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Boundary critical behaviour at m-axial Lifshitz points of semi-infinite systems with a surface plane perpendicular to a modulation axis

H W Diehl[1,2], **M A Shpot**[1,3] **and P V Prudnikov**[1,4]

[1] Fachbereich Physik, Universität Duisburg – Essen, Campus Essen, D-45117 Essen, Germany
[2] Department of Physics and Center for Stochastic Processes in Science and Engineering, Virginia Tech, Blacksburg, VA 24061-0435, USA
[3] Institute for Condensed Matter Physics, 79011 Lviv, Ukraine
[4] Department of Theoretical Physics, Omsk State University, Mira Prospect 55-A, Omsk, 644077, Russia

E-mail: shpot@ph.icmp.lviv.ua

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Abstract

Semi-infinite d-dimensional systems with an m-axial bulk Lifshitz point are considered whose $(d-1)$-dimensional surface hyper-plane is oriented perpendicular to one of the m modulation axes. An n-component ϕ^4 field theory describing the bulk and boundary critical behaviour when (a) the Hamiltonian can be taken to have $O(n)$ symmetry and (b) spatial anisotropies breaking its Euclidean symmetry in the m-dimensional coordinate subspace of potential modulation directions may be ignored is investigated. The long-distance behaviour at the ordinary surface transition is mapped onto a field theory with the boundary conditions that both the order parameter ϕ and its normal derivative $\partial_n\phi$ vanish at the surface plane. The boundary-operator expansion is utilized to study the short-distance behaviour of ϕ near the surface. Its leading contribution is found to be controlled by the boundary operator $\partial_n^2\phi$. The field theory is renormalized for dimensions d below the upper critical dimension $d^*(m) = 4 + m/2$, with a corresponding surface source term $\propto \partial_n^2\phi$ added. The anomalous dimension of this boundary operator is computed to first order in $\epsilon = d^* - d$. The result is used in conjunction with scaling laws to estimate the value of the single independent surface critical exponent $\beta_{L1}^{(\mathrm{ord},\perp)}$ for $d = 3$. Our estimate for the case $m = n = 1$ of a uniaxial Lifshitz point in Ising systems is in reasonable agreement with the published Monte Carlo results.

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1. Introduction

The significance of the n-component ϕ^4 models with $O(n)$ symmetric Hamiltonian derives from the fact that they represent the most common—and probably also most important—universality classes of critical behaviour at bulk critical points of d-dimensional systems with short-range interactions. Prominent examples of such universality classes for given d and $n = 1, 2$ and 3 are those of the Ising, XY and isotropic Heisenberg models, respectively.

When such systems are bounded by free $(d-1)$-dimensional hyper-surfaces or walls, a wealth of distinct boundary critical phenomena can occur [1–4]. A well-studied case is that of the systems with a free surface that can be described by a semi-infinite n-component ϕ^4 model. The Hamiltonian of the latter is of the form

$$\mathcal{H} = \int_{\mathfrak{V}} \mathcal{L}_{\mathrm{b}}(\boldsymbol{x})\,\mathrm{d}V + \int_{\mathfrak{B}} \mathcal{L}_1(\boldsymbol{r})\,\mathrm{d}A, \tag{1}$$

where $\int_{\mathfrak{V}}$ and $\int_{\mathfrak{B}}$ mean volume and surface integrals over the half-space $\mathfrak{V} = \mathbb{R}^d_+ \equiv \{\boldsymbol{x} = (\boldsymbol{r}, z) | \boldsymbol{r} \in \mathbb{R}^{d-1}, 0 \leqslant z < \infty\}$ and the $z = 0$ boundary hyperplane $\mathfrak{B}$, respectively. Provided neither bulk nor surface terms breaking the $O(n)$ symmetry must be included, the bulk and surface densities are given by

$$\mathcal{L}_b = \frac{1}{2}(\nabla\phi)^2 + \frac{\mathring{\tau}}{2}\phi^2 + \frac{\mathring{u}}{4!}|\phi|^4 \tag{2}$$

and

$$\mathcal{L}_1 = \frac{\mathring{c}}{2}\phi^2. \tag{3}$$

Furthermore, one can distinguish three different types of surface transitions that take place at the bulk critical temperature T_c [1, 2]: they are called ordinary, special and extraordinary surface transitions and occur, depending on whether $\mathring{c}$ is larger than, equal to or smaller than a certain critical value $\mathring{c}_{\mathrm{sp}}$.

