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Multicritical Behaviour at Surfaces*

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The critical behaviour of a semi-infinite n-vector model with a surface term $(c/2)\int dS\phi^2$ is studied in $4-\varepsilon$ dimensions near the special transition. It is shown that all critical surface exponents derive from bulk exponents and $\eta_{\|}$, the anomalous dimension of the order parameter at the surface. The surface exponents and the crossover exponent Φ for the variable c are calculated to second order in ε.
It is found that Φ does not satisfy the relation $\Phi=1-\nu$ predicted by Bray and Moore. The order-parameter profile $m(z)=\langle\phi\rangle$ is calculated to first order in ε. In contrast to mean-field theory, $m(z)$ is not flat nor does it satisfy a Neumann boundary condition. General aspects of the field-theoretic renormalization program for systems with surfaces are discussed with particular attention paid to the explanation of the unfamiliar new features caused by the presence of surfaces.

I. Introduction

In a previous paper [1] - hereafter referred to as I - we have described a field-theoretic approach to critical behaviour near free surfaces. This approach is in many respects similar to the usual field-theoretic treatment of bulk critical behaviour [2, 3] and allows one in particular to derive scaling laws for surface exponents in a standard fashion [1, 4].
Apart from obvious computational difficulties, however, the breakdown of translational invariance gives rise to a number of specific problems and novel features. Some, but not all of these, were already manifest in I. It became clear that the usual bulk renormalization functions (for order-parameter, temperature, and coupling-constant renormalization) do not in general suffice to render all interesting correlation functions finite. Thus an additional surface counterterm was needed to renormalize correlation functions involving normal derivatives of the order parameter.
A second unfamiliar phenomenon encountered in I was the appearance of primitively divergent one-particle *reducible* Feynman graphs. This entails that the conventional skeleton expansion [5], in which skeletons are given by classes of primitively divergent one-particle irreducible (vertex) graphs, becomes inadequate [6]. The consequences showed up in a relatively harmless fashion in I because we restricted attention to the asymptotic behaviour at the ordinary transition. They become much more pronounced in the analysis of the *special* (or surface-bulk) transition [4, 7, 8] which is the subject of the present paper.
As in I our analysis is based on the semi-infinite n-vector model defined by the free-energy functional

$$\mathscr{F}\{\phi\}=\int dV\left(\frac{1}{2}(\nabla\phi)^2+\frac{\tau}{2}\phi^2+\frac{g}{4!}(\phi^2)^2-h\cdot\phi\right)+\int dS\left(\frac{c}{2}\phi^2-h_1\cdot\phi\right) \tag{1}$$

in which ϕ is an n-component order-parameter field ($\phi_a(\mathbf{x})$, $a=1,\dots,n$). The volume and surface integrals $\int dV$, $\int dS$ extend over the $d(=4-\varepsilon)$-dimensional half-space $z\geqq 0$ and the plane $z=0$, respectively. The position vector $\mathbf{x}$ will be written as $\mathbf{x}=(\mathbf{r},z)$, $\mathbf{r}$ denoting its $d-1$-dimensional component parallel to the surface. h and h_1 are bulk and surface magnetic

* A brief account of some of the results presented here was given in [4]

fields which we assume to be uniform in their space coordinates **x** and **r**.

The model (1) has been studied previously by a variety of other authors; a fairly complete list of references can be found in [7] (see also [1] and [8]). More recently it has also been used to investigate critical adsorption phenomena [9–11].

The present work has two aims. The first is a detailed *RG* analysis of the special transition. This transition is described by a multicritical point, the 'special' point, at which both the surface variable c *and* h_1 are relevant in addition to the bulk variables h and τ. We will present two-loop calculations from which the scaling indices of all four relevant fields h, τ, h_1, c follow to order ε^2. In particular, we obtain the crossover exponent Φ associated with c, to this order, and show that it deviates from the prediction $\Phi = 1 - \nu$ of Bray and Moore [12]. Previous analyses of the special transition based on the ε-expansion were either limited to first order in ε [12, 13] or else did not consider deviations from the special point [14, 15].

Our second aim is to explain some of the unfamiliar features of the renormalization program mentioned above. To illustrate the appearance of one-particle reducible renormalization parts and to elucidate the consequences thereof we will discuss the renormalization of the surface operator $\phi^2(\mathbf{r}, 0)$ in some detail. A further characteristic problem caused by the presence of surfaces is the necessity to deal with boundary conditions. This was less prominent in I because for $c = \infty$, the value c takes at the fixed point that describes the ordinary transition, both the regularized (finite momentum cut-off Λ) *and* the renormalized correlation functions satisfy Dirichlet boundary conditions order by order in perturbation theory [1, 6]. In the case of the special transition a Neumann boundary condition (vanishing normal derivatives of ϕ) holds at the level of the tree (or mean-field) approximation, but this breaks down already at one-loop order [4, 6, 8]: As we shall see, the cut-off regularized correlation functions satisfy a *cut-off-dependent boundary condition.* This results from the fact that the $(\phi^2)^2$-interaction produces a shift of the critical value $c = c_{\mathrm{sp}}$ for the special transition (which controls the boundary condition). In contrast to mean-field theory, where $c_{\mathrm{sp}} = 0$, the special point is associated with a nonvanishing (and nonuniversal) value $c_{\mathrm{sp}} = c_{\mathrm{sp}}(g, \Lambda)$ of c. It is easy to see that the renormalized correlation functions do also not satisfy Neumann boundary conditions because they become singular near the surface. For example, the order-parameter profile $m(z) = \langle \phi(\mathbf{r}, z) \rangle$ behaves as $z^{(\beta_1 - \beta)/\nu}$ for $z \to 0$ and $h = h_1 = 0$, where ν, β_1, and β are the critical exponent for the bulk correlation length, the surface magnetization $m_1 := m(0)$, and the bulk magnetization $m_b := m(\infty)$.

This behaviour of $m(z)$ follows quite generally from a short-distance expansion (see I and below) and will be explicitly verified by a one-loop calculation of $m(z)$. At the special transition m_b decreases *faster* with temperature than m_1, i.e. $\beta_1 = \beta_1^{\mathrm{sp}} < \beta$. Therefore $m(z)$ as well as its z-derivative $m'(z)$ *diverge* asymptotically for $z \to 0$. In contrast we have $\beta_1 = \beta_1^{\mathrm{ord}} > \beta$ at the ordinary transition, implying $m(z) \to 0$ for $z \to 0$.

In the next section we give some necessary background information and discuss the identification of the special point. Details of our renormalization group approach are described in Section III. Technically, it differs somewhat from the one employed in I because – following Symanzik [6] – we Fourier transform only with respect to parallel momenta ($\mathbf{p}$) and work in a $\mathbf{p}z$-representation rather than in momentum space. Dimensional regularization is preferred in the actual computations, but we frequently indicate the modifications that arise when an ultraviolet cut-off Λ for the parallel momentum integrations is used instead. Results of the ε-expansion of Feynman graphs and some computational details are given in the Appendix.

II. Mean-Field Properties and the Identification of the Multicritical Point

A. Background

The special transition is described by a multicritical point (denoted SB in Fig. 1 of I) which is defined by the critical temperature T_b of the bulk and a critical value c_{sp} [1, 7, 8, 12]. At this point three second-order lines meet, namely a line of ordinary, extraordinary, and surface transitions. The ordinary transition, which was treated in I, occurs at T_b for $c > c_{\mathrm{sp}}$. When $c < c_{\mathrm{sp}}$, the exchange interaction for spins at the surface is sufficiently enhanced (as compared to the bulk) to split off a surface phase. On lowering the temperature, a surface transition first takes place at a critical temperature $T_s(c)$, which is then followed by a so-called 'extraordinary' transition at T_b. Crossover scaling [7, 12] implies that T_s varies as

$$(T_s(c) - T_b)/T_b = \mathrm{const} \cdot (c - c_{\mathrm{sp}})^{1/\Phi} \tag{2}$$

for $c \approx c_{\mathrm{sp}}$. Here Φ is the previously mentioned crossover exponent which we shall calculate below.

