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Universal relations among critical amplitudes of surface quantities

H. W. Diehl
*Institut für Festkörperforschung der Kernforschungsanlage Jülich, Postfach 1913, D-5170 Jülich 1, Federal Republic of Germany**
and Sektion Physik der Universität München, Theresienstrasse 37, D-8000 München 2, Federal Republic of Germany

G. Gompper and W. Speth
Sektion Physik der Universität München, Theresienstrasse 37, D-8000 München 2, Federal Republic of Germany
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Universal relations among critical amplitudes of surface quantities are discussed for d-dimensional semi-infinite systems near their bulk critical temperature T_c^b. Based on the field-theoretic renormalization-group approach, a general derivation of the expected multi-scale-factor universality is given and various universal ratios involving critical amplitudes of the ordinary and special transitions both above and below T_c^b are calculated to first order in $\epsilon=4-d$. In addition, an error in the published one-loop result for the universal order-parameter profile at the ordinary transition of the semi-infinite Ising model is corrected.

I. INTRODUCTION

As is well known, systems showing critical behavior can be divided into equivalence classes such that all members of a class have the same ("universal") critical properties.[1] Aside from critical exponents, scaling functions, and equations of state, the set of universal properties includes combinations of critical amplitudes ("ratios"). The universality of most of these ratios was originally concluded on purely phenomenological grounds.[2] Subsequently, the general origin of universal relations among critical amplitudes was clarified and a systematic derivation of them all was given using the renormalization-group (RG) approach.[3–5] Such relations are not only interesting from a theoretical point of view; they also have experimental significance in that they reduce the number of adjustable parameters of the theory, a fact which allows a more rigorous confrontation between theory and experiment.[6]

The purpose of the present paper is to investigate critical amplitudes of *surface quantities.* We have in mind systems such as a semi-infinite ferromagnet near its critical temperature T_c^b for the appearance of bulk order. In the past few years the theory of surface effects on critical behavior has advanced considerably.[7,8] In particular, it has become clear that the concept of universality classes can be appropriately generalized. However, since a thermodynamic description of surface effect involves, besides the usual bulk fields (bulk magnetic field h, temperature T) and densities (bulk magnetization m_b, bulk energy density), additional *surface fields* (such as a surface magnetic field h_1, surface interaction constant, etc.) and corresponding densities (such as the magnetization at the surface, m_1), universality classes for surface critical behavior are usually narrower than those for bulk critical behavior. For example, in the case of a semi-infinite Ising ferromagnet with short-range interactions, m_1 behaves as $\sim|\tau|^{\beta_1}$ when $\tau=(T-T_c^b)/T_c^b\to 0+$, with an exponent $\beta_1\equiv\beta_1^{\text{ord}}$ characteristic of the *ordinary transition* if the interaction between the spins at the surface is not enhanced too much relative to the bulk, but with a different exponent $\beta_1\equiv\beta_1^{\text{sp}}$ characteristic of the *special transition* if the enhancement takes a critical value—even though all bulk quantities have the same critical behavior in both cases. For still stronger enhancement, a behavior of m_1 characteristic of the *extraordinary transition* is observed.

The universal relations among bulk critical amplitudes near second-order phase transitions can be understood as the result of a *two-scale-factor universality.*[2–5] Roughly speaking, this means that all nonuniversality of the singular part of the bulk free energy and of the asymptotic part of correlation functions can be absorbed in two independent nonuniversal scale factors, which are associated with the two relevant fields h and τ appearing in a scaling or RG analysis. A description of surface critical behavior requires at least one, or more, relevant surface fields in addition to these bulk fields. [Note that we do not consider transitions (such as the surface transition) at which the bulk stays noncritical.] By analogy, one thus expects a *multi-scale-factor universality,* namely a three-scale-factor universality in the cases of the above-mentioned ordinary and extraordinary transitions, at which three fields are relevant, and a four-scale-factor universality in the case of the special transition, which has four relevant fields. We shall give a general derivation of this multi-scale-factor universality using the field-theoretic RG approach.[9] This approach has been extended recently to semi-infinite systems[10–13] and lends itself particularly well to a systematic investigation of universal properties.

Our analysis is based on the Hamiltonian

$$\mathscr{H}=\int dV\left[\frac{1}{2}(\nabla\phi)^2+\frac{1}{2}\tau_0\phi^2+\frac{g}{4!}\phi^4\right]+\frac{1}{2}c_0\int dS\,\phi^2 \quad (1.1)$$

for a scalar order parameter $\phi(x)$. Here, $x=(x_{\parallel},z)$ is a d-dimensional position vector with $x_{\parallel}$, a $(d-1)$-dimensional component, and $z\geq 0$. The volume integral $\int dV$ extends over the d-dimensional half-space $z\geq 0$, the surface integral over the $(d-1)$-dimensional plane $z=0$. The model is the Ising ($n=1$) version of the much-studied semi-infinite n-vector model.[14] Although we shall, for simplicity, only consider the $n=1$ case, those of our results that concern the O(n)-symmetric paramagnetic phase carry over to the general $n\neq 1$ case; this will be indicated by keeping track of the n dependence in the corresponding results. For the sake of simplicity, we shall, moreover, limit ourselves to a computation of critical amplitudes (above and below T_c^b) for the *ordinary* and *special* transitions. Critical amplitudes for the extraordinary transition can be calculated along lines similar to those we take in the computation of the amplitudes below T_c^b.

In contrast to critical bulk amplitudes, critical amplitudes of surface quantities have scarcely been studied previously. The only studies we are aware of are the Monte Carlo work of Landau,[15,16] a recent calculation of the universal ratio $C_{s,\text{sp}}^{(+)}/C_{s,\text{ord}}^{(+)}$ to first order in $\epsilon=4-d$ for the model (1.1), where the $C_{s,\text{sp/ord}}^{(+)}$ mean the amplitudes of the singular part of the (excess) surface specific heat for $\tau\to 0+$, at the special and ordinary transitions,[17] and some preliminary results of Eisenriegler[18] concerning amplitude ratios for polymer quantities.[19]

The remainder of this paper is organized as follows. In Sec. II we briefly recapitulate the necessary field-theoretic tools which are used to derive the promised multi-scale-factor universality. In Sec. III examples of universal ratios involving critical amplitudes of various surface susceptibilities at the ordinary and special transitions, both above and below T_c^b, are given, and the results we obtain for these using the ϵ expansion are summarized. In Sec. IV some of the calculations are outlined. In addition, the universal order-parameter profiles at the ordinary and special transitions are given to order ϵ. While in the case of the special transition our result is in accordance with Ref. 12, we find in the case of the ordinary transition a discrepancy with the profile obtained by Wilson.[20] The source of this discrepancy is explained in Appendix B. Section V is reserved for concluding remarks and a brief summary.

II. THE RENORMALIZATION GROUP, SCALING, AND MULTI-SCALE-FACTOR UNIVERSALITY

We begin with a brief summary of renormalization-group results. Details of the field-theoretic approach we employ may be found in Refs. 10–12. With regard to notations, we follow Ref. 21.

Let

$$G^{(N,M)}(x,r)\equiv\left\langle\prod_{i=1}^{N}\phi(x_i)\prod_{j=1}^{M}\phi(r_j,0)\right\rangle^{\text{conn}} \quad (2.1)$$

denote a connected $(N+M)$-point correlation function (cumulant) with N points $x_i=(x_{i_{\parallel}},z_i)$, $i=1,\ldots,N$, off the surface, and M points $(r_j,0)$, $j=1,2,\ldots,M$, on it. The cumulant average $\langle\ \rangle^{\text{conn}}$ has the usual meaning and is defined relative to the thermodynamic average $\langle\ \rangle$ with the Boltzmann factor $\exp(-\mathscr{H}\{\phi\})$. We use the abbreviations $x=\{x_i\,|\,i=1,\ldots,N\}$, $z=\{z_i\,|\,i=1,\ldots,N\}$, and $r=\{r_j\,|\,j=1,\ldots,M\}$. Introducing $N+M$ $(d-1)$-dimensional parallel momenta p_k, $k=1,\ldots,N+M$—one for each $x_{i_{\parallel}}$ ($p_k=p_i$) and one for each r_j ($p=p_{N+i}$)—we define the parallel Fourier transform $\hat{G}^{(N,M)}(p,z)$, with $p=\{p_k\}$, by

$$\hat{G}^{(N,M)}(p,z)(2\pi)^{d-1}\delta\left[\sum_{k=1}^{N+M}p_k\right]=\int G^{(N,M)}(x,r)\exp\left[-i\sum_{i=1}^{N}p_i\cdot x_{i_{\parallel}}-i\sum_{j=1}^{M}p_{N+j}\cdot r_j\right]\left[\prod_{i=1}^{N}dx_{i_{\parallel}}\right]\left[\prod_{j=1}^{M}dr_j\right]. \quad (2.2)$$

In order to absorb the ultraviolet singularities of $G^{(N,M)}$, the following reparametrizations are needed:

$$\phi=Z_\phi^{1/2}\phi^R\,,\quad \tau_0=\mu^2 Z_\tau\tau+\tau_b\,,\quad g=\mu^\epsilon 2^d\pi^{d/2}Z_u u\,,$$
$$\phi\,|_s=(Z_\phi Z_1)^{1/2}(\phi\,|_s)^R\,,\quad c_0=\mu Z_c c+c_{\text{sp}}\,. \quad (2.3)$$

Here, μ is an arbitrary momentum scale. $\phi\,|_s=\phi(r,0)$ means the order parameter at the surface. Z_w, $w=\phi,\tau,u,1,c$, are bulk and surface normalization factors which are given in Refs. 10 and 11 to two-loop order. τ_b and c_{sp} are the critical values of the multicritical point that describes the special transition; they vanish in dimensional regularization.

The renormalized functions

$$G_R^{(N,M)}(x,r;u,\tau,c,\mu)=Z_\phi^{-(M+N)/2}Z_1^{-M/2}\times G^{(N,M)}(x,r;g,\tau_0,c_0) \quad (2.4)$$

satisfy the RG equations

$$\left[\mu\partial_\mu+\beta_u\partial_u-(2+\eta_\tau)\tau\partial_\tau-(1+\eta_c)c\partial_c+\frac{N+M}{2}\eta_\phi+\frac{M}{2}\eta_1\right]G_R^{(N,M)}=0\,, \quad (2.5)$$

with $\beta_u\equiv\mu\partial_\mu|_0 u$ and $\eta_w\equiv\mu\partial_\mu|_0\ln Z_w$, $w=\phi,\tau,u,1,c$, where $\partial_\mu|_0$ denotes a derivative at fixed bare parameters τ_0,g,c_0. The values $\eta_w^*\equiv\eta_w(u^*)$ of η_w at the infrared-stable fixed point u^* give us the usual bulk exponents $\eta=\eta_\phi^*$, $\nu=(2+\eta_\tau^*)^{-1}$, and $\Delta=(\nu/2)(d+2-\eta)$, as well as the surface exponents $\eta_{\parallel}^{\text{sp}}=\eta+\eta_1^*$, $\Delta_1^{\text{sp}}=(\nu/2)(d-\eta_{\parallel}^{\text{sp}})$ of the special transition, and the crossover exponent $\Phi=\nu(1+\eta_c^*)$.

