrac{1}{2}\big[\,\tfrac{1}{4}\,J'' - J - 3J'\coth y + (15\,J + 9\,I)\coth^2 y - 9\,I'\coth^3 y + 9\,I\coth^4 y\big] \tag{24}$$

with

$$I(y) = \int_{\mathbf{P}} \frac{e^{-2\omega_P y} - e^{-2\Omega y}}{\omega_P(\omega_P^2-1)(\omega_P^2-4)} \tag{25}$$

and

$$J(y) = \int_{\mathbf{P}} \frac{(\omega_P^2-1)\,e^{-2\omega_P y} - (\Omega^2-1)\,e^{-2\Omega y}}{\omega_P(\omega_P^2-1)(\omega_P^2-4)}\ , \tag{26}$$

in which

$$\Omega \equiv \begin{cases} \Omega_+ = 2 & \text{for } \tau_0 > 0\ , \\ \Omega_- = 1 & \text{for } \tau_0 < 0\ . \end{cases} \tag{27}$$

The divergent parts $D_\pm$ are given by

$$D_+(y) = \int_{\mathbf{P}} \left(\frac{1}{2\omega_P} - \frac{3}{2}\,\frac{\mathrm{csch}^2 y}{\omega_P(\omega_P^2-1)}\right) \tag{28}$$

and

$$D_-(y) = \int_{\mathbf{P}} \left(\frac{1}{2\omega_P} - \frac{3}{2}\,\frac{\mathrm{csch}^2 y}{\omega_P(\omega_P^2-4)}\right)\ . \tag{29}$$

These expressions are consistent with Eqs. (17)–(19b) of Ref. 8 provided we suppose the parameter ω_0 in these latter equations stands for $\omega_{P=0}^- = 2$, irrespective of whether $\tau_0 > 0$ or $\tau_0 < 0$. (The choice $\omega_0 = \omega_{P=0}^+ = 1$ for $\tau_0 > 0$ would imply inconsistencies.) No confusion should arise from the fact that our above formulas for τ_0 are not identical to Eqs. (17)–(19b) of Ref. 8: Both sets of equations correspond to different, but equivalent, decompositions into divergent and convergent parts D_- and C_-. Our choice with $\Omega_- = 1$ (rather than $\omega_0 = 2$) has the advantage that the resulting D_- is somewhat easier to calculate and that the contribution to $J(y)$ proportional to $\Omega^2 - 1$ drops out. Otherwise, it is a matter of taste.

The integrals $D_\pm$ can be computed in a straightforward manner with the results

$$\begin{aligned} D_+(y)/s_d &= \Gamma\big(\tfrac{\epsilon}{2}-1\big) - \tfrac{6}{1-\epsilon}\,\Gamma\big(\tfrac{\epsilon}{2}\big)\,\mathrm{csch}^2 y \\ &= \tfrac{-2}{\epsilon}\,(1 + 6\,\mathrm{csch}^2 y) - 1 + C_E \\ &\quad - 6\,(2 - C_E)\,\mathrm{csch}^2 y + O(\epsilon) \end{aligned} \tag{30a}$$

and

$$\begin{aligned} D_-(y)/s_d &= 2^{2-\epsilon}\,\big[2\,\Gamma\big(\tfrac{\epsilon}{2}-1\big) - \tfrac{3}{1-\epsilon}\,\Gamma\big(\tfrac{\epsilon}{2}\big)\,\mathrm{csch}^2 y\big] \\ &= \tfrac{-4}{\epsilon}\,(2 + 3\,\mathrm{csch}^2 y) - 4\,(1 - C_E - 2\ln 2) \\ &\quad - 6\,(2 - C_E - 2\ln 2)\,\mathrm{csch}^2 y + O(\epsilon)\ , \end{aligned} \tag{30b}$$

where C_E means Euler's constant.