The multicritical point requires by its very definition the existence of a surface phase. For models of the

Ising or n-vector type with short-range interactions one expects a surface-ferromagnetic bulk-paramagnetic phase if (and only if) the surface dimension $d-1$ exceeds the lower critical dimension d_* for bulk order. In the Ising case $d_*=1$, and it is known from rigorous work [7, 16] that no surface phase exists in two dimensions. For $n \geqq 2$ the continous $O(n)$ symmetry leads to $d_*=2$ [17], so one expects a surface-ferromagnetic phase for $d>3$. This is corroborated by a low-temperature analysis of the semi-infinite, classical, isotropic Heisenberg ferromagnet. Using a random-phase approximation, Mills and Maradudin [18, 19] showed that spin-waves which are localized near the surface appear in addition to scattering modes. We expect these localized low-energy excitations to destroy surface ferromagnetism for $d \leqq 3$ in a similar fashion as bulk spin-waves destroy bulk long-range order in two dimensions. The case $n=2$ is special; by analogy with the Kosterlitz-Thouless transition [20] of the two-dimensional XY-model, a surface phase with quasi long-range order should be possible for $d=3$ [7]. It must also be mentioned that the assumption of ideal $O(n)$ symmetry throughout the sample is somewhat unrealistic. In general, the interaction will be anisotropic near the surface, even if the bulk is isotropic [21]. However, a hard-axis surface anisotropy should again lead to a surface-ferromagnetic phase for $d=3$. For simplicity, we will nevertheless restrict attention to the isotropic model defined in (1). Since within the ε-expansion one does not see that the special transition ceases to exist for $d=3$ and $n \geqq 2$, one must keep in mind that an extrapolation to $\varepsilon=1$ makes sense only for $n=1$.

B. Identification of the Multicritical Point

In mean-field theory [7, 12, 22] $c_{\mathrm{sp}}=0$ and the special transition has (at least) four characteristic properties each of which can be used for its identification. Since some of these properties are lost beyond mean-field (MF) theory, and to explain the identification of the multicritical point, we will briefly discuss them.

i) The MF magnetization profile is flat [22], i.e. $(h=h_1=0)$

$$m(z)=m_{\mathscr{B}}^{(0)}=(6|\tau|/g)^{1/2} \tag{3}$$

where $m_{\mathscr{B}}^{(0)}$ is the MF bulk magnetization.

ii) The MF correlation functions satisfy Neumann boundary conditions. This follows directly from the fact that the eigenfunctions $\varphi_k(z;c)$ (given by (II.5, 7) of I) which diagonalize the quadratic part of $\mathscr{F}$ become [14, 23, 24]

$$\varphi_k(z;c)=2^{1/2}\,\mathrm{sgn}(k)\cos(kz) \tag{4}$$

for $c=0$. By analogy with (II.4) and (II.10) of I we therefore have $\varphi_k'(z=0^+;0)=0$ and

$$\partial_n \phi=0 \tag{5}$$

where $\partial_n(=\partial_z)$ is the normal derivative along the inner normal.

The Neumann boundary condition follows also from well-known results for the MF propagator (denoted $\mathring{G}^{(2)}(\mathbf{x},\mathbf{x}')$ in I) which we write as $G_c(\mathbf{x},\mathbf{x}')$ for given c. Its parallel Fourier transform reads [22]

$$\tilde{G}_c(\mathbf{p};z,z')=\frac{1}{2\kappa}\left[\mathrm{e}^{-\kappa|z-z'|}+\frac{\kappa-c}{\kappa+c}\,\mathrm{e}^{-\kappa(z+z')}\right] \tag{6}$$

with

$$\kappa=(p^2+c)^{1/2} \tag{7}$$

in the disordered phase, and it satisfies the boundary condition

$$\partial_n G_c(\mathbf{x},\mathbf{x}')=c\,G_c(\mathbf{x},\mathbf{x}') \qquad (\mathbf{x}\in S,\ \mathbf{x}'\notin S). \tag{8}$$

Here the notation $\mathbf{x}\in S$ ($\mathbf{x}\notin S$) was introduced to indicate that $\mathbf{x}$ is ($\mathbf{x}'$ is not) a surface point. For $c=0$, (8) turns into a Neumann boundary condition for the 'Neumann propagator' $G_N:=G_{c=0}$.

iii) The value $c=0$ marks the border-line below which a bound state appears. As discussed in I, the diagonalization of $\delta^2\mathscr{F}/\delta\phi\delta\phi$ involves the eigenfunctions $\varphi(z;c)$ of the operator $-\partial_z^2+\tau$ with the boundary condition $\varphi'(0^+;c)=c\varphi(0;c)$ (see (II.3, 4) of I). For any $c<0$ there exists a bound state [23]

$$\varphi_0(z;c)=(2|c|)^{1/2}\exp(-|c|\,z) \tag{9}$$

with eigenvalue

$$\varepsilon_0=\tau-c^2 \tag{10}$$

in addition to scattering states $\varphi_k(z;c)$ which are again given by (II.5, 7) of I.

The appearance of this bound state is consistent with the expectation that the critical exponents of the surface transition are given by the bulk exponents in $d-1$ dimensions. To see this, note that, in terms of eigenfunctions, $\tilde{G}_c(\mathbf{p};z,z')$ becomes

$$\tilde{G}_c(\mathbf{p};z,z')=\int_0^\infty \frac{dk}{\pi}\,\varphi_k(z;c)(k^2+p^2+\tau)^{-1}\,\varphi_k(z';c)$$
$$+\varphi_0(z;c)(\mathbf{p}^2+\tau-c^2)^{-1}\,\varphi_0(z';c) \tag{11}$$

for $c<0$ and $\tau \geqq c^2$. Along the surface line $\tau=c^2$ ($c<0$) only the bound state gives rise to infra-red singularities. The scattering modes remain massive. This indicates that they are irrelevant degrees of freedom for the surface transition. Decomposing ϕ into bound state and scattering contributions

$$\phi(\mathbf{r}, z)=\psi(\mathbf{r})\,\varphi_0(z; c)+\int_0^\infty \frac{dk}{\pi}\,\phi_k(\mathbf{r})\,\varphi_k(z; c) \tag{12}$$

we may define an effective surface free energy

$$\mathscr{F}_s\{\psi\}=-\ln\left[\left(\prod_k \int d\{\phi_k(\mathbf{r})\}\right)\exp(-\mathscr{F}\{\phi; h=h_1=0\})\right] \tag{13}$$

by integrating out the scattering degrees of freedom. Since $\tau_s:=\tau-c^2$ is small compared to the mass $\tau^{1/2} \approx |c|$ of the scattering states, $\mathscr{F}_s$ can be calculated perturbatively by expanding in powers of $|c|^{-1}$, holding τ_s and $g_s:=gc$ fixed. To leading order one obtains

$$\mathscr{F}_s\{\psi\}=\int dS\left\{\frac{1}{2}(\partial_\parallel \psi)^2+\frac{1}{2}\tau_s\psi^2+\frac{1}{4!}g_s(\psi^2)^2\right\} \tag{14}$$

where $\partial_\parallel$ is the $d-1$-dimensional parallel component of $\nabla=(\partial_\parallel, \partial_z)$. The result confirms the naive expectation that fluctuations in the scattering modes can be ignored. Since $\mathscr{F}_s$ describes a $d-1$-dimensional bulk system with order parameter $\psi(\mathbf{r})$, the above-mentioned well-known result for the critical exponents of the surface transition follows.

iv) The local susceptibility χ_{11} and the bulk susceptibility χ_b both diverge. Recalling that [7]

$$\chi_{11}=(\partial m_1/\partial h_1)_{h=h_1=0} \tag{15}$$

we also introduce, for later use, the layer susceptibilities

$$\chi(z):=(\partial m(z)/\partial h)_{h=h_1=0} \tag{16}$$

$$\chi_1:=\chi(z=0) \tag{17}$$

and the excess susceptibility

$$\chi_s:=\int_0^\infty dz(\chi_b-\chi(z)). \tag{18}$$

For $n \geqq 2$ all χ's are tensors; then (16) e.g. must be interpreted as $\chi^{ab}(z)=[\partial m^a(z)/\partial h^b]_{h=h_1=0}$. Since we are mainly interested in the Ising case we will set $n=1$ whenever we consider temperatures below T_b. The results for $T \geqq T_b$ will be given for general n, however, because the correlation functions (and hence the χ's) are $O(n)$ symmetric for vanishing magnetic fields. Thus $\chi(z)$, for example, can be regarded as the diagonal element of $\chi^{ab}(z)=\chi(z)\,\delta^{ab}$.