Solving the RG equations (5) in the standard fashion,[9] by characteristics, one obtains, for $\hat{G}_R\equiv\hat{G}_R^{(N,M)}$,

$$\hat{G}_R(p,z;u,\tau,c,\mu)=l^{d_G+\eta_G^*}E_G\hat{G}_R(p/l,zl;\bar{u},\bar{\tau},\bar{c},\mu)\,, \quad (2.6)$$

where l is a scale factor and the running variables $\bar{u},\bar{\tau},\bar{c}$

are defined by

$$\ln l=\int_{u}^{\bar u(l)} du'/\beta_u(u') ,$$
$$\bar\tau(l)=l^{-1/\nu}E_\tau \tau , \qquad (2.7)$$
$$\bar c(l)=l^{-\Phi/\nu}E_c c ,$$

with

$$E_\tau \equiv E_\tau(\bar u,u) = \exp\left[-\int_u^{\bar u} du'[2+\eta_\tau(u')-\nu^{-1}]/\beta_u(u')\right] ,$$
$$E_c \equiv E_c(\bar u,u) = \exp\left[-\int_u^{\bar u} du'[1+\eta_c(u')-\Phi/\nu]/\beta_u(u')\right] . \qquad (2.8)$$

We have used the notation d_G for the μ dimension of $\hat G$ and η_G^*, with

$$\eta_G \equiv [(N+M)\eta_\phi+M\eta_1]/2 ,$$

for its anomalous dimension. E_G is given by

$$E_G \equiv E_G(\bar u,u) = \exp\left[\int_u^{\bar u} du'[\eta_G(u')-\eta_G^*]/\beta_u(u')\right] . \qquad (2.9)$$

The result in (2.6) can be easily generalized to include bulk and surface magnetic fields. Given the Hamiltonian

$$\mathscr{H}-h_0\int dV\phi-h_{1,0}\int dS\phi , \qquad (2.10)$$

we can define dimensionless renormalized field h,h_1 and corresponding running variables $\bar h,\bar h_1$ via

$$h=\mu^{-(d+2)/2}Z_\phi^{1/2}h_0 , \quad h_1=\mu^{-d/2}(Z_\phi Z_1)^{1/2}h_{1,0} \qquad (2.11)$$

and

$$\bar h(l)=l^{-\Delta/\nu}E_h h , \quad \bar h_1(l)=l^{-\Delta_1^{\rm sp}/\nu}E_{h_1}h_1 , \qquad (2.12)$$

where

$$E_h \equiv E_h(\bar u,u) = \exp\left[-\int_u^{\bar u} du'\{\tfrac{1}{2}[d+2-\eta_\phi(u')]-\Delta/\nu\}/\beta_u(u')\right] , \qquad (2.13)$$
$$E_{h_1} \equiv E_{h_1}(\bar u,u) = \exp\left[-\int_u^{\bar u} du'\{\tfrac{1}{2}[d-\eta_\phi(u')-\eta_1(u')] - \Delta_1^{\rm sp}/\nu\}/\beta_u(u')\right] .$$

Equation (2.6) remains valid if we add h and h_1 or $\bar h$ and $\bar h_1$ to the variables appearing in the $\hat G_R$'s on the left- or right-hand side.

In the critical domain ($\tau\to 0$), which corresponds to $l\to 0$, we may replace $\bar u$ by u^*, neglecting corrections to scaling. Choosing l such that $\bar\tau$ is no longer critical, namely by

$$\bar\tau(l)=1 , \qquad (2.14)$$

and using dimensional considerations, we find that $\hat G_R$ takes the asymptotic form

$$\hat G_R(p,z;u,\tau,c,h,h_1,\mu)\sim\mu^{d_G}E_G^*\tilde\tau^{\nu(d_G+\eta_G^*)} \times\Xi(p\tilde\tau^{-\nu}/\mu,\mu z\tilde\tau^{\nu}; \tilde c\tilde\tau^{-\Phi},\tilde h\tilde\tau^{-\Delta},\tilde h_1\tilde\tau^{-\Delta_1^{\rm sp}}) , \qquad (2.15)$$

with

$$\tilde\tau=E_\tau^*\tau , \quad \tilde c=E_c^*c , \quad h=E_h^*h , \quad \tilde h_1=E_{h_1}^*h_1 , \qquad (2.16)$$

where the asterisk again indicates the replacement $\bar u\to u^*$. The function $E_G^*\equiv E_G(u^*,u)$, as well as E_τ^*, E_c^*, and $E_{h_1}^*$, depends on the initial coupling u and are therefore *nonuniversal.* By contrast, the scaling function Ξ, which is given by

$$\Xi\equiv\hat G\,|_{u=u^*,\,\tau=1,\,\mu=1} ,$$

is independent of u and μ and therefore *universal.* Note that

$$\eta_G^*=\tfrac{1}{2}(N\eta+M\eta_\parallel^{\rm sp}) \qquad (2.17)$$

and

$$E_G^*=E_h^{*N}E_{h_1}^{*M} . \qquad (2.18)$$

Two important results can therefore be read off from (2.15): First, $\hat G_R$ asymptotically takes the scaling form expected from the phenomenological theory of scaling.[7] This means, in particular, that the critical exponents of the special transition can be expressed in terms of two bulk exponents (ν,Δ) and two surface exponents ($\Delta_1^{\rm sp},\Phi$). Second, we see that apart from the four nonuniversal scales E_τ^*, E_h^*, E_c^*, and $E_{h_1}^*$ (and the trivial μ dependence), the right-hand side of (2.15) is universal. This *four-scale-factor universality* is the obvious analog of the familiar two-scale-factor universality[2] of bulk correlation functions.

To proceed, we need some information about the scaling function Ξ in various limits. If τ, $c=\tilde c\tilde\tau^{-\Phi}$, $\mathscr{h}=\tilde h\tilde\tau^{-\Delta}$, and $\mathscr{h}_1=\tilde h_1\tilde\tau^{-\Delta_1^{\rm sp}}$ are small, one observes a behavior characteristic of the special transition. Thus the limit $c\to 0$ of Ξ should exist:

$$\lim_{c\to 0}\Xi(\mathscr{p},\mathscr{z};c,\mathscr{h},\mathscr{h}_1)=\Xi_0(\mathscr{p},\mathscr{z};\mathscr{h},\mathscr{h}_1) , \qquad (2.19)$$

as do the limits $h\to 0, h_1\to 0$ at fixed $c\neq 0$ or $c=0$. These statements can be, and in some cases have been, checked by perturbation theory. However, as τ decreases at fixed small $c>0$, $c\to\infty$ and one expects a crossover to a behavior characteristic of the ordinary transition when $c\approx 1$. The form of Ξ for $c\to\infty$ follows from the requirement that (2.15) must match with the asymptotic behavior at the ordinary transition (which was analyzed in detail in Ref. 10). Reasoning as in Ref. 21, one finds that

$$\Xi(\mathscr{p},\mathscr{z};c,\mathscr{h},\mathscr{h}_1) \underset{c\to\infty}{\sim} c^{-My}\Xi_\infty(\mathscr{p},\mathscr{z};\mathscr{h},\mathscr{h}_1c^{-y}) +\delta_{M,2}\times{\rm const}\times c^{-\gamma_{11}^{\rm sp}/\Phi} , \qquad (2.20)$$

with[22]

$$y=(\gamma_{11}^{\rm sp}-\gamma_{11}^{\rm ord})/2\Phi=1+\frac{n+2}{n+8}\epsilon+O(\epsilon^2)\ , \tag{2.21}$$

where $\gamma_{11}^{\rm sp}$ and $\gamma_{11}^{\rm ord}$ denote the familiar susceptibility exponent $\gamma_{11}=\nu(1-\eta_{\parallel})$ of the special or ordinary transition, and it should be recalled that M specifies the number of surface points. [The additional term for $M=2$ follows from the fact that $\lim_{\tau\to 0+}\hat{G}_R^{(0,2)}(p=0)$ exists for $c>0$ and $h=h_1=0$; see, e.g., Ref. 21.] An easy way of seeing that $\not{h}_1$ appears in Ξ_∞ in the combination $\not{h}_1 c^{-y}$ is to note that, upon taking a derivative $\partial/\partial\not{h}_1$ of (2.20), M should be replaced by $M+1$ because $\partial\Xi/\partial\not{h}_1$ is the scaling function associated with $\hat{G}^{(N,M+1)}$.

Using well-known scaling laws,[7] we can rewrite $\not{h}_1 c^{-y}$ as

$$\not{h}_1 c^{-y}=E_{h_1}^{\rm ord}h_1\tau^{-\Delta_1^{\rm ord}}\ , \tag{2.22}$$

where

$$E_{h_1}^{\rm ord}\equiv E_{h_1}^{\rm ord}(u,c)=c^{-y}E_{h_1}^{*} \tag{2.23}$$

is a scale factor analogous to $E_{h_1}^{*}$. When (2.20), (2.22), and (2.23) are inserted into (2.15), one sees that, for $c\to\infty$, $\hat{G}$ has a similar scaling form as for $c=0$. The only differences are (i) the scaling function $\Xi\,|_{c=0}\equiv\Xi_0$ in (2.15) is replaced by Ξ_∞, (ii) the surface exponents $\Delta_1^{\rm sp}$ in (2.15) and $\eta_{\parallel}^{\rm sp}$ in the definition (2.17) of η_G^{*} must be substituted by the corresponding exponents $\Delta_1^{\rm ord},\eta_{\parallel}^{\rm ord}$ of the ordinary transition, and (iii) in the definitions (2.16) of $\tilde{h}_1$ and (2.19) of $E_g^{*},E_{h_1}^{*}$ is to be replaced by $E_{h_1}^{\rm ord}$.