We now substitute the self-energy integral (23) into the one-loop contribution (12). Using the above results for $D_\pm$, the z' integration over the contribution $\propto D_\pm$ can be performed analytically. Denoting the mean-field profiles by

$$\sigma(y) \equiv \begin{cases} \sigma_+ = \mathrm{csch}\,y & \text{for } \tau_0 > 0\ , \\ \sigma_- = \coth y & \text{for } \tau_0 < 0\ , \end{cases} \tag{31}$$

let us define the functions

$$F_\pm(y) \equiv \int_0^\infty dy'\,C_\pm(y')\,\big[U_0^\pm(y')\,W_0^\pm(y)\,\theta(y-y') + (y' \leftrightarrow y)\big]\,\sigma_\pm(y')\ . \tag{32}$$

Then the results can be written as

$$m_+^{[1]}(z) = \tfrac{1}{2}\,u_0\,s_d\sqrt{\tfrac{12\tau_0}{u_0}}\,\Big\{\big[\tfrac{2}{\epsilon} + \tfrac{5}{2} - C_E - \ln\tau_0\big]\,\mathrm{csch}\,y - \tfrac{1}{2}\big[\tfrac{2}{\epsilon} - C_E + 1 - \ln\tau_0\big]\,y\,\mathrm{csch}'y - s_d^{-1}\,F_+(y) + O(\epsilon)\Big\}_{y=z\sqrt{\tau_0}} \tag{33a}$$

and

$$m_-^{[1]}(z) = \tfrac{1}{2}\, u_0\, s_d \sqrt{\tfrac{6|\tau_0|}{u_0}}\, \{ [\tfrac{2}{\epsilon} - C_E + 1 - \ln 2|\tau_0|] \coth y - \tfrac{1}{2}[\tfrac{2}{\epsilon} - C_E + 4 - \ln 2|\tau_0|]\, y \coth' y - s_d^{-1} F_-(y) + O(\epsilon) \}_{y=z\sqrt{|\tau_0|/2}} \,. \tag{33b}$$

In expanding the term $\Xi_\pm^{d-2} \propto |\tau_0|^{1-\epsilon/2}$ in powers of ϵ, we assumed that τ_0 is measured in units of the reference scale μ^2 introduced in Eqs. (3a)–(3d). For notational simplicity, we have set $\mu = 1$ and will do so below.

When these results are substituted into Eq. (4) and the bare variables u_0 and τ_0 are expressed in terms of their renormalized analogs using Eqs. (3b) and (3a), the poles are found to cancel. The resulting renormalized profiles are

$$\begin{aligned} m(z;u,\tau) = {} & m^{[0]}(z; u_0 = u/s_d,\ \tau_0 = \tau) \\ & + \mathrm{FP}\{m^{[1]}(z; u_0 = u/s_d,\ \tau_0 = \tau)\} \\ & + O(u^{3/2}) \,, \end{aligned} \tag{34}$$

where FP means finite (regular) part.

In order to improve these perturbative results by means of the RG, we recall that the RG equation satisfied by $m(z)$ yields the asymptotic scaling form

$$m(z;u,\tau) \approx M_-\, |\tau|^\beta\, P_\pm(z/\xi_\pm) \,, \tag{35}$$

in which M_- is the same nonuniversal metric factor that appears in the equation

$$m_b^- = m_-(z = \infty) \approx M_-\, |\tau|^\beta \tag{36}$$

for the bulk order parameter, while

$$\xi_\pm \approx \xi_0^\pm\, |\tau|^{-\nu} \tag{37}$$

are the bulk correlation lengths for $\tau \gtrless 0$. All nonuniversality in Eq. (35) is contained in the two nonuniversal amplitudes M_- and ξ_0^+. The amplitude ratio[20]

$$\xi_0^+/\xi_0^- = 2^\nu \left[1 + \tfrac{5}{24}\,\epsilon + O(\epsilon^2)\right] \tag{38}$$

is a well-known universal quantity.

Using Eqs. (35) and (36) in conjunction with standard RG arguments, we can express the scaling functions as

$$P_\pm(\zeta) = m_\pm(\zeta\, \xi_*^\pm; u^*, \tau = \pm 1)/m_-(\infty; u^*, -1) \,, \tag{39}$$

where $u^* = \epsilon/3 + O(\epsilon^2)$ is the value of u at the infrared-stable fixed point, while $\xi_\pm^* \equiv \xi_\pm(u^*, \tau = \pm 1)$ is the appropriate value of $\xi_0^\pm$ for our renormalized theory with $u = u^*$. By a straightforward calculation one finds that the two nonuniversal amplitudes involved in Eq. (39) are given by[21]

$$\xi_+^* = 1 + \tfrac{u^*}{4}\,(1 - C_E) + O(\epsilon^2) \tag{40}$$

and

$$m_-(\infty; u^*, -1) = \sqrt{\frac{6 s_d}{u^*}} \left[1 + \frac{1 - C_E - \ln 2}{2}\, u^* + O(\epsilon^2) \right] . \tag{41}$$