Among these properties *(iv)* is best suited for the identification of the multicritical point. The first two are lost beyond the MF approximation, as already mentioned in the Introduction. The third is tailored for MF theory and less useful because an appropriate generalization would require that we consider the inverse of the two-point correlation function. Loosely speaking *(iv)* says that bulk and surface are both critical. This should be contrasted with the conditions at the surface transition where χ_{11} diverges while χ_b is analytic and at the ordinary transition where χ_b diverges while χ_{11} remains finite (though nonanalytic).

Specifically, the multicritical point can be identified as follows. Working in $\mathbf{p}z$-space let us cut off the parallel momentum integrations at $|\mathbf{p}|=\Lambda$. We then determine the critical value $\tau_b=\tau_b(g, \Lambda)$ of τ as usual from

$$\chi_b^{-1}(\tau_b, g, \Lambda)=0. \tag{19}$$

Then $c_{sp}=c_{sp}(g, \Lambda)$ follows from

$$\chi_{11}^{-1}(\tau_b, c_{sp}, g, \Lambda)=0. \tag{20}$$

A straightforward calculation (see Eqs. (4.3–7) of Ref. 12) gives, to one-loop order,

$$c_{sp}=-\Lambda\frac{n+2}{3}\mathring{u}+O(\mathring{u}^2) \tag{21}$$

where

$$\mathring{u}=\Lambda^{-\varepsilon}2^{-d}\pi^{-d/2}g \tag{22}$$

is the dimensionless bare coupling constant.

In dimensional regularization, where momentum-independent terms $\propto \Lambda$ are thrown away, $c_{sp} \equiv 0$ to all orders. This is completely analogous to the result $\tau_b \equiv 0$ for the shift of the critical temperature.

III. Renormalization Group Analysis of the Special Transition

A. Surface Singularities and Surface Counterterms

We begin with a brief exposition of some basic features of the RG program for semi-infinite systems, following partly Symanzik's reasoning [6].

To go beyond MF theory one can set up a perturbation expansion in terms of $\tilde{G}_c$. Alternatively, one can expand in powers of c and use $\tilde{G}_N$ as free propagator. Since $\tilde{G}_c$ is fairly complicated the latter is preferable unless one wants to keep the full c-dependence of the correlation functions. In either case one finds from (6) that the free propagator differs from the corresponding translationally invariant 'bulk' propagator

$$\tilde{G}_{\mathscr{E}}(\mathbf{p}; z, z') = (2\kappa)^{-1} \exp(-\kappa|z-z'|) \tag{23}$$

by an image term, i.e.

$$G_{\text{free}} = G_{\mathscr{E}} + G_{\mathscr{S}}. \tag{24}$$

Specifically for $G_{\text{free}} = G_N$, one has

$$G_{\mathscr{S}}(\mathbf{x}, \mathbf{x}') = G_{\mathscr{E}}(\hat{\mathbf{x}} - \mathbf{x}') \tag{25}$$

where $\hat{\mathbf{x}} = (\mathbf{r}, -z)$ is the image point of $\mathbf{x} = (\mathbf{r}, z)$.

Let us consider one-particle irreducible (1PI) graphs (defined diagrammatically in the usual way). Using the decomposition (24) for each propagator line one obtains, among others, graphs that involve exclusively $G_{\mathscr{E}}$. These 'bulk' graphs are precisely the 1PI graphs of the corresponding translationally invariant theory. Unregularized or for $\Lambda \to \infty$, $G_{\mathscr{E}}$ behaves as

$$G_{\mathscr{E}}(\mathbf{x} - \mathbf{x}') \sim |\mathbf{x} - \mathbf{x}'|^{-2+\varepsilon} \quad (\mathbf{x} \to \mathbf{x}') \tag{26}$$

at short distances. This singular behaviour is known to produce ultra-violet (uv) singularities in the perturbation series. Apart from obvious Λ^2 singularities in tadpole graphs (for $\varepsilon = 0$), nonintegrable singularities result from products of $G_{\mathscr{E}}$'s. For bulk graphs the remedy is well-known [5, 25]: The uv singularities can be absorbed by a few counterterms related to order-parameter, temperature, and coupling-constant renormalization. For the discussion that follows it is helpful to recall two facts: *a)* Counterterms are distributions with support only at the vertices of 'contracted' graphs, i.e. graphs in which the vertices are contracted to a point, and therefore can be represented by *local* interactions. *b)* It is sufficient to renormalize 1PI graphs. Once all primitively divergent 1PI graphs – the skeletons [5] – have been renormalized, all other graphs and in particular those of correlation functions are automatically finite.

While property *a)* continues to be true for our semi-infinite model (or more generally for similar models with surfaces [6]) *b)* breaks down, as we shall see. Note that this break-down is to be expected because *b)* is a consequence of translational invariance (see e.g. [25]).

Next, consider graphs that involve also $G_{\mathscr{S}}$. As is obvious from (25), $G_{\mathscr{S}}$ becomes singular when $\mathbf{x}'$ approaches the image point of $\mathbf{x}$; i.e. when $\mathbf{x}$ and $\mathbf{x}'$ approach one and the same surface point. $G_{\mathscr{S}}$ will therefore produce *additional uv singularities at the surface.* To understand the consequences note that the approach to renormalization theory associated with Bogoliubov and Shirkov [25] is essentially a position space procedure. In particular, the arguments leading to *a) do not depend on translational invariance.* By analogy with *a)* one thus concludes that these surface singularities can be absorbed by (a finite number of) local surface counterterms. Power counting [1, 4, 6] implies that – apart from the usual bulk renormalization functions – two additional renormalization factors Z_c, Z_1 for the variable c and the order parameter $\phi|_{\mathscr{S}} := \phi(\mathbf{r}, z=0)$ at the surface are needed:

$$\mathring{c} = \mu Z_c c^{\mathscr{R}} + c_{\text{sp}} \tag{27}$$

$$\mathring{\phi}|_{\mathscr{S}} = (Z_\phi Z_1)^{1/2} \phi|_{\mathscr{S}}^{\mathscr{R}} = Z_1^{1/2} \phi^{\mathscr{R}}|_{\mathscr{S}}. \tag{28}$$

Here μ is an arbitrary momentum scale, and we have slightly changed the notation for the bare quantities $\mathring{c}$, $\mathring{\phi}$ in order to distinguish them clearly from their renormalized counterparts $c^{\mathscr{R}}$, $\phi^{\mathscr{R}}$. To simplify the notation we will henceforth drop the index '$\mathscr{R}$' on $c^{\mathscr{R}}, \phi^{\mathscr{R}}$, and the renormalized dimensionless magnetic fields

$$h^{\mathscr{R}} = \mu^{-1+\varepsilon/2} Z_\phi^{1/2} \mathring{h} \tag{29}$$

$$h_1^{\mathscr{R}} = \mu^{-2+\varepsilon/2} (Z_\phi Z_1)^{1/2} \mathring{h}_1. \tag{30}$$

The renormalized action then becomes

$$\begin{aligned} \mathscr{F}^{\mathscr{R}} = &\int dV \{\tfrac{1}{2} Z_\phi (\nabla\phi)^2 + \tfrac{1}{2}(\mu^2 Z_t t + \tau_{\mathscr{E}}) Z_\phi \phi^2 \\ &+ \mu^\varepsilon (u/4!)\, 2^d \pi^{d/2} Z_u Z_\phi^2 (\phi^2)^2 - \mu^{1-\varepsilon/2} h \cdot \phi\} \\ &+ \int dS \{\tfrac{1}{2}(\mu Z_c c + c_{\text{sp}}) Z_\phi \phi^2 - \mu^{2-\varepsilon/2} Z_1^{-1/2} h_1 \cdot \phi\}. \end{aligned} \tag{31}$$

Within the dimensional renormalization scheme $Z_{\phi,t,u}$ are given by (III.18a–c) of I to two-loop order. Z_1 should be well distinguished from the Z-factor Z_1 of I. The results given in the appendix yield [4]

$$Z_1 = 1 + \frac{n+2}{3\varepsilon} u + \left(\frac{(n+2)(n+5)}{9} - \frac{n+2}{3}\,\varepsilon\right) \varepsilon^{-2} u^2 + O(u^3) \tag{32}$$

$$Z_c = 1 + \frac{n+2}{3\varepsilon} u + \left(\frac{(n+2)(n+5)}{9} + \frac{n+2}{36}\,\varepsilon(1-4\pi^2)\right) \varepsilon^{-2} u^2 + O(u^3). \tag{33}$$

We have deliberately omitted a surface counterterm $\propto \int dS \phi \partial_n \phi$ in (31). Such a counterterm is allowed by power counting and would in fact be needed to renormalize 1PI graphs. This is easy to see by considering the tadpole graph in Fig. 1 which is proportional to $G_N(\mathbf{x}, \mathbf{x})$ which in turn is proportional to $z^{-2+\varepsilon} = -\varepsilon^{-1} \delta'(z) + O(\varepsilon^0)$, according to (B.1, 2) (For simplicity we set $c = \tau = 0$ and use dimensional regularization here).