The result confirms what one would naively expect for the ordinary transition according to the phenomenological theory of scaling, namely that all critical exponents can be expressed in terms of three exponents (two bulk exponents, ν and Δ, and one surface exponent, $\Delta_1^{\rm ord}$) and that all nonuniversality is contained in three nonuniversal scales (E_h^{*}, E_τ^{*}, and $E_{h_1}^{\rm ord}$). Thus, in contrast to the special transition, the universality class of the ordinary transitions is, in fact, characterized by a *three-scale-factor universality.*

III. UNIVERSAL AMPLITUDE RATIOS

Using the results of the preceding section, it is straightforward to construct universal amplitude ratios. The only carriers of nonuniversality are the scale factors $E_\tau^{*},\ldots,E_{h_1}^{*}$ and μ. Consequently, a ratio is universal whenever these scale factors and the powers of μ cancel out. We shall mostly be concerned with susceptibility amplitudes and therefore begin by recalling the definition of local, layer, and excess susceptibilities.

Let $m(z)=\langle\phi(x_{\parallel},z)\rangle_{h,h_1}^{R}$ be the renormalized order-parameter profile and $\chi(z)$ be the layer susceptibility

$$\chi(z)=\left.\frac{\partial m(z)}{\partial h}\right|_{h=h_1=0}\ . \tag{3.1}$$

In the following we shall always assume that $h=h_1=0$, unless the contrary is said (or evident from the context). In terms of $m(z)$ and $\chi(z)$, the bulk, surface, and excess magnetizations m_b, m_1, and m_s, or susceptibilities χ_b, χ_1, and χ_s, are given by[23]

$$m_b=m(\infty)\ ,\quad \chi_b=\chi(\infty)\ ,$$
$$m_1=m(0)\ ,\quad \chi_1=\chi(0)\ , \tag{3.2}$$
$$m_s=\int_0^\infty dz[m(z)-m_b]\ ,\quad \chi_s=\int_0^\infty dz[\chi(z)-\chi_b]=\frac{\partial m_s}{\partial h}\ .$$

We also define the local susceptibility by

$$\chi_{11}=\frac{\partial m_1}{\partial h_1}\ . \tag{3.3}$$

Writing the singular part of any of these quantities in the form

$$\chi_{11}\sim\chi_{11,{\rm ord/sp}}^{(\pm)}|\tau|^{-\gamma_{11}^{\rm ord/sp}}\ , \tag{3.4}$$

we introduce critical amplitudes $\chi_{11,{\rm ord/sp}}^{(\pm)}$, $m_{s,{\rm ord/sp}}^{(-)}$, etc. Here the plus or minus sign refers to $\tau>0$ or $\tau<0$, and ord or sp to the ordinary or special transition. In the analogous definitions of the critical amplitudes of the quantities m_b, χ_b, m_1, χ_1, m_s, and χ_s, the appropriate bulk or surface exponents β, γ, β_1, γ_1, $\beta_s=\beta-\nu$, and $\gamma_s=\gamma+\nu$ must, of course, be substituted for γ_{11}.

As an example, let us demonstrate that the ratio $\chi_s^{(\pm)}\chi_{11}^{(\pm)}/(\chi_1^{(\pm)})^2$ is universal. The susceptibilities χ_s, χ_{11}, and χ_1 can be expressed in terms of $\hat{G}_R^{(2,0)}$, $\hat{G}_R^{(0,2)}$, and $\hat{G}_R^{(1,1)}$, respectively, and satisfy the same RG equations as these. Let $\Xi_s^{(\pm)}(c)$, $\Xi_{11}^{(\pm)}(c)$, and $\Xi_1^{(\pm)}(c)$ be the scaling functions of χ_s, χ_{11}, and χ_1, i.e., the analog of Ξ in (2.15) for $h=h_1\equiv 0$. Using the well-known scaling law $\gamma_s+\gamma_{11}=2\gamma_1$ and (2.15)–(2.18), one concludes that

$$[\chi_s^{(\pm)}\chi_{11}^{(\pm)}(\chi_1^{(\pm)})^{-2}]_{\rm sp}=\Xi_s^{(\pm)}(0+)\Xi_{11}^{(\pm)}(0+)\times[\Xi_1^{(\pm)}(0+)]^{-2}\ . \tag{3.5}$$

All nonuniversality has dropped out of $\lim_{\tau\to 0\pm}\lim_{c\to 0+}\chi_s\chi_{11}/\chi_1^2$, leaving a universal ratio. The universality of this ratio at the ordinary transition can be derived in an analogous fashion. According to (2.20), we expect, for $c\to\infty$, the asymptotic behavior

$$\Xi_s^{(\pm)}(c)=\Xi_{s,\infty}^{(\pm)}+o(c^0)\ ,$$
$$\Xi_1^{(\pm)}(c)=\Xi_{1,\infty}^{(\pm)}c^{-y}+o(c^{-y})\ , \tag{3.6}$$
$$\Xi_{11}^{(\pm)}(c)={\rm const}\times c^{-\gamma_{11}^{\rm sp}/\Phi}+\Xi_{11,\infty}^{(\pm)}c^{-2y}+o(c^{-2y})\ ,$$

where $\Xi_{s,\infty}^{(\pm)}$, $\Xi_{1,\infty}^{(\pm)}$, and $\Xi_{11,\infty}^{(\pm)}$ are (universal) constants and the symbol $o(\ )$—which should not be confused with $O(\ )$—has the usual meaning. [A function $f(c)$ is said to be $o(g(c))$ for $c\to\infty$ if $f(c)/g(c)\to 0$; it is said to be $O(g(c))$ if $f(c)/g(c)\to$const.] We must now take into account that because of $\gamma_{11}^{\rm ord}<0$, χ_{11} does not diverge at the ordinary transition. Its leading singular part (for $c\to\infty$), $\chi_{11}^{\rm sing}$, in terms of which the exponent $\gamma_{11}^{\rm ord}$ and the amplitude $\chi_{11,{\rm ord}}^{(\pm)}$ are defined, follows from the term $\propto c^{-2y}$ of $\Xi_{11}^{(\pm)}(c)$. Upon inserting (3.6) in $\lim_{\tau\to 0\pm}\lim_{c\to\infty}\chi_s\chi_{11}^{\rm sing}/\chi_1^2$, one sees that all nonuniversal factors (contained in c, for example) cancel again out, giving

$$[\chi_s^{(\pm)}\chi_{11}^{(\pm)}(\chi_1^{(\pm)})^{-2}]_{\rm ord}=\Xi_{s,\infty}^{(\pm)}\Xi_{11,\infty}^{(\pm)}(\Xi_{1,\infty}^{(\pm)})^{-2}\ . \tag{3.7}$$

The universality of other ratios—in particular, of those presented below—can be derived along the same lines.

We next present the ϵ expansion of a variety of universal ratios. The results are based on the one-loop calculations described in the next section. We find[24]

$$[\chi_s^{(+)}\chi_{11}^{(+)}(\chi_1^{(+)})^{-2}]_{\rm ord}=1+\frac{n+2}{n+8}\epsilon\frac{\pi}{2}+O(\epsilon^2), \quad (3.8a)$$

$$[\chi_s^{(-)}\chi_{11}^{(-)}(\chi_1^{(-)})^{-2}]_{\rm ord}=-0.09\epsilon+O(\epsilon^2)\ , \quad (3.8b)$$

$$[\chi_s^{(+)}\chi_{11}^{(+)}(\chi_1^{(+)})^{-2}]_{\rm sp}=\frac{n+2}{n+8}\epsilon\frac{\pi}{2}+O(\epsilon^2)\ , \quad (3.8c)$$

$$[\chi_s^{(-)}\chi_{11}^{(-)}(\chi_1^{(-)})^{-2}]_{\rm sp}=-0.25\epsilon+O(\epsilon^2)\ . \quad (3.8d)$$

Note that the ϵ^0 terms in (3.8b)—(3.8d) are identically zero because the Landau approximation[7] predicts that χ_{11} is analytic in τ for $\tau<0$ and $c>0$, and yields $\chi_s(\tau,c=0)\equiv 0$, both above and below T_c^b.

Other universal ratios we have calculated are

$$(\chi_s^{(+)}/\chi_s^{(-)})_{\rm ord}=-\frac{4\sqrt{2}}{3}(1-0.15\epsilon)+O(\epsilon^2)\ , \quad (3.9a)$$

$$(\chi_s^{(+)}/\chi_s^{(-)})_{\rm sp}=-4\sqrt{2}\epsilon^0+O(\epsilon)\ , \quad (3.9b)$$

$$(\chi_1^{(+)}/\chi_1^{(-)})_{\rm ord}=\frac{1}{\sqrt{2}}(1+0.11\epsilon)+O(\epsilon^2)\ , \quad (3.10a)$$

$$(\chi_1^{(+)}/\chi_1^{(-)})_{\rm sp}=2(1+0.92\epsilon)+O(\epsilon^2)\ , \quad (3.10b)$$

$$(\chi_{11}^{(+)}/\chi_{11}^{(-)})_{\rm ord}=3.1\epsilon^{-1}+O(\epsilon^0)\ , \quad (3.11a)$$

$$(\chi_{11}^{(+)}/\chi_{11}^{(-)})_{\rm sp}=\sqrt{2}(1+0.56\epsilon)+O(\epsilon^2)\ . \quad (3.11b)$$

In each case, a calculation of the next term in the ϵ expansion [for example, the $O(\epsilon)$ term in (3.9b)] would involve a two-loop calculation.