Combining the above results, we finally obtain

$$P_+(\zeta) = \sqrt{2} \left\{ \left[1 + u^*(\tfrac{3}{4} + \tfrac{\ln 2}{2})\right] \mathrm{csch}\zeta - \tfrac{u^*}{2 s_d}\, F_+(\zeta) \right\} \tag{42a}$$

and

$$P_-(\zeta) = \coth\frac{\zeta}{2} + \frac{11}{16}\, u^* \zeta\, \mathrm{csch}^2 \frac{\zeta}{2} - \frac{u^*}{2 s_d}\, F_-\left(\frac{\zeta}{2}\right) . \tag{42b}$$

In Figs. 1 and 2 we have plotted these functions for $\epsilon = 1$ ($d = 3$). As already mentioned in the Introduction, both P_+ and P_- cross over from the short distance to the long-distance behavior in a *monotonic and physically reasonable* manner. This refutes the contradictory results for P_+ by Peliti and Leibler.[16]

III. ASYMPTOTIC BEHAVIOR OF PROFILES AND TEMPERATURE SINGULARITY OF SURFACE MAGNETIZATION

According to Eqs. (35) and (36), P_- is normalized such that

$$P_-(\infty) = 1 \,, \tag{43}$$

whereas $P_+(\infty) = 0$, of course. Since we have scaled the distance z from the surface by the true bulk correlation length (defined via the exponential decay of the bulk correlation function[21,22]), $P_\pm$ should behave asymptotically as

$$P_\pm(\zeta) - P_\pm(\infty) \sim e^{-\zeta} \tag{44}$$

in the limit $\zeta \to \infty$. In Appendix B we determine the asymptotic behavior of both F_+ and F_-. Exploiting the results in Eqs. (42a) and (42b), one easily deduces the asymptotic forms

$$P_+(\zeta) \underset{\zeta\to\infty}{\approx} 2\sqrt{2} \left\{ 1 + u^* \left[\tfrac{3}{4} + \tfrac{\ln 2}{2} + \tfrac{\pi}{4} \left(1 - 2\sqrt{3} + \tfrac{2\sqrt{3}}{\pi} \ln \tfrac{2\sqrt{3}+3}{2\sqrt{3}-3} \right) \right] \right\} e^{-\zeta} \tag{45a}$$

and

$$P_-(\zeta) \underset{\zeta\to\infty}{\approx} 1 + \left\{ 2 + u^* \left[\tfrac{11}{4}\,\zeta - \tfrac{\pi}{2} \left(\sqrt{3}\,\zeta + 4 - 1/\sqrt{3} \right) \right] \right\} e^{-\zeta} \,, \tag{45b}$$

in conformity with our expectations.

We proceed by analyzing the short-distance behavior of $P_\pm$, in order to determine the temperature singularity of the surface magnetization m_1 (or near-surface magnetization). In order for $P_\pm$ to be compatible with the asymptotic behavior of m_1 in Eq. (1), it must have the limiting form

$$P_\pm(\zeta) \underset{\zeta\to 0}{\approx} \zeta^{-\beta/\nu}(c_\pm + a_\pm\,\zeta^{1/\nu} + a'_\pm\,\zeta^{2/\nu} + b_\pm\,\zeta^d + \text{l.s.t}) , \tag{46}$$

where l.s.t. means less singular terms. Since the scaling functions $P_\pm$ are universal, so are the constants $a_\pm$, $a'_\pm$, $b_\pm$, and $c_\pm$, which evidently can be expressed as universal ratios of nonuniversal amplitudes related to $m_\pm$, m_b, and $\xi_\pm$. Comparison with Eq. (1) yields the relations

$$\frac{c_+}{c_-} = \left(\frac{\xi_0^+}{\xi_0^-}\right)^{-\beta/\nu} , \tag{47a}$$

$$\frac{a_+}{a_-} = -\frac{A_+}{A_-}\left(\frac{\xi_0^+}{\xi_0^-}\right)^{(1-\beta)/\nu} , \tag{47b}$$

$$\frac{a'_+}{a'_-} = -\frac{A'_+}{A'_-}\left(\frac{\xi_0^+}{\xi_0^-}\right)^{(2-\beta)/\nu} , \tag{47c}$$

and

$$\frac{b_+}{b_-} = \frac{B_+}{B_-}\left(\frac{\xi_0^+}{\xi_0^-}\right)^{d-\beta/\nu} . \tag{47d}$$