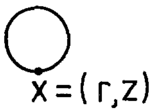

Fig. 1. A 1PI graph containing a surface singularity $\propto\delta'(z)$

The pole term is absorbed by the above counterterm. Hence, if we insist on having renormalized 1PI functions which are well defined in the distribution sense, then we clearly need this counterterm.

Ultimately, however, we want to renormalize correlation functions, and for that purpose this counterterm turns out to be completely unnecessary. This follows from the observation that the 1PI functions are integrated with free propagators G_N or G_c in regularized correlation function graphs. Utilizing the boundary condition (8) one recognizes that the vertex $\phi\partial_n\phi$ attached to G_c on either end has the same effect as the vertex $\mathring{c}\phi^2|_{\sigma}$. An appropriate choice of the counterterm $\propto\phi^2|_{\sigma}$ will therefore guarantee that the coefficient of $\phi\partial_n\phi$ can be taken to vanish. Alternatively, we can argue that $\phi\partial_n\phi$ gives a vanishing contribution when attached to two G_N's whose other arguments are off the surface. Consequently, if we take the surface interactions $\propto\phi^2|_{\sigma}$ and $\phi|_{\sigma}$ at an infinitesimal distance from the surface and let this distance shrink to zero *after* the normal derivatives have been taken at $z=0$, then the counterterm will remain completely ineffective. (The previous argument based on G_c amounts to letting $\phi^2|_{\sigma}$ approach the surface before taking normal derivatives.) Anyhow, the conclusion is that this counterterm is not needed, and we will therefore not discuss it any further.

B. The Appearance of One-Particle Reducible Renormalization Parts

Having constructed the necessary counterterms we will now discuss the break-down of property *b)*. The reason for this break-down is the appearance of one-particle *reducible* (1PR) renormalization parts (primitively divergent 1PR graphs) [1, 6]. As a first example consider the graph in Fig. 2, in which the crossed circle indicates a surface point and the left external point (uncrossed) is separated by a distance $z>0$ from the surface. If the right external point were also off the surface, then the graph would require only bulk subtractions for $c=t=0$ and, therefore, would have no pole term at all in dimensional regularization. As the right external point becomes a surface point, a pole term $\propto\delta(z)$ develops. This is absorbed by the counterterm $\propto(Z_1^{-1/2}-1)$ in (31).

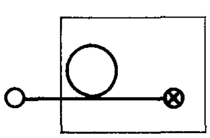

Fig. 2. The box contains a one-particle reducible renormalization part. The crossed (uncrossed) circle denotes an external point on (off) the surface

Next, we introduce the notation $G^{(N,M;K)}$ for the connected correlation functions

$$\left\langle \prod_{i=1}^{N}\phi(\mathbf{x}_i)\prod_{j=1}^{M}\phi(\mathbf{r}_j,0)\prod_{k=1}^{K}\frac{1}{2}\phi^2(\mathbf{R}_k,0)\right\rangle^{\text{conn}}$$

with N external points off the surface, M external surface points, and K insertions of $\frac{1}{2}\phi^2|_{\sigma}$ (The definition is analogous to (III.15) of I). The graphs of $G^{(2,0;1)}$ are shown in Fig. 3 to two-loop order. Let us specifically consider graph (10). In the translationally invariant theory it has uv singularities coming exclusively from the upper closed loop, and it vanishes for $t=0$. From (A2) and (A14) of the appendix one sees that, in our case, the graph has first and second order poles in ε. Moreover, the ε^{-1}-pole term of the amputated graph obtained by removing the external legs involves the distribution z_+^{-1} (For a definition of z_+^{-1} see Ref. [26]). The reason is that this graph contains a divergent subgraph, namely the 1PR graph inside the box of Fig. 4. The latter corresponds to the graphs (3) and $(\hat{3})$ of Fig. 3 which have first-order pole terms and in conjunction with graph (2) determine the counterterm $\propto\phi^2|_{\sigma}$ to one-loop order. (Note for comparison that in the translationally invariant theory (3) and $(\hat{3})$ do not contribute to the ϕ^2 counterterm.) To eliminate the pole terms of graph (10) that come from the divergent subgraph we must: *(i)* contract

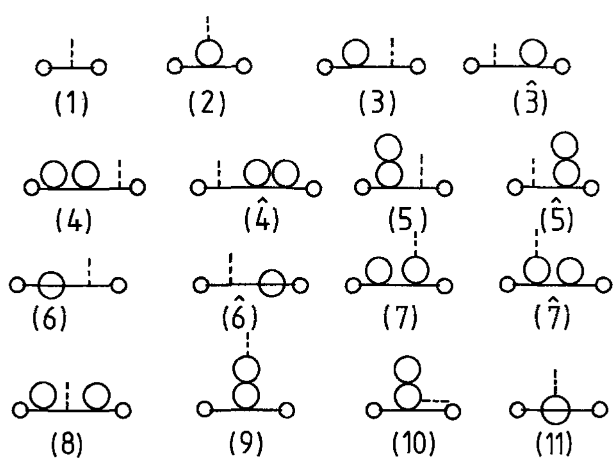

Fig. 3. Graphs of $G^{(2,0;1)}$ to two-loop order. The dashed lines denote insertions of the surface operator $\frac{1}{2}\phi^2|_{\sigma}$

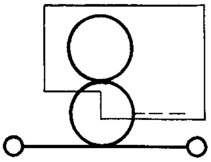

Fig. 4. The graph has an ε^{-2} pole term because it contains the primitively divergent one-particle reducible subgraph inside the box

the interior of the box in Fig. 4 to a point, *(ii)* multiply the resulting reduced graph (which is graph (2) of Fig. 3) by the pole term of the subgraph, and *(iii)* subtract the result from graph (10). With the help of the results given in the appendix one can easily check that the pole term $\propto z_+^{-1}$ – which would be impossible to absorb by a local counterterm – then vanishes (Similar cancellations must and do occur for the other two-loop graphs).

An obvious consequence of these findings is that $\Gamma^{(2;1)}$, the 1PI analogue of $G^{(2,0;1)}$, *is not multiplicatively renormalizable* and therefore *does not satisfy a homogeneous RG equation.*

C. Renormalization Group Equations and Results

Although the 1PI functions are not multiplicatively renormalizable, the relations between the bare and renormalized correlation functions $G^{(N,M;K)}_{\text{bare}/\mathscr{R}}$ have a familiar form. From (31) one finds

$$G^{(N,M;K)}_{\mathscr{R}} = Z_\Phi^{-(N+M)/2} Z_1^{-M/2} Z_c^K G^{(N,M;K)}_{\text{bare}} \tag{34}$$

which entails the renormalization group (RG) equations*

$$\{\mu\partial_\mu + \beta_u \partial_u + \sum_w (\mu\partial_\mu|_0 \ln w) w\partial_w + \tfrac{1}{2}[(N+M)\eta_\Phi + M\eta_1] - K\eta_c\} G^{(N,M;K)}_{\mathscr{R}} = 0. \tag{35}$$

Here the sum runs over $w = t, c, h, h_1$ and $\partial\mu|_0$ denotes a μ-derivative at fixed bare variables $g, \tau, \mathring{h}, \mathring{h}_1$. β_u and η_Φ are the same as in I. η_1 and η_c are defined by

$$\eta_{1,c}(u) = \mu\partial_\mu|_0 \ln Z_{1,c}. \tag{36}$$

Using (32, 33) one finds

$$\eta_1(u) = -\frac{n+2}{3}u + 2\frac{n+2}{3}u^2 + O(u^3), \tag{37}$$

$$\eta_c(u) = -\frac{n+2}{3}u + \frac{n+2}{18}(4\pi^2 - 1)u^2 + O(u^3). \tag{38}$$

* This holds for all $G^{(N,M;K)}_{\mathscr{R}}$ except $G^{(0,0;k)}_{\mathscr{R}}$, $k = 1, 2, 3$, which require additional additive renormalizations and hence satisfy inhomogeneous RG equations