Since $\gamma_s=\gamma+\nu$, both at the ordinary and the special transition, the ratios $\chi_{s,\rm ord}^{(\pm)}/\chi_{s,\rm sp}^{(\pm)}$ are also universal. Their ϵ expansion reads

$$\chi_{s,\rm ord}^{(+)}/\chi_{s,\rm sp}^{(+)}=-\left[\frac{n+2}{n+8}\epsilon\frac{\pi}{2}\right]^{-1}+O(\epsilon^0)\ , \quad (3.12a)$$

$$\chi_{s,\rm ord}^{(-)}/\chi_{s,\rm sp}^{(-)}=-5.8\epsilon^{-1}+O(\epsilon^0)\ . \quad (3.12b)$$

We also give some examples of mixed universal ratios involving amplitudes of both bulk and excess surface quantities. For $c=\infty$ or $c=0$ the order-parameter profile $m(z)$ and the layer susceptibility $\chi(z)$ can be written as

$$m(z)=m_b\sigma_{\rm ord/sp}(z/2\xi)\ , \quad (3.13)$$

$$\chi(z)=\chi_b X_{\rm ord/sp}^{(\pm)}(z/2\xi)\ , \quad (3.14)$$

where $\xi=\xi^{(\pm)}|\tau|^{-\nu}$ is the bulk correlation length. Since aside from the scale $\xi^{(\pm)}$, the scaling functions $\sigma_{\rm sp/ord}$ and $X_{\rm sp/ord}^{(\pm)}$ are universal, the following ratios are also universal:

$$m_{s,\rm ord/sp}^{(-)}/(m_b^{(-)}\xi^{(-)})=2\int_0^\infty d\zeta[\sigma_{\rm ord/sp}(\zeta)-1]\ , \quad (3.15a)$$

$$\chi_{s,\rm ord/sp}^{(\pm)}/(\chi_b^{(\pm)}\xi^{(\pm)})=2\int_0^\infty d\zeta[X_{\rm ord/sp}^{(\pm)}(\zeta)-1]\ . \quad (3.15b)$$

Our results for these ratios read

$$m_{s,\rm ord}^{(-)}/m_b^{(-)}\xi^{(-)}=-2\ln 2(1-0.05\epsilon)+O(\epsilon^2)\ , \quad (3.16a)$$

$$m_{s,\rm sp}^{(-)}/(m_b^{(-)}\xi^{(-)})=\frac{\pi}{6}\epsilon+O(\epsilon^2)\ , \quad (3.16b)$$

$$\chi_{s,\rm ord}^{(+)}/(\chi_b^{(+)}\xi^{(+)})=-\left[1-\frac{n+2}{n+8}\epsilon\pi\left[\frac{1}{\sqrt{3}}-\frac{1}{2}\right]\right]+O(\epsilon^2)\ , \quad (3.17a)$$

$$\chi_{s,\rm ord}^{(-)}/(\chi_b^{(-)}\xi^{(-)})=\tfrac{3}{2}(1+0.94\epsilon)+O(\epsilon^2)\ , \quad (3.17b)$$

$$\chi_{s,\rm sp}^{(+)}/(\chi_b^{(+)}\xi^{(+)})=\frac{n+2}{n+8}\epsilon\frac{\pi}{2}+O(\epsilon^2)\ , \quad (3.17c)$$

$$\chi_{s,\rm sp}^{(-)}/(\chi_b^{(-)}\xi^{(-)})=-\frac{\pi}{12}\epsilon+O(\epsilon^2)\ . \quad (3.17d)$$

As already indicated in the Introduction, no previous estimates of the above universal amplitude ratios other than Landau's[15,16] Monte Carlo (MC) results $(\chi_s^{(+)}/\chi_s^{(-)})_{\rm ord}\approx 3.14$ ($d=2$) and ≈ 0.78 ($d=3$) of the two- and three-dimensional Ising model seem to exist in the literature. In Fig. 1(a) we compare these with our result (3.9a). The agreement is unfortunately extremely poor. Particularly puzzling is the fact that these MC estimates and the (exact) mean-field result for $d=4$ appear to fall on a straight line whose slope differs appreciably from the one predicted by (3.9a) at $d=4$. While we certainly cannot expect that a simple linear extrapolation of our first-order result, (3.9a), gives accurate results for $d=3$ or even $d=2$, the slope at $d=4$ should come out correctly. Landau also gives the estimates $4|m_{s,\rm ord}^{(-)}|\approx 0.60+0.05$ and $m_b^{(-)}\approx 1.20$, for $d=2$, and $6m_{s,\rm ord}^{(-)}|\approx 2.3\pm 0.2$ and $m_b^{(-)}\approx 1.57$,[25] for $d=3$. These can be combined with the

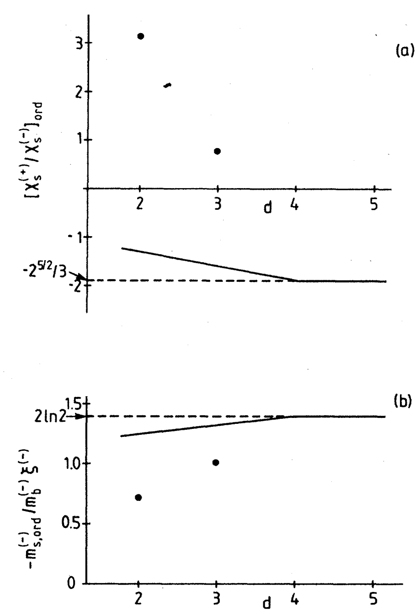

FIG. 1. Universal amplitude ratios (a) $(\chi_s^{(+)}/\chi_s^{(-)})_{\rm ord}$ and (b) $m_{s,\rm ord}^{(-)}/m_b^{(-)}\xi^{(-)}$ as a function of the space dimension d. The straight lines below $d=4$ are linear extrapolations of the ϵ expansions given in (3.9a) and (3.16a). The arrow and the dashed line indicate the respective mean-field results which are exact for $d\geq 4$. The dots represent values which were obtained from the MC results of Refs. 15 and 16 and the results of Ref. 26 for $\xi^{(-)}$.

results $\xi^{(-)}(d=2) = 0.176\pm0.005$ and $\xi^{(-)}(d=3) = 0.244\pm0.001$ of Tarko and Fisher[26] to obtain the estimates $m_{s,\mathrm{ord}}^{(-)}/m_b^{(-)}\xi^{(-)} \approx 0.71$ $(d=2)$ and ≈ 1.0 $(d=3)$. The same $d=3$ estimate is obtained from the more recent data of Binder and Landau[27] through numerical integration of their profile $\sigma_{\mathrm{ord}}(\xi)$, using (3.15a). In Fig. 1(b) these estimates are compared with the linear extrapolation of the $O(\epsilon)$ result in (3.16a). While the agreement is much better than in Fig. 1(a), it is again somewhat disturbing that the estimates based on the MC data seem to fall on a straight line through the exact $d=4$ result, with a slope different from the one predicted by the ϵ expansion. It would be interesting to see whether the $d=4$ results in Figs. 1(a) and 1(b) can be confirmed by MC calculations. For completeness we also note that the exact results of McCoy and Wu on the two-dimensional Ising model[28] imply that $(\chi_{11}^{(+)}/\chi_{11}^{(-)})_{\mathrm{ord}} \equiv 1$.

IV. OUTLINE OF THE CALCULATIONS

We next give a brief outline of our calculations, omitting uninteresting technical details. The interested reader may consult Refs. 10—12 and 29 for further information on technicalities.

Being specifically concerned with susceptibility amplitudes, we begin by recalling how the surface susceptibilities χ_{11}, χ_1, and χ_s read in terms of the correlation functions $\hat{G}^{(N,M)}$ introduced in Eqs. (2.1) and (2.2). We have

$$\chi_{11} = \hat{G}_R^{(0,2)}(p=0;0,0) \tag{4.1}$$

and

$$\chi_1 = \int_0^\infty dz\, \hat{G}_R^{(1,1)}(p=0;z,0)\ . \tag{4.2}$$

χ_s is given by the last line of Eq. (3.2), with

$$\chi(z) = \int_0^\infty dz'\, \hat{G}_R^{(2,0)}(p=0;z,z')\ . \tag{4.3}$$

These relations hold above and below T_c^b. We first describe the calculations for the disordered phase $T > T_c^b, c \geq 0$. These are technically easier because below T_c^b, as in any ordered phase (including the surface-ordered and bulk-disordered phase), the $\hat{G}^{(N,M)}$'s also depend (in a functional way) on the order-parameter profile $m(z)$.

A. The disordered phase ($T > T_c^b$, $c \geq 0$)

The strategy outlined in Sec. III requires the calculation of the scaling functions associated with χ_{11}, χ_1, etc. This can be done in a perturbative fashion by computing the latter quantities for $u=u^*$ and arbitrary $c\geq 0$, $\tau > 0$, using the free propagator

$$\hat{G}(p;z,z') = \frac{1}{2\kappa}\left[e^{-\kappa|z-z'|} + \frac{\kappa - c_0}{\kappa + c_0} e^{-\kappa(z+z')}\right]\ , \tag{4.4a}$$

with

$$\kappa = (p^2+\tau_0)^{1/2}\ . \tag{4.4b}$$

In fact, to one-loop order, with which we will be satisfied throughout, χ_{11}, χ_1, and χ_s can be worked out analytically; χ_{11} may be found in Ref. 39, χ_s in Ref. 29, and χ_1 can be calculated along similar lines.

However, for the evaluation of the amplitudes, detailed knowledge about the c dependence of these quantities is actually not needed. It is sufficient to know their asymptotic behavior for c equal or close to the respective fixed-point value $c=0$ or $c=\infty$ of the special or ordinary transition. In the case of the special transition, the amplitudes are, because of (2.19), entirely given by $c=0$ quantities. Since we use the dimensional regularization scheme, $c=0$ implies $c_0=0$. Hence, only Feynman graphs with the Neumann propagator $\hat{G}_N = \hat{G}\,|_{c_0=0}$ have to be evaluated. This procedure, in which one sets $c=0$ from the outset, gives the same results as the previous one of keeping the full c_0 dependence first, then renormalizing, and finally taking the limit $c\to 0$.