The extraordinary transition is a transition from a surface-ordered, bulk-disordered high-temperature phase to a low-temperature phase with long-range order both at the surface and in the bulk. It—and hence also the special transition—can occur only for those choices of d and n for which fluctuations do not destroy long-range order at the surface at all nonzero temperatures T. This requires $d - 1 > 1$ in the scalar case $n = 1$, and $d - 1 > 2$ in the continuous-symmetry case $n > 1$.

Suppose n and d are such that all three of these transitions can occur. Then the critical behaviour that surface quantities exhibit at any of these is representative of a separate surface universality class, although their bulk critical behaviour is the same. Thus the bulk universality class associated with this choice of n and d splits into three distinct surface universality classes.

In this paper, we shall be concerned with the surface critical behaviour of n-vector systems at m-axial bulk Lifshitz points. A Lifshitz point (LP) is a multicritical point at which a disordered, a homogeneous ordered and a modulated ordered phase meet [5–7]. A family of natural extensions of the bulk models defined on $\mathbb{R}^d$ by the bulk density (2) that have such LPs was introduced decades ago [8, 9], but investigated in greater detail via field-theoretic renormalization group (RG) only in the past few years (see [10–13] and references therein). Their bulk density is given by

$$\mathcal{L}_{\mathrm{b}}(\boldsymbol{x}) = \frac{\mathring{\sigma}}{2}\left(\sum_{\alpha=1}^{m}\partial_\alpha^2\phi\right)^2 + \frac{1}{2}\sum_{\beta=m+1}^{d}(\partial_\beta\phi)^2 + \frac{\mathring{u}}{4!}|\phi|^4 + \frac{\mathring{\rho}}{2}\sum_{\alpha=1}^{m}(\partial_\alpha\phi)^2 + \frac{\mathring{\tau}}{2}\phi^2, \tag{4}$$

where the position vector $\boldsymbol{x}$ has the representation $(x_\gamma) = (x_\alpha, x_\beta)$ in Euclidean coordinates x_γ. We use the convention that α and β denote coordinate indices γ with $1 \leqslant \alpha \leqslant m$ and

$m < \beta \leqslant d$, respectively. Likewise, ∂_α and ∂_β mean the corresponding spatial derivatives $\partial_\gamma = \partial/\partial x_\gamma$. At the level of Landau theory, the model has a continuous transition from a disordered to a homogeneous ordered phase for $\mathring{\rho} > 0$ at $\mathring{\tau} = 0$. For negative $\mathring{\rho}$, a continuous transition to a modulated ordered phase occurs at a nonzero value of $\mathring{\tau}$. The transition lines between these phases merge at $\mathring{\tau} = \mathring{\rho} = 0$, which is an m-axial LP within Landau theory.

At LPs, systems exhibit scale invariance of the *strong anisotropic kind*: coordinate difference Δx_α within the α-subspace scale as a nontrivial power $(\Delta x_\beta)^\theta$ of the complementary ones Δx_β, where θ, the anisotropy exponent, generally differs from 1, and in Landau theory has the mean-field value $\theta^{\mathrm{MF}} = 1/2$.

Owing to this anisotropic scale invariance, boundary critical phenomena at LPs are richer than at critical points (CPs). For example, in the CP case, the orientation of the surface relative to the coordinate axes does not play any important role on the level of a description in terms of a ϕ^4 field theory. However, for systems at LPs the surface's orientation matters in an essential way, just as it does quite generally for systems with anisotropic scale invariance: two fundamentally distinct orientations can be distinguished—one for which all α-directions are parallel to the surface (which we shall refer to as parallel) and another one for which the surface normal $\boldsymbol{n}$ is along one of the m α-directions (which we shall refer to as perpendicular).