The remaining RG functions can be written

$$\mu\partial_\mu|_0 \ln t = -(2+\eta_t), \tag{39a}$$

$$\mu\partial_\mu|_0 \ln c = -(1+\eta_c), \tag{39b}$$

$$\mu\partial_\mu|_0 \ln h = -1 + (\varepsilon + \eta_\Phi)/2, \tag{39c}$$

$$\mu\partial_\mu|_0 \ln h_1 = -2 + (\varepsilon + \eta_\Phi + \eta_1)/2. \tag{39d}$$

Standard arguments show that the values, the exponent functions take at the infra-red stable fixed point u^*, give the critical exponents. One has $\nu = (2+\eta_t(u^*))^{-1}$, $\eta = \eta_\Phi(u^*)$ (as in I),

$$\eta_\parallel = \eta + \eta_1(u^*), \tag{40}$$

and

$$\Phi = \nu[1 + \eta_c(u^*)]. \tag{41}$$

This gives

$$\eta_\parallel = -\frac{n+2}{n+8}\varepsilon - \frac{5(n+2)(n-4)}{2(n+8)^3}\varepsilon^2 + O(\varepsilon^3), \tag{42}$$

$$\Phi = \frac{1}{2} - \frac{n+2}{4(n+8)}\varepsilon + \frac{n+2}{8(n+8)^3} \cdot [8\pi^2(n+8) - (n^2 + 35n + 156)]\varepsilon^2 + O(\varepsilon^2). \tag{43}$$

The result in (42) has been derived independently by Reeve [14, 15]. Φ differs from $1-\nu$ at order ε^2, as pointed out previously. The estimates $\eta_\parallel \approx 0.2$, $\Phi \approx 0.68$ one obtains from (42, 43) for the three-dimensional Ising ($n=1$) exponents $\eta_\parallel, \Phi$ agree reasonably well with Monte Carlo data of Binder and Landau [7]. (For a more detailed comparison see [7] and [8].)

With the help of the RG equations (35) one can derive the familiar scaling laws $\eta_\perp = (\eta + \eta_\parallel)/2$, $\gamma_{11} = \nu(1-\eta_\parallel)$, $\gamma_1 = (2-\eta_\perp)$, $\beta_1 = \nu(d-2+\eta_\parallel)/2$ etc. in a similar fashion as in I. Moreover, one finds that the correlation functions take scaling forms at $u = u^*$. Skipping derivations we give some representative examples. The renormalized magnetization profile can be written

$$m(z; u^*, t, c, h, h_1) = |t|^\beta \sigma(\mu z|t|^\nu, c|t|^{-\Phi}, h|t|^{-\Delta}, h_1|t|^{-\Delta_1}) \tag{44}$$

with $\Delta_1 = \nu(d - \eta_\parallel)/2$ and the usual bulk exponents β, Δ. The profile has been calculated to order ε by Brézin and Leibler [11] for $h = t \equiv 0$. We will present a one-loop calculation of $m(z)$ for $h = h_1 = c = 0$, $t < 0$ in the next subsection.

To analyze the behaviour of $m(z)$ near the surface we use the short-distance expansion proposed in I.

Writing [1, 6, 11]

$$\langle\phi(\mathbf{r}, z)\rangle \sim C(z)\langle\phi(\mathbf{r}, 0)\rangle \quad (45)$$

and specializing for simplicity to $h=h_1=c=0$, one obtains

$$[\mu\partial_\mu+\beta_u\partial_u-(2+\eta_t)t\partial_t-\eta_1/2]\,C(z)=0 \quad (46)$$

from the RG equations (35) of the two correlation functions in (45). The solution at the fixed point becomes

$$C(z; u^*, t)=(\mu z)^{\eta_1^*/2} D(\mu z|t|^\nu) \quad (47)$$

with

$$\eta_1^*=-\frac{n+2}{n+8}\varepsilon-\frac{3(n^2-4)}{(n+8)^3}\varepsilon^2+O(\varepsilon^3) \quad (48)$$

and since $\eta_1^*/2=(\beta_1-\beta)/\nu$, the magnetization behaves as

$$m(z)\sim \mathrm{const}\,(\mu z)^{(\beta_1-\beta)/\nu}|t|^{\beta_1} \quad (49)$$

for $\mu z \ll |t|^{-\nu}$. The result seems to imply that the surface magnetization m_1 is infinite (which it is of course not). However, it must be kept in mind that (49) is only valid in the scaling regime where z is large compared to the lattice constant (though small on the scale of the correlation length). In the derivation of (49) we have tacitly assumed that the scaling function $D(\zeta)$ approaches a constant for $\zeta\to 0$. This and (49) will be verified to order ε below.

Taking into account that χ_σ, χ_1 and χ_{11} satisfy the same RG equations as $G_{\mathscr{R}}^{(2,0;0)}$, $G_{\mathscr{R}}^{(1,1;0)}$, and $G_{\mathscr{R}}^{(0,2;0)}$ respectively, one also finds the usual scaling expressions for these functions, namely

$$\chi_\sigma(u^*; t, c)=\mu^{-3}|t|^{-\gamma_\sigma} X_\sigma(c|t|^{-\Phi}) \quad (50)$$

where

$$\gamma_\sigma=\gamma+\nu \quad (51)$$

and similar results for χ_{11}, χ_1 with γ_σ replaced by γ_1 and γ_{11}.

Logarithmic corrections in four dimensions can be analyzed in the same way as in I. One obtains (for $c=h=h_1\equiv 0$)

$$\chi_\sigma(t)\sim\mu^{-3}|t|^{-3/2}\,|\ln|t||^{(n-10)/(2n+16)} \quad (52)$$

$$\chi_1(t)\sim\mu^{-2}|t|^{-1}|\ln|t||^{3(n+2)/(2n+16)} \quad (53)$$

$$\chi_{11}(t)\sim\mu^{-1}|t|^{-1/2}|\ln|t||^{3(n+2)/(2n+16)} \quad (54)$$

$$m_1(t)\sim\mu^{1-\varepsilon/2}|t|^{1/2}|\ln|t||^{1/2} \quad (55)$$

In the derivation of (52) we have used the fact that the u^0 term in the perturbation expansion of χ_σ vanishes. The line of surface transitions (i.e. $T_\sigma(c)$) follows from the flow equations for c, t, u, and the behaviour of χ_{11} for $u=0$. Instead of (2) one has

$$\mathring{c}-c_{\mathrm{sp}}\approx-\mathrm{const}\,t^{1/2}|\ln t|^{(n+2)/(2n+16)} \quad (56)$$

D. Magnetization Profile for $n=1$

In this final subsection we calculate the renormalized magnetization profile for $c=h=h_1\equiv 0$ to one-loop order. For the sake of simplicity we will restrict attention to the Ising ($n=1$) case. Similar calculations have been carried out for $h_1=\infty$ in [9] and for $t=0$, $h_1\neq 0$, $c\neq 0$ in [11].

The bare magnetization profile $\mathring{m}(z)$ satisfies at one-loop order the differential equation

$$[-\partial_z^2+\tau+(g/6)\mathring{m}^2+(g/2)\,Q(z)]\,\mathring{m}=0 \quad (57)$$

with the boundary condition

$$\mathring{m}'(0)=c_{\mathrm{sp}}\mathring{m}(0) \quad (58)$$

Here

$$Q(z)=\int_{\mathbf{p}}\tilde{G}(\mathbf{p}; z, z; \{\mathring{m}\}) \quad (59)$$

in which

$$\int_{\mathbf{p}}=\int d^{d-1}p/(2\pi)^{d-1}$$

while $\tilde{G}(\{\mathring{m}\})$ is a solution of

$$[-\partial_z^2+\mathbf{p}^2+\tau+(g/2)\mathring{m}^2]\,\tilde{G}(\mathbf{p}; z, z'; \{\mathring{m}\})=\delta(z-z') \quad (60a)$$

with the boundary condition

$$\partial_n G(\{\mathring{m}\})=c_{\mathrm{sp}\,\sigma}|G(\{\mathring{m}\}) \quad (60b)$$

In dimensional renormalization (58, 60b) turn again into Neumann boundary conditions.