The case of the ordinary transition is more subtle. Here one would like to set $c_0=\infty$ from the outset, so that only Feynman graphs with the Dirichlet propagator[30] $G_D = G\,|_{c_0=\infty}$ must be computed. While this turns out to be possible, two interrelated difficulties are encountered. First, the amplitudes cannot entirely be expressed in terms of the functions $G_R^{(N,M)}|_{c=\infty}$ because these vanish identically whenever $M>0$. Nevertheless, the asymptotic behavior of $G_R^{(N,M)}$ can be related to $c_0=\infty$ quantities in the way described in Refs. 10, 21, and 31: One expands the bare $G^{(N,M)}$'s in powers of c_0^{-1}. The leading term in this expansion is $c_0^{-M} G_\infty^{(N,M)}$, where $G_\infty^{(N,M)}$ is the Fourier transform of the $c_0=\infty$ function

$$G_\infty^{(N,M)} = \left\langle \prod_{i=1}^{N} \phi(x_i) \prod_{j=1}^{M} \partial_n \phi(r_j,0) \right\rangle_{c_0=\infty}\ ,$$

and $\partial_n = \partial_z$ means a normal derivative. The desired information then follows upon renormalization of $G_\infty^{(N,M)}$. However, the two methods—first renormalizing, then taking the limit $c\to\infty$, or first expanding in powers of c_0^{-1}, then renormalizing the expansion coefficients $G_\infty^{(N,M)}$—do not, in general, give identical results. The reason, roughly speaking, is that the limits $\Lambda\to\infty$ and $c_0\to\infty$ do not commute. [The c_0^{-1} expansion fails to capture terms $\propto \ln(1+\Lambda/c_0)$ which become singular in the limit $c_0/\Lambda\to 0$. These are precisely singularities of the sort that are absorbed by Z_c.] Exceptions are quantities such as $G_R^{(N,0)}$, whose limit $c\to\infty$ exists and is nonvanishing. For those, both methods yield the same results because the contributions from the additional counterterms one has for $c<\infty$ vanish as $c\to\infty$. For other quantities (such as $G_R^{(N,M)}$, $M>0$, or χ_1) the two methods yield different nonuniversal amplitudes. The difference amounts to a different choice of the scale factor $E_{h_1}^{\mathrm{ord}}$ in (2.23): Aside from an overall proportionality factor (which depends on the choice of Z_c, Z_1, and the corresponding renormalization factor[10] needed to renormalize $\partial_n\phi$ for $c_0=\infty$), the two scale factors $E_{h_1}^{\mathrm{ord}}$ differ in that c^{-y} in (2.23) is replaced by $(c_0/\mu)^{-1}$ if one uses the method based on the c_0^{-1} expansion. Of course, we are free to use either one of these two methods for calculating the universal amplitude ratios at the ordinary transition *as long as we consistently use the same method for all nonuniversal amplitudes involved.* However, caution must be exercised in calculating universal ratios which involve amplitudes at both the special and ordinary transitions. Here, one must really insert the values which follow from the large-c behavior of the renormalized quantities for the amplitudes at the ordinary transition. If one nevertheless wishes to use the c_0^{-1} expansion, one must know the precise relation between the respective nonuniversal amplitudes. In the case of the amplitude ratios (3.12a) and (3.12b), no problem arises, since $\lim_{c\to\infty}\mathcal{X}_s$ exists and is nonvanishing, both methods yield the same $\mathcal{X}_{s,\mathrm{ord}}^{(\pm)}$.

Our results for the susceptibilities at $u=u^*$ and $c=0$ read

$$\mathcal{X}_{11}=\tau^{-\gamma_{11}^{\mathrm{sp}}}\left[1+\frac{n+2}{n+8}\epsilon\tfrac{1}{4}(5-3C_E)+O(\epsilon^2)\right], \tag{4.5a}$$

$$\mathcal{X}_{1}=\tau^{-\gamma_{1}^{\mathrm{sp}}}\left[1+\frac{n+2}{n+8}\epsilon\left[1-\tfrac{3}{4}C_E+\frac{\pi}{2}3^{-1/2}\right]+O(\epsilon^2)\right], \tag{4.5b}$$

$$\mathcal{X}_{s}=\tau^{-\gamma_{s}}\left[\frac{n+2}{n+8}\frac{\pi}{2}\epsilon+O(\epsilon^2)\right], \tag{4.5c}$$

where $C_E=0.577\,215\ldots$ is Euler's constant and we have set $\mu=1$. The corresponding results for the ordinary transition are

$$\mathcal{X}_{11}^{\mathrm{sing}}=-(E_{h_1}^{\mathrm{ord}*})^2\tau^{-\gamma_{11}^{\mathrm{ord}}}\times\left[1+\frac{n+2}{n+8}\epsilon\tfrac{1}{4}(3-C_E)+O(\epsilon^2)\right], \tag{4.6a}$$

$$\mathcal{X}_{1}=E_{h_1}^{\mathrm{ord}*}\tau^{-\gamma_{1}^{\mathrm{ord}}}\left[1-\frac{n+2}{n+8}\epsilon\tfrac{1}{2}(C_E+\pi 3^{-1/2}-\tfrac{3}{2})+O(\epsilon^2)\right], \tag{4.6b}$$

$$\mathcal{X}_{s}=-\tau^{-\gamma_{s}}\left[1+\frac{n+2}{n+8}\epsilon[\tfrac{3}{4}(1-C_E)+\pi(\tfrac{1}{2}-3^{-1/2})]+O(\epsilon^2)\right]. \tag{4.6c}$$

The results in (4.6a) and (4.6b) were obtained using the c_0^{-1} expansion. $E_{h_1}^{\mathrm{ord}*}$ should therefore be interpreted as c_0^{-1}.

B. The ordered phase ($T<T_c^b$, $c\geq 0$)

The computation of the amplitudes for the ordered phase requires as a first step the calculation of the order-parameter profile. Since one-loop calculations of the profiles at the ordinary and special transitions were already described in Refs. 10, 12, 20, 29, and 32, we only give a brief summary of the equations which must be solved. As stated, we will only consider the case $n=1$. (The profile for $n\geq 2$ may be found in Ref. 29 to one-loop order.)

In the absence of bulk and surface magnetic fields the (bare) profile $\langle\phi(x)\rangle=\langle\phi(0,z)\rangle$ satisfies the equation

$$\Gamma^{(1)}(x;\{\langle\phi\rangle\})=0, \tag{4.7}$$

with the boundary condition

$$\partial_n\langle\phi\rangle=c_0\langle\phi\,|_s\rangle, \tag{4.8}$$

where $\Gamma^{(1)}$ is the usual (bare) one-point vertex function. Writing $\Gamma^{(1)}=\Gamma_0^{(1)}+\Gamma_1^{(1)}+\cdots$, $\langle\phi\rangle=\langle\phi\rangle_0+\langle\phi\rangle_1+\cdots$, etc., we split all quantities into tree ($\equiv 0$ loop), one-loop, and higher contributions. We then expand Eq. (4.7) about $\langle\phi\rangle_0$. Since $\Gamma_0^{(1)}(x;\{\langle\phi\rangle_0\})=0$, we obtain, to one-loop order,

$$\left[-\partial_z^2+\tau+\frac{g}{2}\langle\phi\rangle_0^2\right]\langle\phi(x)\rangle_1=-\Gamma_1^{(1)}(x;\{\langle\phi\rangle_0\}). \tag{4.9}$$

On the left-hand side the mean-field expression for the ($p=0$) Fourier transform of the two-point vertex function is recognizable; its inverse is the free propagator $\widetilde{G}_0^{(2)}(p;z,z';\{\langle\phi\rangle_0\})$ defined by

$$\left[-\partial_z^2+p^2+\tau+\frac{g}{2}\langle\phi\rangle_0^2\right]\widehat{G}_0^{(2)}(p;z,z';\{\langle\phi\rangle_0\})=\delta(z-z'), \tag{4.10}$$

together with the boundary condition (4.8) for $z\to 0$, $z'>0$, or vice versa. The right-hand side can also be expressed in terms of $\widehat{G}_0^{(2)}$. With the notation

$$\int_p\equiv\int d^{d-1}p/(2\pi)^{d-1},$$

it reads

$$\Gamma_1^{(1)}(x;\{\langle\phi\rangle\}_0)=\frac{g}{2}\langle\phi(0,z)\rangle_0\int_p\widehat{G}_0^{(2)}(p;z,z;\{\langle\phi\rangle_0\}). \tag{4.11}$$

Using $G_0^{(2)}$, Eq. (4.9) can be solved for $\langle\phi\rangle_1$. Upon substitution of Eq. (4.11), the profile becomes

$$\langle\phi(x)\rangle=\langle\phi(0,z)\rangle_0-\frac{g}{2}\int_0^\infty dz'\,\widehat{G}_0^{(2)}(0;z,z';\{\langle\phi\rangle_0\})\langle\phi(0,z')\rangle_0\times\int_p\widehat{G}_0^{(2)}(p;z',z';\{\langle\phi_0\rangle\})+O(\text{2-loop}). \tag{4.12}$$

The mean-field quantities $\langle\phi\rangle_0$ and $\widehat{G}_0^{(2)}$ are known for all values of $c_0\geq 0$.[33] Specifically for $c_0=\infty$, they may be found, for instance, in Refs. 10 and 20, and for $c_0=c_{\mathrm{sp}}$, they are given in Ref. 12. In a similar fashion the two-point correlation function $\widehat{G}^{(2)}(p;z,z';\{\langle\phi\rangle\})$, which, for $z>0$ and $z'>0$, is precisely the function $\widehat{G}^{(2,0)}$ defined by Eqs. (2.1) and (2.2), can be expressed in terms of $\langle\phi\rangle_0$ and $\widehat{G}_0^{(2)}$. The result is represented graphically in Fig. 2.

To obtain the renormalized profiles for $c=\infty$ and $c=0$ from (4.12), we isolated the poles in ϵ which occur for $c_0=\infty$ or $c_0=0$ in the dimensionally regularized theory and verified that these poles vanish when the bare order parameter, temperature, and coupling constant are, according to Eq. (2.3), expressed in terms of their renormalized counterparts. We then set $u=u^*$ and exponentiated the logarithms in τ to arrive at (3.13) with

$$m_b = m_b^{(-)} |\tau|^{\beta} , \tag{4.13a}$$

where

$$m_b^{(-)} = (6/2^d \pi^{d/2} u^*)^{1/2} \left[1 - \frac{\epsilon}{6}(\ln 2 + C_E - 1) + O(\epsilon^2) \right] , \tag{4.13b}$$

and

$$\xi = \xi^{(-)} |\tau|^{-\nu} , \tag{4.14a}$$

with

$$\xi^{(-)} = 2^{-\nu}[1 - (\tfrac{1}{12}C_E + \tfrac{1}{8})\epsilon + O(\epsilon^2)] . \tag{4.14b}$$

(The bulk correlation length is normalized such that

$$\xi^{-2} = \left. \frac{\partial \ln \Gamma_{\text{bulk}}^{(2)}(q^2,\tau)}{\partial q^2} \right|_{q^2=0} ,$$

where $\Gamma_{\text{bulk}}^{(2)}$ is the renormalized two-point vertex function of the translationally invariant ϕ^4 theory in momentum space.) Our result for $\sigma_{\text{ord}}(\zeta)$ can be written as

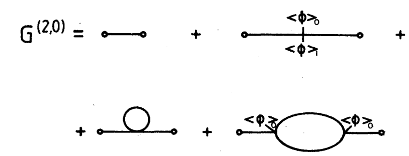

FIG. 2. Expansion of $G^{(2,0)}$, for $T < T_c^b$, to one-loop order. The lines represent the free propagator $G_0^{(2,0)}$. The weight of the two-point vertex in the second graph is $g\langle\phi\rangle_0\langle\phi\rangle_1$, and that of the three-point vertex in the last graph is $g\langle\phi\rangle_0$.