In Appendix A we determine the asymptotic expansions of the functions $F_\pm$ and the renormalized profiles $m_\pm(z)$. These results confirm that $P_\pm$ has the anticipated limiting form (46), with the coefficients having the ϵ expansions

$$a_+ = \sqrt{2}\,\left[-\tfrac{1}{6} + \tfrac{\epsilon}{216}\,(1 - 6\,C_E - 6\,\ln 2)\right] + O(\epsilon^2) , \tag{48a}$$

$$a_- = \tfrac{1}{6} + \tfrac{\epsilon}{36}\,\left(C_E - \tfrac{17}{12}\right) + O(\epsilon^2) , \tag{48b}$$

$$a'_+ = \tfrac{\sqrt{2}}{36} + O(\epsilon) , \tag{48c}$$

$$a'_- = -\tfrac{1}{72} + O(\epsilon) , \tag{48d}$$

$$b_+ = -\tfrac{\sqrt{2}}{120} + O(\epsilon) , \tag{48e}$$

$$b_- = -\tfrac{1}{60} + O(\epsilon) , \tag{48f}$$

$$c_+ = \sqrt{2}\,\left[1 + \tfrac{\epsilon}{12}\,(6\,C_E + 2\,\ln 2 - 13)\right] + O(\epsilon^2) , \tag{48g}$$

and

$$c_- = 2 + \epsilon\,\left(C_E - \tfrac{7}{4}\right) + O(\epsilon^2) . \tag{48h}$$

As immediate consequences, Eqs. (47a)–(47d) are found to hold with

$$A_+ = A_- \equiv A \tag{49a}$$

and

$$A'_+ = A'_- \equiv A' . \tag{49b}$$

Since these latter findings are at variance with those of Ohno and Okabe,[8] we have verified that their method of calculation (which uses a cutoff regularization) leads to equivalent results. The source of the discrepancy with Ref. 8 is discussed in Appendix C.

Let us also note that the ϵ expansions of the universal amplitude ratios $c_\pm$ given in Eqs. (48g) and (48h) were obtained previously through a completely independent calculation by Ciach and one of the authors.[19] The result for c_+ has been used in a recent analysis[13] of experimental data on critical adsorption. This analysis found the theoretical values for c_+ in fair agreement with the experimental ones.

IV. SUMMARY AND CONCLUSIONS

Using the field-theoretic RG approach in $4-\epsilon$ dimensions, we were able to compute the universal order-parameter profiles $P_\pm(\zeta)$ to first order in ϵ both for the extraordinary transition in the semi-infinite ϕ^4 model and for critical adsorption. Our principal findings and conclusions may be summarized as follows.

First, to the order of our calculation we find complete agreement with the scaling picture for the extraordinary transition suggested by Bray and Moore.[7] In particular, the universal profiles $P_\pm$ pertaining to the extraordinary transition fixed point $\mathcal{P}^*_{\text{ex}}$ at $h_1 = 0$ and $c = -\infty$ and to the critical-adsorption fixed point $\mathcal{P}^*_{\text{ca}}$ at $h_1 = \infty$ and $c = +\infty$ agree.

Second, the short-distance behavior of $P_\pm$ is fully consistent with Bray and Moore's prediction that the surface magnetization m_1 has a $|\tau|^{2-\alpha}$ singularity plus regular background terms. This refutes claims[8] that $\partial_\tau m_1$ at order ϵ has a jump singularity at T_{cb}.

Third, the profiles $P_\pm(\xi;\epsilon = 1)$ obtained by naive extrapolation to three dimensions display a smooth monotonous crossover from the behavior at short distances $\xi \ll 1$ to the behavior at long distances $\xi \gg 1$, just as expected on physical grounds. The results of Peliti and Leibler,[16] yielding a nonmonotonous profile P_+ in three dimensions, are incorrect.

Finally, it seems worthwhile to point out that our results for $P_\pm$ may be utilized in the analysis of experimental data on the critical adsorption of fluids. An example of such an analysis is provided by Ref. 13, in which the universal amplitude ratio c_+, whose ϵ expansion is given in Eq. (48g), is extracted from experimental data.