To solve (57) we make the ansatz

$$\mathring{m}(z)=\mathring{m}_{\mathscr{B}}\,\Sigma(z) \quad (61)$$

with

$$\mathring{m}_{\mathscr{B}}=(6|\tau|/g)^{1/2}[1+gA+O(g^2)] \quad (62)$$

and

$$\Sigma(z)=\Sigma^{(0)}(z)+g\,\Sigma^{(1)}(z)+O(g^2) \quad (63)$$

$\mathring{m}_{\mathscr{B}}$ is the bare bulk magnetization. From the well-known MF solution for the profile [7, 24] one derives

$$\Sigma^{(0)}(z)=1+c_{\mathrm{sp}}(2|\tau|)^{-1/2}\exp(-(2|\tau|)^{1/2}z)+O(c_{\mathrm{sp}}^2) \quad (64)$$

Hence

$$\lim_{z\to\infty} \Sigma^{(1)}(z)=0 \tag{65}$$

The term $\propto c_{sp}$ in Eq. (64) is needed in the cut-off regularized theory to cancel the linear divergence of the one-loop term (see below).
In (60a, 59) we may use the MF result for $\mathring{m}(z)$. One thus finds

$$A=-(8|\tau|)^{-1}\int_{\mathbf{p}} \kappa_2^{-1} \tag{66}$$

$$\kappa_2=(\mathbf{p}^2+2|\tau|)^{1/2} \tag{67}$$

and the equation

$$(-\partial_z^2+2|\tau|)\,\Sigma^{(1)}(z)+\int_{\mathbf{p}}(4\kappa_2)^{-1}\exp(-2\kappa_2 z)=0 \tag{68}$$

which is easily solved. Utilizing the boundary condition (58) and (21) one arives at

$$\Sigma(z)=1+(g/8)\{\int_{\mathbf{p}}(\mathbf{p}^2+3|\tau|/2)^{-1}(2\kappa_2)^{-1}e^{-2\kappa_2 z} -(2|\tau|)^{-1/2}\exp(-(2|\tau|)^{1/2}z)\int_{\mathbf{p}}[(\mathbf{p}^2+3|\tau|/2)^{-1}-p^{-2}]\} \tag{69}$$

The subtraction in the last bracket, which makes the $\mathbf{p}$-integral convergent, results from the term $\propto c_{sp}$ in (64). (The Λ^2 divergence in A is cancelled by the mass counterterm $\propto\tau_{\mathscr{E}}$, as usual.)
We now insert the Z-factors of the dimensionally regularized theory. The renormalized magnetization profile then follows in a straightforward way. For $u=u^*$ the result can be written

$$m(z)=m_{\mathscr{E}}\,\sigma(\zeta) \tag{70}$$

with

$$\zeta=\mu z(|t|/2)^{\nu}, \tag{71}$$

$$m_{\mathscr{E}}=\mu^{1-\varepsilon/2}(18\,\vartheta_d/\varepsilon)^{1/2} \cdot[1+(\varepsilon/6)(1-C_E-\ln 2)+O(\varepsilon^2)]\,|t|^{\beta} \tag{72}$$

and

$$\sigma(\zeta)=1+(\varepsilon/6)\,[K_0(4\zeta)-3J(\zeta)+(3^{1/2}\pi/2)\,e^{-2\zeta}] +O(\varepsilon^2) \tag{73}$$

where $\vartheta_d=2^{-d}\pi^{-d/2}$,

$$J(\zeta):=\int_0^{\infty} dp\,\frac{\exp(-2\zeta(p^2+4)^{1/2})}{(p^2+3)(p^2+4)^{1/2}}, \tag{74}$$

C_E is Euler's constant, and K_0 denotes a modified Bessel function.
Since

$$K_0(4\zeta)\sim-[C_E+\ln(2\zeta)] \quad (\zeta\to 0) \tag{75}$$

the scaling function $\sigma(\zeta)$ behaves as

$$\sigma(\zeta)\sim C_0\,\zeta^{-\varepsilon/6+O(\varepsilon^2)} \quad (\zeta\to 0) \tag{76}$$

with

$$C_0=1-(\varepsilon/12)(2C_E+6J(0)+\ln 4-3^{1/2}\pi)+O(\varepsilon^2) \tag{77}$$

at short distances. This agrees with (49) at order ε.

IV. Summary and Conclusions

Using field-theoretic methods we have studied the semi-infinite n-vector model near the special transition. We have shown how to renormalize correlation functions with insertions of the surface operators $\phi|_{\mathscr{S}}$ and $\phi^2|_{\mathscr{S}}$. From the associated renormalization group equations the surface exponents and their scaling laws could be obtained in a standard and straightforward fashion. All surface exponents and the crossover exponent Φ follow from the Z-factors Z_1, Z_c for $\phi|_{\mathscr{S}}$ and $\phi^2|_{\mathscr{S}}$, and the familiar bulk renormalization functions. They were calculated to second order in ε and it was found that Φ differs from $1-\nu$ at order ε^2. Bray and Moore's [12] conjecture $\Phi=1-\nu$ is therefore not generally valid.
We also derived the logarithmic corrections of the susceptibilities χ_{11}, χ_1, $\chi_{\mathscr{S}}$, and the surface magnetization m_1 in four dimensions, and calculated, for the special case of a scalar order parameter ($n=1$), the magnetization profile $m(z,t)$ for $\varepsilon>0$, $h=h_1=0$, $\mathring{c}=c_{sp}$. It was found that $\mathring{m}(z,t)$, the regularized profile, satisfies a cut-off dependent boundary condition. The renormalized magnetization which describes the asymptotic behaviour in the scaling regime (where z is large compared to the lattice constant but small on the scale of the correlation length) behaves as $m(z,t)\sim|t|^{\beta_1}(\mu z)^{(\beta_1-\beta)/\nu}$, however. This behaviour is expected from scaling and was confirmed via a short-distance expansion.
Although the approach described here, in I, and in [6] is very similar to the well-known field-theoretic treatment of bulk critical behaviour [2, 3], we have seen that the presence of surfaces gives rise to a number of novel features which require modifications of the standard renormalization theory: The scattering off of the surface leads to additional uv singularities. Those can be absorbed by local surface counterterms. However, not only one-particle irreducible graphs but also one-particle reducible ones contribute to these counterterms. As already pointed out by Symanzik [6], this implies a break-down of the conventional skeleton expansion into classes of primitively divergent 1PI graphs. That is to say, the skeleton expansion must be modified in an appro-

priate way due to the appearance of one-particle reducible renormalization parts. Symanzik has described how this can be done [6]. The main rule for the identification of surface renormalization parts is the following: Graphs that are composed of several 1 PI subgraphs which are one-particle reducibly linked and have singularities on the surface will in general *not* become finite by renormalization of their divergent subgraphs. In Symanzik's words, the surface acts as an additional line, and therefore the graph itself may require a (final) subtraction. We have tried to illustrate this here by discussing the renormalization of $\phi^2|_{\mathscr{S}}$. A consequence of these findings is that 1PI functions such as $\langle \phi\,\phi\,\phi^2|_{\mathscr{S}}/2\rangle_{1\mathrm{PI}}$ satisfy inhomogeneous rather than homogeneous RG equations. For practical purposes it appears most convenient to focus on correlation functions which still satisfy homogeneous RG equations.

In summary we conclude that the field-theoretic approach to critical phenomena near surfaces is well established and as efficient as the analogous methods for the treatment of bulk critical behaviour.

Appendix

We first summarize our results for the dimensionally regularized one and two-loop graphs of $G^{(1,1;0)}$ and $G^{(2,0;1)}$ for $\tau=c=0$ and then present some technical details of our calculations.