$$\sigma_{\text{ord}}(\zeta) = \sigma_{\text{ord}}^{(0)}(\zeta) + \epsilon\sigma_{\text{ord}}^{(1)}(\zeta) + O(\epsilon^2) , \tag{4.15a}$$

$$\sigma_{\text{ord}}^{(0)}(\zeta) = \tanh\zeta , \tag{4.15b}$$

$$\sigma_{\text{ord}}^{(1)}(\zeta) = \frac{1}{3}\left[\frac{1}{4}(\pi\sqrt{3} - \tfrac{11}{2})\zeta\,\text{sech}^2\zeta - \frac{\pi}{2\sqrt{3}}\tanh\zeta\,\text{sech}^2\zeta + \frac{1}{2}\int_0^\infty dz'\, R(\zeta')\tanh(\zeta')2|\tau|\hat{G}_0^{(2)}(0,z,z',\{\langle\phi\rangle_0\}) \right] , \tag{4.15c}$$

with

$$R(\zeta) = \left[9\tanh^2\zeta[I(\zeta)(1+\tanh^2\zeta) - I'(\zeta)\tanh\zeta] + 3K_0(4\zeta)(1+5\tanh^2\zeta) + 12K_1(4\zeta)\tanh\zeta + \frac{1}{\zeta}K_1(4\zeta) \right] , \tag{4.16}$$

where K_0 and K_1 are modified Bessel functions and $I(\zeta)$ is defined by

$$I(\zeta) = \int_0^\infty dp \frac{\exp[-2\zeta(p^2+4)^{1/2}]}{(p^2+4)^{1/2}(p^2+3)} . \tag{4.17}$$

$\sigma_{\text{sp}}(\xi)$ was already given in Ref. 12; it reads

$$\sigma_{\text{sp}}(\xi) = 1 + \frac{\epsilon}{6}\left[K_0(4\zeta) - 3I(\zeta) + \frac{\sqrt{3}\pi}{2}e^{-2\zeta} \right] + O(\epsilon^2) . \tag{4.18}$$

[Note that the variable ζ of Ref. 12 differs from the one employed here by a factor $1+O(\epsilon)$. Nevertheless, the two functions $\sigma_{\text{sp}}(\zeta)$ are the same to first order in ϵ, the implied difference being of order ϵ^2.]

The shape function $\sigma_{\text{ord}}(\zeta)$ was previously calculated by Wilson,[20] who used a different method and obtained a slightly different result. Instead of solving Eq. (4.9) by means of the Green's function $\hat{G}_0^{(2)}$, Wilson made an ansatz for $\langle\phi\rangle_1$ in the form of a linear combination of hyperbolic functions and then tried to solve for the coefficients. In Appendix A we repeat the calculation of $\sigma_{\text{ord}}(\zeta)$ along these lines and correct Wilson's result. The corrected result is given in Eq. (A11). We checked by numerical evaluation that the latter is equivalent to Eq. (4.15). In Figs. 3 and 4 extrapolations of $\sigma_{\text{ord}}(\zeta)$ and $\sigma_{\text{sp}}(\zeta)$ to $d=3$ are depicted and compared with the recent Monte Carlo results of Binder and Landau.[27] To ensure that the extrapolation complies with the exponentiated short-distance form[10,12,29] $\sigma(\zeta) \sim \zeta^{(\beta_1-\beta)/\nu}$ of $\sigma_{\text{ord/sp}}(\zeta)$ we expanded the logarithm of $\sigma(\zeta)$, reexponentiated to obtain $\sigma(\zeta) = \sigma^{(0)}\exp(\epsilon\sigma^{(1)}/\sigma^{(0)})$, and then set $\epsilon=1$. In both cases the one-loop result compares better with the Monte Carlo data than the mean-field result. Perfect agreement between our one-loop $\sigma_{\text{ord}}(\zeta)$ and the Monte Carlo data cannot be expected, because the one-loop approximation to[10]

$$(\beta_1^{\text{ord}} - \beta)/\nu = 1 - \tfrac{1}{6}\epsilon - \tfrac{17}{162}\epsilon^2 + O(\epsilon^3) \tag{4.19}$$

is not very accurate. If we neglect the $O(\epsilon^2)$ terms in

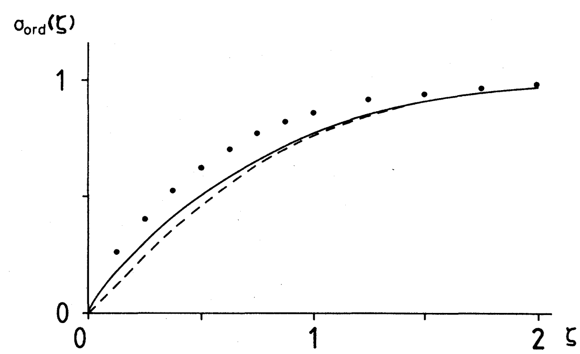

FIG. 3. Order-parameter profile at the ordinary transition, $\sigma_{\text{ord}}(\zeta)$, in tree (dashed curve) and one-loop approximations (solid curve). The dots are Monte Carlo results taken from Ref. 27.

(4.19) and then set $\epsilon=1$, we obtain $(\beta_1^{\rm ord}-\beta)/\nu\approx 0.83$; if we include them, we obtain instead ≈ 0.73. Since this latter value is much closer to the Monte Carlo estimate[27] 0.67, a two-loop approximation should give much better agreement. In the case of $\sigma_{\rm sp}(\zeta)$ the corresponding $O(\epsilon)$ and $O(\epsilon^2)$ estimates for

$$(\beta_1^{\rm sp}-\beta)/\nu=-\tfrac{1}{6}\epsilon+\tfrac{1}{162}\epsilon^2+O(\epsilon^3) \tag{4.20}$$

are ≈ -0.17 and ≈ -0.16, and are virtually indistinguishable from the slope ≈ -0.17 of the Monte Carlo data [cf. Fig. 5(b) of Ref. 27].

Substitution of Eqs. (4.15) and (4.18) into Eq. (3.15a) yields the amplitudes

$$m_{s,\rm ord}^{(-)}=-(3/2^d\pi^{d/2}u^*)^{1/2}2\ln 2[1-0.32\epsilon+O(\epsilon^2)] \tag{4.21a}$$

and

$$m_{s,\rm sp}^{(-)}=(3/2^d\pi^{d/2}u^*)^{1/2}\left[\epsilon\frac{\pi}{6}+O(\epsilon^2)\right]. \tag{4.21b}$$

The susceptibility amplitudes can be calculated along similar lines. One starts with the expression for the bare two-point function given in Fig. 2. The computation of χ_s and χ_1 involves z integrals over external points. It is advantageous to do these integrals first because the corresponding external lines of the one-loop graphs in Fig. 2 are then simply replaced by the mean-field susceptibility

$$\chi_0(z)=(2\,|\,\tau_0\,|\,)^{-1}{\rm sech}^2y[\sinh y\cosh^3 y+\tfrac{3}{2}(y+\sinh y\cosh y)-\cosh^4 y+1] \tag{4.22}$$

for $c_0=\infty$, or

$$\chi_0(z)=(2\,|\,\tau_0\,|\,)^{-1} \tag{4.23}$$

for $c_0=0$, where $y=|\,\tau_0/2\,|^{1/2}z$. External legs that connect a surface point with an internal point $z>0$ correspond to

$$c_0^{-1}\partial_{z'}\hat G_0^{(2)}(p=0;z',z;\{\langle\phi\rangle_0\})\,|_{z'=0,c_0=\infty}=c_0^{-1}{\rm sech}^2y \tag{4.24}$$

in the case of the ordinary transition and to $\chi_0(z=0)$ in the case of the special transition. Care must be exercised in the calculation of χ_s to properly extract the divergent bulk piece $\int_0^\infty dz\,\chi_0$. By isolating the poles in ϵ and removing these via the reparametrizations (2.3), one can bring the renormalized susceptibilities χ_s, χ_1, and χ_{11} into a form which contains only convergent integrals. These can then be evaluated by numerical integration. Since the calculations are fairly lengthy, we refrain from presenting them in detail. As an example, we only describe the calculation of χ_1 in Appendix B. [To make Appendix B self-contained, there we use $\sigma_{\rm ord}(\zeta)$ in the corrected Wilson form (A11) as input. However, we checked again that the alternative computational method outlined above and based on Eq. (4.15) gives the same results.]

Our susceptibility results for $u=u^*$ and $c=0$ are

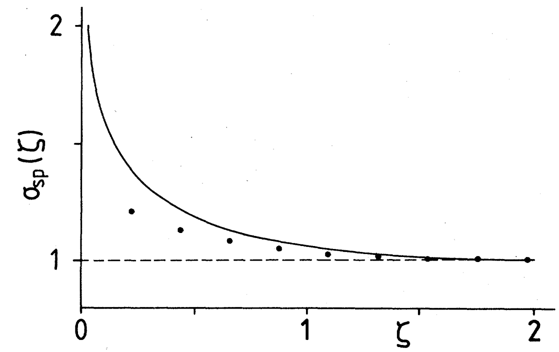

FIG. 4. Order-parameter profile at the special transition, $\sigma_{\rm sp}(\zeta)$, in tree (dashed curve) and one-loop approximations (solid curve). The dots are Monte Carlo results taken from Ref. 27.

$$\chi_{11}=|\,\tau\,|^{-\gamma_{11}^{\rm sp}}(1/\sqrt{2})[1-0.294\epsilon+O(\epsilon^2)]\,, \tag{4.25a}$$

$$\chi_1=|\,\tau\,|^{-\gamma_1^{\rm sp}}\tfrac{1}{2}[1-0.4319\epsilon+O(\epsilon^2)]\,, \tag{4.25b}$$

$$\chi_s=-|\,\tau\,|^{-\gamma_s}\left[\frac{\pi}{24\sqrt{2}}\epsilon+O(\epsilon^2)\right]. \tag{4.25c}$$

At the ordinary transition we find

$$\chi_{11}^{\rm sing}=-(E_{h_1}^{\rm ord*})^2\,|\,\tau\,|^{-\gamma_{11}^{\rm ord}}[0.321\epsilon+O(\epsilon^2)]\,, \tag{4.26a}$$

$$\chi_1=E_{h_1}^{\rm ord*}\,|\,\tau\,|^{-\gamma_1^{\rm ord}}2^{1/2}[1-0.259\epsilon+O(\epsilon^2)]\,, \tag{4.26b}$$

$$\chi_s=3\times 2^{-5/2}\,|\,\tau\,|^{-\gamma_s}[1+0.177\epsilon+O(\epsilon^2)]\,. \tag{4.26c}$$

From Eqs. (4.13b), (4.14b), (4.21a), (4.21b), (4.25a)–(4.25c), and (4.26a)–(4.26c) the ϵ expansions of the universal amplitudes given in Sec. III follow in a straightforward fashion.