As a consequence of the different scaling behaviour of distances along the α- and β-directions, it depends on whether the orientation of the surface is parallel or perpendicular which boundary contributions $\mathcal{L}_1$ are potentially infrared relevant below the upper critical dimension $d^*(m) = 4 + m/2$ and hence must be included in the action. The problem of constructing semi-infinite extensions of the models with bulk density (4) for $d = d^*(m) - \epsilon$ that are '*minimal*' in the sense that all irrelevant and marginal boundary contributions not compatible with the presumed $O(n)$ and Euclidean[5] symmetries are discarded was considered for the case of parallel surface orientation in [15, 16], where it was found that a contribution $\propto \sum_\alpha (\partial_\alpha \phi)^2$ had to be included in the corresponding surface density $\mathcal{L}_1 \equiv \mathcal{L}_1^{\parallel}$, in addition to the one in equation (3). The so obtained semi-infinite model, defined by equation (4) in conjunction with the boundary density

$$\mathcal{L}_1^{\parallel} = \frac{\mathring{c}}{2}\phi^2 + \frac{\mathring{\lambda}}{2}\sum_{\alpha=1}^{m}(\partial_\alpha\phi)^2, \tag{5}$$

was then utilized in [16, 17] to determine the ϵ expansion of the surface critical exponents of the corresponding ordinary and special transitions to second and first order, respectively. This extends or complements the previous work based on the mean-field approximation [18] and Monte Carlo simulations for the axial-next-nearest-neighbour Ising (ANNNI) model [19].

The model is a natural and simple-looking generalization of the semi-infinite n-vector model defined by equations (2) and (3), to which it reduces when $m = 0$. The following fluctuating boundary conditions [2, 3] one obtains for it:

$$\partial_n \phi = (\mathring{c} - \mathring{\lambda}\partial_\alpha\partial_\alpha)\phi, \tag{6}$$

where ∂_n $(=\partial_z)$ is the derivative along the inward normal $\boldsymbol{n}$, are of the Robin type, generalizing the familiar ones of the CP ($m = 0$) case to nonzero values of $\mathring{\lambda}$.[6] As shown in [16, 17], the new boundary term $\propto \mathring{\lambda}$ has the effect of moving the fixed points onto which the ordinary, special

[5] We presume that the bulk and the boundary contributions breaking the rotational invariance in the α-subspace may be ignored. When $m > 1$, spatial anisotropies lead, in particular, to nonisotropic bulk contributions of the form $T_{\alpha_1\alpha_2\alpha_3\alpha_4}(\partial_{\alpha_1}\partial_{\alpha_2}\phi)\cdot\partial_{\alpha_3}\partial_{\alpha_4}\phi$, where $T_{\alpha_1\alpha_2\alpha_3\alpha_4}$ is a tensor whose symmetry is that of an m-cube or lower. The $O(\epsilon^2)$ results of [14] for the bulk model indicate that such terms are relevant in the infrared for $\epsilon > 0$.

[6] Here and below we utilize the summation convention that pairs of the same α- and β-indices are to be summed from $\alpha = 1$ to m and $\beta = m + 1$ to d, respectively.

and extraordinary transitions are mapped to a nontrivial value $\lambda^* = O(\epsilon^0)$ of the renormalized counterpart λ of $\mathring{\lambda}$.

In the following we shall consider the case of *perpendicular* surface orientation. Previous work on it either was restricted to an investigation of the corresponding ordinary transition of the semi-infinite ANNNI model on the level of the mean-field approximation [20, 21], or else employed Monte Carlo simulations to study both the ordinary and special transitions of this model [19].

Our aim is to construct and analyse an appropriate minimal semi-infinite model for general values of n, m and d. This turns out to be a greater challenge and more interesting than in the case of parallel surface orientation. Since the classical equation of motion of the order-parameter profile now involves a differential equation of fourth order in ∂_z, two, rather than one, boundary conditions are required (aside from two analogous ones at $z = \infty$). Furthermore, being an x_α coordinate, $z \equiv x_m$ now scales naively as $\mu^{-1/2}$, where μ is an arbitrary momentum unit making μx_β dimensionless. Compared to the case of parallel surface orientation (where $z \sim \mu^{-1}$), power counting gives more potentially relevant or marginal surface terms. Recently, one of us has suggested an appropriate surface density $\mathcal{L}_1^{\perp}$ and the associated boundary conditions [22]. In section 2, we recall this density and derive the fluctuating boundary conditions it implies. Using the latter, we show that the existing additional surface contributions that are compatible with symmetry and short-rangedness of interactions, and not irrelevant according to power counting, are redundant.