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APPENDIX A: SHORT-DISTANCE BEHAVIOR OF PROFILES

In order to determine the asymptotic behavior of $P_\pm(\zeta)$ for $\zeta \to 0$, we need information about how $F_\pm(y)$ behaves for small values of y. This can be gained by expanding the integrand in Eq. (32) and integrating termwise. To expand $C_\pm(y)$ we use the fact that $I(y)$ is the solution of the differential equation

$$I''(y) - 4\,\Omega^2\, I(y) = 4\, K_{d-1}\, K_0\left(\frac{4y}{\Omega}\right) \tag{A1}$$

for the initial values $I(0) = 0$ and $I'(0)$ as implied by Eq. (25). [The latter initial value can be determined by numerical integration of the expression for $I'(0)$ resulting from Eq. (25), but will not be needed in the following.] Here

$$K_{d-1} \equiv 2\,(4\pi)^{(1-d)/2}/\Gamma\left(\tfrac{d-1}{2}\right)\,, \tag{A2}$$

and Ω means the quantity defined in Eq. (27). Further, $K_0(x)$ is a modified Bessel function whose asymptotic expansion for small x reads

$$K_0(x) = -\ln\tfrac{x}{2}\sum_{k=0}^{\infty}\tfrac{x^{2k}}{2^{2k}(k!)^2} + \sum_{k=0}^{\infty}\tfrac{x^{2k}}{2^{2k}(k!)^2}\,\psi(k+1)\,, \tag{A3}$$

where $\psi(x) \equiv d\ln\Gamma(x)/dx$ is the usual ψ (digamma) function.

Using the ansatz

$$I(y) = -\ln\left(\tfrac{2y}{\Omega}\right)\sum_{n=1}^{\infty} a_n\, y^{2n} + \sum_{n=1}^{\infty} b_n\, y^{2n} + \tfrac{I'(0)}{2\Omega}\sinh(2\Omega y) \tag{A4}$$

we find

$$\begin{aligned} I(y) = &-(2y^2 + 3y^4 + \tfrac{49}{30}y^6)\,(C_E + \ln y) \\ &+ (3y^2 + \tfrac{37}{12}y^4 + \tfrac{292}{75}y^6) \\ &+ \tfrac{I'(0)}{2\Omega}\,(4y + \tfrac{32}{3}y^3 + \tfrac{128}{15}y^5 + \tfrac{1024}{315}y^7) \\ &+ O(y^8, y^8\ln y) \end{aligned} \tag{A5a}$$

for $\tau_0 > 0$ and

$$\begin{aligned} I(y) = &-(2y^2 + 2y^4 + \tfrac{4}{5}y^6)\,(C_E + \ln 2y) \\ &+ (3y^2 + \tfrac{7}{2}y^4 + \tfrac{39}{25}y^6) \\ &+ \tfrac{I'(0)}{2\Omega}\,(2y + \tfrac{4}{3}y^3 + \tfrac{4}{15}y^5 + \tfrac{8}{315}y^7) \\ &+ O(y^8, y^8\ln y) \end{aligned} \tag{A5b}$$

for $\tau_0 < 0$. The corresponding expansion of $J(y)$ can be obtained upon substitution of these results into

$$I''(y) - 4\,I(y) = 4\,J(y)\,. \tag{A6}$$

The resulting expansions for $F_\pm$ are

$$\begin{aligned} -\tfrac{1}{8s_d}\,y\,F_+(y) = &\;1 - \tfrac{5}{144}y^2 - \tfrac{421}{10800}y^4 \\ &-(\tfrac{3}{8} + \tfrac{1}{48}y^2 + \tfrac{1}{2880}y^4)\ln y \\ &-(\tfrac{3}{8} + \tfrac{1}{48}y^2 + \tfrac{179}{1440}y^4)\,C_E \\ &+O(y^6, y^6\ln y) \end{aligned} \tag{A7a}$$

and

$$\begin{aligned} -\tfrac{1}{8s_d}\,y\,F_-(y) = &\;(1 - \tfrac{1}{18}y^2 - \tfrac{247}{5400}y^4) \\ &-(\tfrac{3}{8} + \tfrac{1}{24}y^2 + \tfrac{13}{36}y^4)\ln y \\ &-(\tfrac{3}{8} + \tfrac{1}{24}y^2 + \tfrac{4}{225}y^4)\,(C_E + \ln 2) \\ &+O(y^6, y^6\ln y)\,. \end{aligned} \tag{A7b}$$