V. SUMMARY AND CONCLUDING REMARKS

In this work we have shown that universal relations exist among critical amplitudes of surface quantities. By applying field-theoretic RG methods to semi-infinite model systems we were able to elucidate the general origin of these relations and to give a systematic derivation of the expected multi-scale-factor universality. Within our field-theoretic approach this multi-scale-factor universality arises as a natural consequence in much the same way as the familiar two-scale-factor universality at bulk critical points. With each relevant field (h,τ,h_1,c at the special transition or h,τ,h_1 at the ordinary transition) is associated one independent critical exponent (which follows from the anomalous dimension of the bulk or surface operator to which it couples) and one independent nonuniversal scale factor. Similarly, as all critical exponents can be expressed in terms of the four (special transition) or three (ordinary transition) "basic" exponents $\eta,\nu,\eta_\parallel^{\rm sp},\Phi$ or $\eta,\nu,\eta_\parallel^{\rm ord}$, say, all nonuniversal amplitudes are expressible in terms of these four or three scale factors. Ratios from which these scale factors drop out are universal.

We also worked out the ϵ expansion to one-loop order of a number of universal ratios. Owing to the shortness of the series, extrapolations to three dimensions are very uncertain. This can, in principle, be improved by extending the ϵ expansion to the next order, a task which appears feasible but extremely laborious. To obtain more accurate estimates of the universal ratios that we calculated. Monte Carlo calculations along the lines of Binder and Landau[27] might be very useful. An experimental determination of susceptibility amplitudes is clearly difficult but seems absolutely within reach of present experimental techniques. In particular, the proposed x-ray scattering at grazing angles[34] should have some potential usefulness in this respect. Another type of experimentally accessible universal amplitude ratios are those for the surface tension of polymer solutions discussed recently by Eisenriegler.[18] [The statistics of such polymer solutions is described by the $n \to 0$ limit of the semi-infinite n-vector model (1.1);[7,18,35] their nice feature is that the analog of the surface enhancement c may be experimentally varied.]

Finally, we have presented, within the one-loop approximation, the universal order-parameter profiles at the ordinary and special transitions. These compare reasonably well with the Monte Carlo results of Binder and Landau.[27]

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APPENDIX A: ORDER-PARAMETER PROFILE AT THE ORDINARY TRANSITION

In this appendix the order-parameter profile $\sigma_{\rm ord}(\zeta)$ is calculated along the lines taken by Wilson.[20] The main difference between his and our approach is that we again use dimensional regularization, whereas he cuts off the parallel momentum integrations at $|p|=\Lambda$.

To calculate the bare profile we set $c_0=\infty$. At zero-loop order we then have

$$\langle\phi(x)\rangle_0=(6\,|\tau_0|\,/g)^{1/2}\tanh y_0\ , \tag{A1}$$

where here and below y_0 means

$$y_0=Bz\ ,\quad B=(\,|\tau_0|\,/2)^{1/2}\ . \tag{A2}$$

The free propagator reads

$$\hat G_0^{(2)}(p;z,z';\{\langle\phi\rangle_0\})=f(p;z,z')-f(p;z,-z')\ , \tag{A3}$$

with

$$f(p;z,z')=[\exp(-w_p\,|z-z'|\,)/2w_p(w_p^2-B^2)(w_p^2-4B^2)]\{[3B^2\tanh^2Bz-B^2+w_p^2+{\rm sgn}(z-z')3w_pB\tanh Bz](z\rightleftarrows z')\}\ , \tag{A4}$$

where $w_p^2=p^2+4B^2$. This agrees with Eqs. (12) and (17) of Ref. 20 up to an obvious misprint in the last line of Eq. (17) $[-3\,{\rm sgn}(z'-z)$ should have a plus sign].

We now wish to solve Eq. (4.9). Inserting Eqs. (A1) and (A3) into Eq. (4.11), we obtain, for the right-hand side of Eq. (4.9),

$$\begin{aligned}-\Gamma_1^{(1)}(x;\{\langle\phi\rangle_0\})&=-\frac{g}{2}\left[\frac{6\,|\tau_0|}{g}\right]^{1/2}\tanh y_0 Q(y_0)\ ,\\ Q(y_0)/\,|\tau_0|\,2^{-d}\pi^{-d/2}&=\epsilon^{-1}(-4+6\,{\rm sech}^2y_0)+2C_E-2+2\ln|2\tau_0|+(6-\pi 3^{1/2}-3C_E-3\ln|2\tau_0|\,){\rm sech}^2y_0\\ &\quad+\pi 3^{1/2}{\rm sech}^4y_0-\tfrac{1}{2}J''(y_0)+2J(y_0)+6J'(y_0)\tanh y_0-[\tfrac{9}{2}I''(y_0)+12J(y_0)]\tanh^2y_0\\ &\quad+18I'(y_0)\tanh^3y_0-18I(y_0)\tanh^4y_0\ .\end{aligned} \tag{A5}$$

The functions I and J are the same as in Ref. 20; I was already introduced in Eq. (4.17), and J is defined by

$$J(y_0)=\int_0^\infty dp(p^2+4)^{-1/2}\exp[-2y_0(p^2+4)^{1/2}]\ . \tag{A6}$$

Equation (A5) may be compared with Eq. (A2) of Ref. 20. In the latter the first term inside the curly brackets should be increased by 1, so that it becomes $1-2\ln(\Lambda/B)$. Aside from some additional terms in our Eq. (A5) resulting from products of the form $O(\epsilon^{-1})\times O(\epsilon)$, the $O(\epsilon^0)$ terms then agree in both equations, as they should.

Following Wilson, let us take

$$\begin{aligned}\langle\phi(x)\rangle_1=&\,g2^{-d}\pi^{-d/2}(6\,|\tau_0|\,/g)^{1/2}\\ &\times 2[a_1(y_0)+b(y_0)\tanh y_0+c(y_0){\rm sech}^2y_0\\ &+d_1(y_0){\rm sech}^2y_0\tanh y_0]\end{aligned} \tag{A7}$$

as a trial solution to Eq. (4.9). Inserting an ansatz of this form in his Eq. (A2), the analog of our Eq. (4.9), and comparing the coefficients of $\tanh^r y_0$, $r=0,1,\ldots,5$, on both sides, Wilson derived his set of equations, (A9). If a solution to these latter equations exists, then the ansatz clearly solves his Eq. (A2). However, since (A9) constitutes six conditions for the four unknowns $a_1(y_0)$, $b(y_0)$, $c(y_0)$, and $d_1(y_0)$, a solution to (A9) need not exist. Conversely, if $\langle\phi\rangle_1$ in Eq. (A7) is a solution to Eq. (4.9) [or Wilson's Eq. (A2)], the coefficients $a_1(y_0),\ldots,d_1(y_0)$ do not necessarily have to satisfy his six conditions (A9). In fact, this is precisely what happens. We find that the solution to Eq. (4.9) takes the form (A7), with

$$a_1(y_0)=\tilde{a}_1(y_0)-\tilde{a}_1(\infty)\tanh^2 y_0 \ , \tag{A8a}$$

in which

$$\tilde{a}_1(y_0)=3\int_0^{y_0}dy'[4I(y')+J(y')+3H(y')] \ , \tag{A9}$$

with

$$H(y)=\int_0^\infty dp(p^2+3)^{-2}(p^2+4)^{-1/2}\exp[-2y(p^2+4)^{1/2}] \ . \tag{A10}$$

The other coefficients are

$$b(y_0)=(2\epsilon)^{-1}-\tfrac{1}{4}(C_E-1+\ln|2\tau_0|)+b_1(y_0) \ , \tag{A8b}$$

$$b_1(y_0)=-\tfrac{1}{4}[15I(y_0)+J(y_0)+18H(y_0)] \ ,$$

$$c(y_0)=\tfrac{1}{8}y_0(C_E+\tfrac{3}{2}+\ln|2\tau_0|-2/\epsilon)+c_1(y_0) \ , \tag{A8c}$$

$$c_1(y_0)=-\tfrac{1}{2}\int_0^{y_0}dy'[18I(y')+5J(y')+9H(y')] + \tfrac{1}{8}y_0(\pi\sqrt{3}-\tfrac{11}{2}) \ ,$$

$$d_1(y_0)=\tfrac{3}{2}I(y_0)-(\pi/12)\sqrt{3} \ , \tag{A8d}$$

where we have defined c_1 in such a way that $\sigma_{\rm ord}^{(1)}(\zeta)$ takes the concise form given below.

The main difference between Wilson's and our result for $\langle\phi\rangle_1$ shows up in $a_1(y_0)$.[36] His $a_1(y_0)$ differs from ours in Eq. (A8a) in that $\tanh^2 y_0$ is replaced by $\exp(-2y_0)-1$. To see that Wilson's $a_1(y_0)$ is incorrect, note simply that the terms $\propto\exp(-2y_0)$ to which it gives rise cancel neither in his Eq. (A9a) nor in (A9c); they only vanish in the difference (A9a)—(A9c), as a solution to which his $a_1(y_0)$ was constructed. On the other hand, replacement of his $a_1(y_0)$ by ours does not lead to a solution of his set of equations (A9); otherwise the terms that result from the $\tanh^2 y_0$ piece of $a_1(y_0)$ would have to vanish identically. While, therefore, our coefficients $a_1(y_0),\ldots,d_1(y_0)$ likewise do not satisfy the analogs of Wilson's conditions(A9), it is a matter of straightforward algebra to verify that our result in Eq. (A7), with the coefficients (A8a)—(A8d), is a solution to Eq. (4.9).