A. Summary of Results for Feynman Graphs

The graphs for $G^{(1,1;0)}$ and $G^{(2,0;1)}$ are shown in Figs. 5 and 3, respectively. To two-loop order our results can be written in the form

$$\tilde{G}^{(1,1;0)}_{ab}(\mathbf{p},z;\mathbf{p}')=\delta^{ab}(2\pi)^{d-1}\,\delta(\mathbf{p}+\mathbf{p}')\,p^{-1}\,\mathrm{e}^{-pz}\cdot\left\{1+\sum_{i=2}^{4}J_i(\mathbf{p},z)\right\} \tag{A.1}$$

$$\tilde{G}^{(2,0;1)}_{ab}(\mathbf{p}_1,z_1;\mathbf{p}_2,z_2;P)=\delta^{ab}(2\pi)^{d-1}\,\delta(\mathbf{p}_1+\mathbf{p}_2+\mathbf{P})\cdot(p_1p_2)^{-1}\,e^{-(p_1z_1+p_2z_2)}\Big[1+\sum_{v\neq 1}I_v(\mathbf{p}_1,z_1;\mathbf{p}_2,z_2)\Big] \tag{A.2}$$

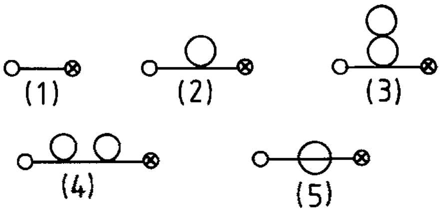

Fig. 5. Graphs of $G^{(1,1;0)}$ to two-loop order. The crossed circle indicates a surface point, the other external point is off the surface

Here i and $v=2,3,\hat{3},\dots,11$ label the graphs in Figs. 5 and 3 such that the terms that involve J_i or I_v represent the contributions from the graphs i or v. We express the J_i's and I_v's in terms of $\mathring{u}=\mu^{-\varepsilon}2^{-d}\pi^{-d/2}g$, Euler's constant $C_E=0.5772\dots$, and the functions

$$\mathscr{A}(\mathbf{p},z)=2-C_E-2\,\mathrm{Ei}(-2pz)\,\mathrm{e}^{2pz}-\ln(2p)^2 \tag{A.3}$$

$$\mathscr{B}(\mathbf{p}_1,z_1;\mathbf{p}_2,z_2)=p_1\,p_2\,e^{(p_1z_1+p_2z_2)}\cdot\int_0^\infty dz\,z_+^{-1}\,G_N(\mathbf{p}_1;z_1,z)\,G_N(\mathbf{p}_2;z_2,z)\,\mathrm{e}^{-Pz} \tag{A.4}$$

where Ei is the exponential-integral function in the notation of Ref. (27) and $P=|-\mathbf{p}_1-\mathbf{p}_2|$. The integral in (A.4) involves the distribution $z_+^{-1}=\lim_{\varepsilon\to 0}\left(z^{-1+\varepsilon}-\frac{1}{\varepsilon}\delta(z)\right)$ defined in Ref. 26.

Our results are:

$$J_2=\mathring{u}\frac{n+2}{3}\{\tfrac{1}{2}\varepsilon^{-1}+\tfrac{1}{4}\mathscr{A}+O(\varepsilon)\} \tag{A.5}$$

$$J_3=\mathring{u}^2\left(\frac{n+2}{3}\right)^2\{\tfrac{1}{8}\varepsilon^{-2}+\tfrac{1}{8}\varepsilon^{-1}(\mathscr{A}-1)+O(\varepsilon^0)\} \tag{A.6}$$

$$J_4=\mathring{u}^2\left(\frac{n+2}{3}\right)^2\{-\tfrac{1}{4}\varepsilon^{-2}+\tfrac{1}{8}\varepsilon^{-1}(1-2\mathscr{A})+O(\varepsilon^0)\} \tag{A.7}$$

$$J_5=\mathring{u}^2\frac{n+2}{3}\{-\tfrac{1}{2}\varepsilon^{-2}-\tfrac{1}{2}\varepsilon^{-1}(\mathscr{A}+\tfrac{7}{6})+O(\varepsilon^0)\} \tag{A.8}$$

$$I_2=-\mathring{u}\frac{n+2}{3}\{2\varepsilon^{-1}+2+C_E+2\mathscr{B}+O(\varepsilon)\} \tag{A.9}$$

$$I_{j+1}=J_j(p_1,z_1),\quad j=2,3,4,5 \tag{A.10}$$

$$I_7=\mathring{u}^2\left(\frac{n+2}{3}\right)^2\{-\tfrac{1}{2}\varepsilon^{-2}-\tfrac{1}{2}\mathscr{A}(\mathbf{p}_1,z_1)\,\varepsilon^{-1}+O(\varepsilon^0)\} \tag{A.11}$$

$$I_8=J_2(\mathbf{p}_1,z_1)\,J_2(\mathbf{p}_2,z_2) \tag{A.12}$$

$$I_9=\mathring{u}^2\left(\frac{n+2}{3}\right)^2\{3\varepsilon^{-2}+(7+3C_E+6\mathscr{B})\,\varepsilon^{-1}+O(\varepsilon^0)\} \tag{A.13}$$

$$I_{10}=\mathring{u}^2\left(\frac{n+2}{3}\right)^2\{-\varepsilon^{-2}-(3+C_E+2\mathscr{B})\,\varepsilon^{-1}+O(\varepsilon^0)\} \tag{A.14}$$

$$I_{11}=\mathring{u}^2\frac{n+2}{3}\left\{2\varepsilon^{-2}+\left(5+2C_E+\frac{\pi^2}{3}+4\mathscr{B}\right)\varepsilon^{-1}+O(\varepsilon^0)\right\} \tag{A.15}$$

and

$$I_v(\mathbf{p}_1,z_1;\mathbf{p}_2,z_2)=I_v(\mathbf{p}_2,z_2;\mathbf{p}_1,z_1) \tag{A.16}$$

Using these results in conjunction with the results for Z_ϕ and Z_u given in I one easily verifies that

$G_{\mathscr{R}}^{(1,1;0)}$ and $G_{\mathscr{R}}^{(2,0;1)}$ as defined in (34) are renormalized to two-loop order.

B. Some Technical Details

The technical problems that had to be overcome to obtain some of the results presented above were considerable. As a rule of thumb one can say that a l-loop calculation for a semi-infinite system is (at least) as difficult as a $l+1$-loop calculation for the corresponding translationally invariant system. To understand this consider any graph of $G^{(2,0;1)}$. Since z and z' are both positive we can amputate the free Neumann propagator at either end. The remaining amputated graph then is a *distribution* in z and z' whose ε-expansion must be determined. In some cases the amputated graphs can be evaluated in closed form and one obtains simple power distributions $z^{-m+\varepsilon}$ $(m=1, 2, \ldots)$ whose ε-expansion is well-known [26]:

$$z^{-m+\varepsilon}=\frac{(-1)^{m-1}}{(m-1)!}\varepsilon^{-1}\delta^{(m-1)}(z)+z_{+}^{-m}+O(\varepsilon) \tag{B.1}$$

Here $\delta^{(m-1)}(z)$ is the $(m-1)^{\text{th}}$ derivative of the δ-function $\delta(z)$, and the distribution z_{+}^{-m} is defined in [26]. In general, however, we know of no systematic way to evaluate the ε-expansion of these distributions other than to apply them to test functions. As compared to the calculation of translationally invariant graphs this adds at least one more integration (apart from the fact that the amputated graphs themselves are more difficult to calculate).
For illustrative purposes we will sketch the calculation of two graphs, namely the graphs (2) of Fig. 5 and (11) of Fig. 3. The former involves a closed loop, giving

$$G_N(\mathbf{x},\mathbf{x})=\sigma_d\Gamma\left(1-\frac{\varepsilon}{2}\right)z^{-2+\varepsilon}. \tag{B.2}$$

Here $\mathbf{x}=(\mathbf{r}, z)$, $\sigma_d=2^{-d}\pi^{-d/2}$, and we have set $\mu=1$. Use of (B.1) in (B.2) would readily yield the pole term of J_2 given in (A.5) upon integration. But since we also need the $O(\varepsilon^0)$ term it is more convenient to calculate directly

$$\int_0^\infty dz'\,\tilde{G}_N(\mathbf{p}; z, z')\,\tilde{G}_N(\mathbf{p}; z', 0)\,G_N(\mathbf{x}', \mathbf{x}')$$
$$=\sigma_d\frac{\Gamma\left(1-\frac{\varepsilon}{2}\right)}{4p^2}e^{-pz}\left\{\frac{z^{-1+\varepsilon}}{\varepsilon-1}+(2p)^{1-\varepsilon}\right.$$
$$\left.\cdot\left[e^{2pz}\Gamma(\varepsilon-1, 2pz)+\Gamma(\varepsilon-1)\right]\right\}. \tag{B.3}$$

The incomplete Γ-function has the ε-expansion*

$$\Gamma(\varepsilon-1, 2pz)=\mathrm{Ei}(-2pz)+(2pz)^{-1}e^{-2pz}+O(\varepsilon) \tag{B.4}$$