Utilizing these results one finds that the renormalized profiles behave as

$$\begin{aligned} m_+(z) \underset{z\to 0}{\approx} \sqrt{\tfrac{12s_d}{u}}\,\tfrac{1}{z}\Big[&1 - \tfrac{5}{2}u + \tfrac{3}{4}C_E\,u + \tfrac{3}{2}u\ln z - \left(\tfrac{1}{6} + \tfrac{u}{36} + \tfrac{u}{24}C_E + \tfrac{u}{12}\ln z\right)\tau z^2 \\ &+\left(\tfrac{7}{360} + \tfrac{1789}{10800}u - \tfrac{323}{7200}C_E\,u + \tfrac{u}{240}\ln\tau - \tfrac{u}{720}\ln z\right)\tau^2 z^4\Big] \end{aligned} \tag{A8a}$$

and

$$\begin{aligned} m_-(z) \underset{z\to 0}{\approx} \sqrt{\tfrac{12s_d}{u}}\,\tfrac{1}{z}\Big[&1 - \tfrac{5}{2}u + \tfrac{3}{4}C_E\,u + \tfrac{3}{2}u\ln z - \left(\tfrac{1}{6} + \tfrac{u}{36} + \tfrac{u}{24}C_E + \tfrac{u}{12}\ln z\right)\tau z^2 \\ &-\left(\tfrac{1}{180} + \tfrac{43}{1350}u - \tfrac{59}{3600}C_E\,u - \tfrac{u}{60}\ln|\tau| + \tfrac{u}{600}\ln 2 - \tfrac{13}{360}u\ln z\right)\tau^2 z^4\Big], \end{aligned} \tag{A8b}$$

respectively. From these expressions the equality of A_+ and A_- as well as of A'_+ and A'_- can be read off directly. The results for the asymptotic behavior of $P_\pm$ given in Eqs. (46)–(48h) can be deduced in a straightforward fashion using the well-known ϵ expansions of the bulk exponents.

APPENDIX B: LONG-DISTANCE BEHAVIOR OF $F_\pm$

In order to derive from Eqs. (42a) and (42b) for the profiles $P_\pm(\zeta)$ their asymptotic long-distance forms given in Eqs. (45a) and (45b), we must determine how the functions $F_\pm(y)$ behave in the limit $y \to \infty$.

Using a steepest descent approximation we find

$$I(y) \underset{y\to\infty}{\approx} -\frac{K_{d-1}}{6}\sqrt{\frac{\pi}{y}}e^{-2y} \tag{B1}$$

for $\tau > 0$ and

$$I(y) \underset{y\to\infty}{\approx} -\frac{K_{d-1}}{6\sqrt{3}}e^{-2y} \tag{B2}$$

for $\tau < 0$.

Inserting this into Eq. (32) we arrive at

$$F_+(\zeta) \underset{\zeta\to\infty}{\approx} \pi s_d \left(1 - 2\sqrt{3} + \frac{2\sqrt{3}}{\pi}\ln\frac{2\sqrt{3}+3}{2\sqrt{3}-3}\right) e^{-\zeta} \tag{B3}$$

and

$$F_-(\zeta/2) \underset{\zeta\to\infty}{\approx} \pi s_d \left(\sqrt{3}\,\zeta + 4 - 1/\sqrt{3}\right) e^{-\zeta}\,. \tag{B4}$$

APPENDIX C: COMPARISON WITH OHNO AND OKABE'S WORK

In order to resolve the discrepancy with Ref. 8 we follow their line of calculation but take their integrals $D_>$ and $D_<$ to be defined by the cutoff-regularized right-hand sides of our Eqs. (28) and (29) for $D_\pm$, with our choice (27) of Ω. Expanding all functions we arrive at the same expressions as Ohno and Okabe but

$$D_<(y) = K_3\left[\tfrac{1}{2} - \tfrac{1}{2y^2}(3 + y^2 + \tfrac{1}{5}y^4)\ln\tfrac{\Lambda}{2\,\Xi_-}\right] + O(y^4), \tag{C1}$$

$$D_>(y) = K_3\left[\tfrac{1}{8} - \tfrac{1}{2y^2}(3 - \tfrac{1}{2}y^2 + \tfrac{1}{5}y^4)\ln\tfrac{\Lambda}{\Xi_+}\right] + O(y^4) \tag{C2}$$

instead of their results. [The term proportional to $I'(0)$ in Eqs. (A5a) and (A5b) cancels and thus does not affect the result.] Integrating termwise we find $m_+^{[1]}$ and $m_-^{[1]}$ to have the same expansion

$$-\tfrac{3}{2}K_3\tfrac{\sqrt{2u}}{z}\left[2 + \tfrac{1}{36}\tau z^2 + (-\tfrac{3}{4} + \tfrac{1}{24}\tau z^2)\ln\Lambda z\right] \tag{C3}$$

up to second order in the temperature, where Λ is the momentum cutoff. Thus the statement that the coefficients of the terms linear in τ differ is refuted.

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