When Eq. (A5) is combined with Eqs. (A7) and (A8a)—(A8d), and the expressions from Eq. (2.2) are substituted for τ_0 and g ($Z_\phi\equiv 1$) at this order), the poles in ϵ are found to cancel. After setting $u=u^*$, Eqs. (3.13), (4.13a), (4.13b), (4.15a), and (4.15b) are recovered, with

$$\sigma_{\rm ord}^{(1)}(\zeta)=\tfrac{2}{3}[a_1(\zeta)+b_1(\zeta)\tanh\zeta+c_1(\zeta)\mathrm{sech}^2\zeta + d_1(\zeta)\tanh\zeta\,\mathrm{sech}^2\zeta] \ . \tag{A11}$$

APPENDIX B: CALCULATION OF $\chi_1(T<T_c^b)$ AT THE ORDINARY TRANSITION

Following the strategy explained in Sec. IV, we expand the bare susceptibility $\chi_{1,\rm bare}$ in powers of c_0^{-1}. This gives

$$\chi_{1,\rm bare}=c_0^{-1}\chi_{1,\infty}+O(c_0^2) \ , \tag{B1}$$

with

$$\chi_{1,\infty}=\int_0^\infty dz\,\hat{G}_\infty^{(1,1)}(p=0;z) \ , \tag{B2}$$

where $\hat{G}_\infty^{(1,1)}$ is the Fourier transform of

$$\langle\partial_n\phi(x'_{\parallel},0)\phi(x_{\parallel},z)\rangle_{c_0=\infty} \ .$$

The graphs of $\chi_{1,\infty}$ follow from those given in Fig. 2 by taking a normal derivative at one external point and integrating the other external point over z. One thus finds

$$\chi_{1,\infty}=B^{-1}-(g/B)\int_0^\infty dy[\langle\phi(0,y)\rangle_0\langle\phi(0,y)\rangle_1+\tfrac{1}{2}Q(y)]\mathrm{sech}^2 y\chi_0(y) + 6g\int_0^\infty dy_1\int_0^\infty dy_2\tanh y_1\tanh y_2\,\mathrm{sech}^2 y_1\chi_0(y_2)R(y_1,y_2) \ , \tag{B3}$$

where $\chi_0(y)$ was defined in (4.23a), and

$$R(y_1,y_2)=\int_p[\hat{G}_0^{(2)}(p=0;z_1,z_2;\{\langle\phi\rangle_0\})|_{c_0=\infty}]^2=2^{-d}\pi^{-d/2}\left[4\pi^{1/2}\Big/\Gamma\left[\frac{d-1}{2}\right]\right]B^{1-\epsilon}\int_2^\infty r(x,y_1,y_2)dx \ . \tag{B4}$$

The function r is symmetric with respect to interchange of y_1 and y_2, and for $y_1\ge y_2$ is given by

$$r(x,y_1,y_2)=[(x^2-4)^{-(3+\epsilon)/2}/x(x^2-1)^2]e^{-2xy_1}(3\tanh^2 y_1+x^2-1+3x\tanh y_1)^2 \times[(3\tanh^2 y_2+x^2-1)\sinh(xy_2)-3x\tanh y_2\cosh(xy_2)]^2 \ . \tag{B5}$$

$R(y_1,y_2)$ contains a bulk singularity, as may be seen from the fact that the x integral in (B4) diverges for $\epsilon=0$ when $y_1=y_2$. We extract this singularity by rewriting the x integral as follows:

$$\int_2^\infty dx\,r(x,y_1,y_2)=\tfrac{1}{4}\int_2^\infty x^{-\epsilon}\exp(-2x|y_1-y_2|)dx+\int_2^\infty[r(x,y_1,y_2)-\tfrac{1}{4}\exp(-2x|y_1-y_2|)]dx+O(\epsilon) \ . \tag{B6}$$

The second integral is convergent, so we set $\epsilon=0$ there. The first integral, considered as a distribution in y_1-y_2, has the expansion

$$\tfrac{1}{4}\int_2^\infty x^{-\epsilon}\exp(-2x|y_1-y_2|)dx=2^{\epsilon-3}[2(\epsilon^{-1}+C_E)\delta(y_1-y_2)+|y_1-y_2|_\pm^{-1}\exp(-4|y_1-y_2|)+O(\epsilon)] \ , \tag{B7}$$

in which $|y_1-y_2|_{\pm}^{-1}$ is the generalized function denoted by $|y_1-y_2|^{-1}$ in Ref. 37.

Another problem arises in the y integral in (B3). Aside from the explicit pole terms in $\langle\phi\rangle_1$ and $Q(y)$, there is a singularity coming from the term $\propto J''(y)$ in Q. To see this, note that since $J''(y)\sim y^{-2}$ and $\mathrm{sech}^2 y\chi_0(y)\sim y$ as $y\to 0$, the integral diverges at the lower bound. In Eq. (A5) we gave the ϵ expansion that results when $Q(y)$ is considered as a *function.* The appearance of the above singularity—a typical surface singularity—tells us that $Q(y)$, considered as a *distribution,* has an additional singularity $\propto\epsilon^{-1}\delta'(y)$. To evaluate the latter pole term, we must go one step back and replace $|\tau|_0 J''(y)$ by the corresponding d-dimensional term from which it originated, namely by

$$|\tau_0|^{1-\epsilon/2}J_d''(y)=2^d\pi^{d/2}\frac{1}{2}\frac{\partial^2}{\partial z^2}\int_p\frac{\exp[-2z(p^2+2|\tau_0|)^{1/2}]}{2p^2(p^2+2|\tau_0|)^{1/2}}\ . \tag{B8}$$

The y integration can now be done before the p integration. One thus finds

$$|\tau_0|^{1-\epsilon/2}\int_0^\infty dy\,J_2''(y)\mathrm{sech}^2 y\chi_0(y)=\frac{2}{\epsilon}-C_E+2-\ln|2\tau_0|-8\int_0^\infty dy\,K_1'(4y)[2|\tau_0|\chi_0(y)\mathrm{sech}^2 y-4y]\ . \tag{B9}$$

Using this in conjunction with Eqs. (B2)—(B8) and Eqs. (A7)—(A9), one is led to

$$\chi_{1,\infty}=(|\tau_0|/2)^{-1/2}[1+u(\epsilon^{-1}-\tfrac{1}{2}\ln|\tau_0|+A)]\ , \tag{B10}$$

with

$$\begin{aligned}A=&-\tfrac{1}{2}\int_0^\infty dy\,\mathrm{sech}^2 y\,2|\tau_0|\chi_0(y)\{\tanh y[24\sigma_{\mathrm{ord}}^{(1)}(\zeta)+\tfrac{1}{8}y(C_E+\tfrac{3}{2}+\ln 2)\mathrm{sech}^2 y]+C_E-1+\ln 2\\&\qquad+\tfrac{3}{2}(2-\pi 3^{-1/2}-C_E-\ln 2)\mathrm{sech}^2 y+(\pi/2)\sqrt{3}\mathrm{sech}^4 y+3J'(y)\tanh y\\&\qquad-[\tfrac{9}{4}I''(y)+6J(y)]\tanh^2 y+9I'(y)\tanh^3 y-9I(y)\tanh^4(y)\}\\&+\tfrac{1}{2}-\tfrac{1}{4}\ln 2-C_E/4-2\int_0^\infty dy\,K_1'(4y)[2|\tau_0|\chi_0(y)\mathrm{sech}^2 y-4y]-\tfrac{1}{2}\int_0^\infty dy\,K_0(4y)2|\tau_0|\chi_0(y)\mathrm{sech}^2 y\\&+(\tfrac{3}{2}\ln 2+\tfrac{3}{2}C_E+3)(\tfrac{31}{30}-\tfrac{4}{5}\ln 2)+\tfrac{3}{2}\int_0^\infty dy\int_0^\infty dy'\,f(y,y')|y-y'|_{\pm}^{-1}e^{-4|y-y'|}\\&+12\int_0^\infty dy\int_0^\infty dy'\int_2^\infty dx\,f(y,y')[r(x,y,y')-\tfrac{1}{4}e^{-2x|y-y'|}]\ ,\end{aligned} \tag{B11}$$

where

$$f(y,y')=2|\tau_0|\chi_0(y')\tanh y'\tanh y\,\mathrm{sech}^2 y\ . \tag{B12}$$

Numerical evaluation gives

$$A\approx-0.77\ . \tag{B13}$$

The renormalized function $\chi_{1,\infty}^R$ is given by[10] $[1-(u/2\epsilon)]\chi_{1,\infty}$ at this order. At the fixed point $u^*=\epsilon/3+O(\epsilon^2)$, it becomes

$$\chi_{1,\infty}^R=2^{1/2}(1-Au^*)|\tau|^{-(1/2+\epsilon/6)}\ . \tag{B14}$$

This implies Eq. (4.26b).

APPENDIX C: CALCULATION OF $\chi_1(T>T_c^b)$ AT THE ORDINARY TRANSITION

Above T_c^b the calculations are much easier and can be done analytically. Specifically for χ_1, we have again Eqs. (B1) and (B2), where now

$$\chi_{1,\infty}=\tau_0^{-1/2}[1-\tfrac{1}{2}g2^{-d}\pi^{-d/2}\tau_0^{-\epsilon/2}\times\int_0^\infty dy\,e^{-y}(1-e^{-y})Q_1(y)+O(g^2)]\ , \tag{C1}$$

with

$$\begin{aligned}Q_1(y)&\equiv\tau_0^{-1+\epsilon/2}2^d\pi^{d/2}\int_p\hat{G}(p;y,y;\tau_0=1)\\&=\Gamma(\epsilon/2-1)-2y^{-1+\epsilon/2}K_{1-\epsilon/2}(2y)\ .\end{aligned} \tag{C2}$$

Aside from an elementary integral, we need

$$\begin{aligned}\int_0^\infty dy\,e^{-\lambda y}y^{\epsilon/2-1}K_{1-\epsilon/2}(2y)&=\pi^{1/2}4^{1-\epsilon/2}\frac{\Gamma(\epsilon-1)}{(2+\lambda)\Gamma((1+\epsilon)/2)}\\&\quad\times{}_2F_1\left[1,\frac{3-\epsilon}{2};\frac{1+\epsilon}{2};\frac{\lambda-2}{\lambda+2}\right]\end{aligned} \tag{C3}$$

for $\lambda=1$ and 2. Here, Eq. 6.621.3 of Gradshteyn and Ryzhik[38] was used. The ϵ expansion of the hypergeometric function ${}_2F_1$ may be worked out as in Eq. (2.12) of Ref. 39. It can be written in the form

$$\begin{aligned}&{}_2F_1\left[1,\frac{3-\epsilon}{2};\frac{1+\epsilon}{2};x\right]\Gamma\left[\frac{3-\epsilon}{2}\right]\Gamma(\epsilon-1)\Big/\Gamma\left[\frac{1+\epsilon}{2}\right]\\&\quad=(1-x)^{-2}\left[-\left[\frac{1}{2\epsilon}+\ln 2\right](1+x)+x^{1/2}\ln\frac{1+x^{1/2}}{1-x^{1/2}}+O(\epsilon)\right]\ .\end{aligned} \tag{C4}$$

From here on the calculation proceeds in a straightforward fashion. Upon going over to renormalized quantities, the result in Eq. (4.6b) is recovered.

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