From these results (A.5) follows in a straightforward way.
To calculate graph (11) of Fig. 3 we amputate the two external Neumann lines and divide by $g^2(n+2)/3$. For simplicity, we also set P, the momentum of the inserted operator $[\phi^2]_{\mathbf{p}}$, equal to zero. We are then left with the calculation of

$$I(\mathbf{p}_1; z, z')=\int_{\mathbf{p}} h(\mathbf{p}; z, z')\,\tilde{G}_N(\mathbf{p}_1-\mathbf{p}; 0, z)$$
$$\cdot\tilde{G}_N(\mathbf{p}_1-\mathbf{p}; 0, z') \tag{B.5}$$

in which

$$h(\mathbf{p}; z, z')=\int d^{d-1}r\exp(-i\,\mathbf{p}\cdot\mathbf{r})\,G_N^2((\mathbf{r}, z), (0, z')) \tag{B.6}$$

is the parallel Fourier transform $[G_N^2]_{\mathbf{p}}$ of G_N^2. We split G_N into its bulk and surface parts: $G_N=G_{\mathscr{b}}+G_{\mathscr{s}}$. Upon insertion into (B.6), h then becomes

$$h=h_{\mathscr{b}\mathscr{b}}+2h_{\mathscr{b}\mathscr{s}}+h_{\mathscr{s}\mathscr{s}} \tag{B.7}$$

with $h_{\mathscr{b}\mathscr{b}}=[G_b^2]_{\mathbf{p}}$, $h_{\mathscr{b}\mathscr{s}}=[G_{\mathscr{b}}G_{\mathscr{s}}]_{\mathbf{p}}$ etc. A straightforward calculation gives

$$h_{\mathscr{b}\mathscr{b}}(\mathbf{p}; z, z')=C_\varepsilon\,\mathrm{B}\left(1-\frac{\varepsilon}{2}, 1-\frac{\varepsilon}{2}\right)[p/|z-z'|]^{(1-\varepsilon)/2}$$
$$K_{\frac{1-\varepsilon}{2}}(p|z-z'|) \tag{B.8}$$

$$h_{\mathscr{s}\mathscr{s}}(\mathbf{p}; z, z')=h_{\mathscr{b}\mathscr{b}}(\mathbf{p}; z, -z') \tag{B.9}$$

$$h_{\mathscr{b}\mathscr{s}}(\mathbf{p}; z, z')=C_\varepsilon\,p^{(1-\varepsilon)/2}$$
$$\cdot\int_0^1 d\alpha[\alpha(1-\alpha)]^{-\varepsilon/2}[(z+z')^2-4\alpha zz']^{(\varepsilon-1)/4}$$
$$\cdot K_{\frac{1-\varepsilon}{2}}(p[z^2+2(1-2\alpha)zz'+z'^2]^{1/2}) \tag{B.10}$$

with

$$C_\varepsilon=2^{(\varepsilon-7)/2}\pi^{(\varepsilon-5)/2} \tag{B.11}$$

B and $\mathrm{K}_{(1-\varepsilon)/2}$ denote the beta function [27] and a modified Bessel function, respectively. In the derivation of (B.11) Feynman's well-known method for folding two denominators into one has been used.

Substitution of (B.7) into (B.5) implies a similar decomposition for $\mathrm{I}(\mathbf{p}_1; z, z')$:

$$I=I_{\mathscr{b}\mathscr{b}}+2I_{\mathscr{b}\mathscr{s}}+I_{\mathscr{s}\mathscr{s}}. \tag{B.12}$$

---

* Note that $z>0$ and that all terms on the right-hand side of Eq. (B.3) are treated as ordinary functions here. In the distribution sense $\Gamma(\varepsilon-1, 2pz)$ has a pole term $\varepsilon^{-1}\delta(2pz)$

The pole terms of the distributions $I_{\mathscr{E}\mathscr{E}}$, $I_{\mathscr{E}\mathscr{O}}$ are independent of $\mathbf{p}_1$. We therefore set $\mathbf{p}_1=\mathbf{0}$. The $\mathbf{p}$-integrations can then be carried out and one obtains

$$I_{\mathscr{E}\mathscr{E}}(\mathbf{p}_1=\mathbf{0}; z, z')=D_\varepsilon \mathrm{B}\left(1-\frac{\varepsilon}{2}, 1-\frac{\varepsilon}{2}\right) f(z, z') \tag{B.13}$$

with

$$D_\varepsilon=2^\varepsilon \pi^{1/2} \frac{\Gamma(1-\varepsilon)\,\Gamma(2-2\varepsilon)}{\Gamma\left(\frac{3-\varepsilon}{2}\right)\Gamma\left(2-\frac{3\varepsilon}{2}\right)} \tag{B.14}$$

and

$$f(z, z')=z_{\max}^{-2+2\varepsilon}\,{}_2F_1\left(2-2\varepsilon, 1-\frac{\varepsilon}{2}; 2-3\frac{\varepsilon}{2}; z_{\min}/z_{\max}\right) \tag{B.15}$$

Here ${}_2F_1$ is a hypergeometric function [27] and $z_{\min}, z_{\max}$ denote the minimum or maximum value of z and z'. Similarly, one finds

$$I_{\mathscr{O}\mathscr{O}}(\mathbf{0}; z, z')=D_\varepsilon(z+z')^{-2+2\varepsilon} \tag{B.16}$$

and

$$I_{\mathscr{E}\mathscr{O}}(\mathbf{0}; z, z')=2^{2-2\varepsilon} D_\varepsilon(z^2+z'^2)^{-1+\varepsilon}\, Y_\varepsilon(z'/z) \tag{B.17}$$

with

$$Y_\varepsilon(\psi)=[1+2\psi/(1+\psi^2)]^{-1+\varepsilon}\int_0^1 d\alpha\{[\alpha(1-\alpha)]^{-\varepsilon/2}$$
$$\cdot(1+w)^{-2+2\varepsilon}\,{}_2F_1\left(2-2\varepsilon, 1-\frac{\varepsilon}{2}; 2-\frac{3\varepsilon}{2}; \frac{1-w}{1+w}\right) \tag{B.18}$$

where

$$w:=1-4\alpha\psi/(1-\psi)^2 \tag{B.19}$$

and $\psi=z'/z$. Equation (B.15) has the ε-expansion

$$f(z, z')=(\varepsilon^{-2}+\tfrac{1}{2}\varepsilon^{-1})\,\delta(z)\,\delta(z')$$
$$+2\varepsilon^{-1} z_+^{-1}\,\delta(z-z')+O(\varepsilon^0) \tag{B.20}$$

To obtain this result one first shows that the pole terms of f have the form $a_1\,\delta(z)\,\delta(z')+a_2 z_+^{-1}\,\delta(z-z')$. The coefficients a_1 and a_2 can then be determined by integrating (B.15) over the square $0\leqq z\leqq \Delta$, $0\leqq z'\leqq \Delta$.

The ε-expansion of $I_{\mathscr{O}\mathscr{O}}$ is easy and needs no explanation. It reads

$$I_{\mathscr{O}\mathscr{O}}(\mathbf{p}_1; z, z')=\varepsilon^{-1}\,\delta(z)\,\delta(z')+O(\varepsilon^0) \tag{B.21}$$

$I_{\mathscr{E}\mathscr{O}}$ has a pole term $\propto\varepsilon^{-1}\,\delta(z)\,\delta(z')$. To obtain its strength we integrate over the region $\mathscr{R}:=\{(z^2+z'^2)^{1/2}\leqq R_0;\ z\geqq 0,\ z'\geqq 0\}$.

This gives

$$\int_{\mathscr{R}} dz\,dz'\,I_{\mathscr{E}\mathscr{O}}/(2^{2-2\varepsilon} D_\varepsilon)$$
$$=(2\varepsilon)^{-1}\int_0^\infty d\psi\; Y_{\varepsilon=0}(\psi)/(1+\psi^2)+O(\varepsilon^0) \tag{B.21}$$

A lengthy but straightforward calculations gives

$$\int_0^\infty d\psi\; Y_0(\psi)/(1+\psi^2)=\int_0^1 dx(2x)^{-1}\ln(1+x)=\frac{\pi^2}{24} \tag{B.22}$$

Using (B.14, 21) and (B.22) one arrives at

$$I_{\mathscr{E}\mathscr{O}}(\mathbf{p}_1; z, z')=\varepsilon^{-1}(\pi^2/6)\,\delta(z)\,\delta(z')+O(\varepsilon^0) \tag{B.23}$$

Equations (B.12–14, 20, 21) and (B.23) then imply the final result

$$I(\mathbf{p}_1; z, z')=[2\varepsilon^{-2}+\varepsilon^{-1}(2C_E+5+\pi^2/3)]\,\delta(z)\,\delta(z')$$
$$+4\varepsilon^{-1} z_+^{-1}\,\delta(z-z')+O(\varepsilon^0) \tag{B.24}$$

which is consistent with (A.2, 4) and (A.15).

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