In section 3 we determine the free propagator subject to these boundary conditions, at the LP for general values of the surface interaction constants. Owing to its rather complicated form, explicit perturbative RG calculation for dimensions $d = d^*(m) - \epsilon$ are difficult to perform with it. In section 4 we show, following a suggestion made in [22], how this problem can be by-passed to some extent in the case of the ordinary transition. The asymptotic large-scale behaviour at this transition can be argued to be described by a theory with boundary conditions,

$$\phi = \partial_n \phi = 0. \tag{7}$$

Hence, one can work with the corresponding simplified free propagator at the price of having to deal with correlation functions involving, besides the field ϕ, also the boundary operator $\partial_n^2 \phi$. From the anomalous dimension of the latter the required single independent surface critical exponent $\beta_{\mathrm{L1}}^{(\mathrm{ord},\perp)}$ of this transition can be inferred. Performing a one-loop RG analysis, we compute in section 5 the ϵ expansion of this exponent to $O(\epsilon)$ for general values of m. The result is used to estimate its value for the case $m = n = 1$ of the three-dimensional semi-infinite ANNNI model. Section 6 contains concluding remarks. Finally, there is an appendix explaining how the required one-loop integral was calculated.

While it is quite common to investigate field theories with Dirichlet boundary conditions (see [2, 3, 23, 24] and references therein), we are not aware of previous studies of field theories satisfying the boundary conditions (7), barring familiar examples of hydrodynamic equations for fluids [25]. It is therefore not unlikely that the work described below might also be of interest for other problems.

2. Boundary density and fluctuating boundary conditions

The boundary density suggested in [22] is

$$\mathcal{L}_1^{\perp} = \frac{\mathring{c}_\perp}{2}\phi^2 + \mathring{b}\phi\partial_n\phi + \sum_{\alpha=1}^{m-1}\left[\frac{\mathring{\lambda}_\parallel}{2}(\partial_\alpha\phi)^2 + \mathring{f}(\partial_\alpha\phi)\partial_n\partial_\alpha\phi\right] + \frac{\mathring{\lambda}_\perp}{2}(\partial_n\phi)^2 \tag{8}$$

with $\mathring{f} = 0$. We have added the term $\propto \mathring{f}$ since it cannot be ruled out. Contributions breaking the symmetry among the $m-1$ α-directions parallel to the surface have been excluded. That different values should be allowed for the coupling constants $\mathring{\lambda}_\perp$ and $\mathring{\lambda}_\parallel$ should be obvious because the surface breaks the symmetry between α-directions parallel to it and the z-direction. Besides the monomials included in equation (8), there are a number of other surface operators one has to worry about, namely

$$\mathcal{O}_1 = \phi\partial_n^2\phi, \quad \mathcal{O}_2 = (\partial_n\phi)\partial_n^2\phi, \quad \mathcal{O}_3 = \phi\partial_n^3\phi. \tag{9}$$

Before discussing these, let us first derive the fluctuating boundary conditions that apply to the model defined by equations (1), (4) and (8).

To this end, we compute the variation $\delta\mathcal{H}$ of the Hamiltonian. By integrations by parts, one gets

$$\begin{aligned}\delta\mathcal{H} = \int_{\mathfrak{V}} \delta\phi \left\{\frac{\partial\mathcal{L}_b}{\partial\phi} + \sum_{\alpha=1}^{m}\partial_\alpha^2\frac{\partial\mathcal{L}_b}{\partial\left(\partial_\alpha^2\phi\right)} - \sum_{\gamma=1}^{d}\partial_\gamma\frac{\partial\mathcal{L}_b}{\partial(\partial_\gamma\phi)}\right\}\\ + \int_{\mathfrak{B}}\delta\phi\left[\frac{\partial\mathcal{L}_1^\perp}{\partial\phi} - \frac{\partial\mathcal{L}_b}{\partial(\partial_n\phi)} + \partial_n\frac{\partial\mathcal{L}_b}{\partial\left(\partial_n^2\phi\right)} - \sum_{\alpha=1}^{m-1}\partial_\alpha\frac{\partial\mathcal{L}_1^\perp}{\partial(\partial_\alpha\phi)}\right]\\ + \int_{\mathfrak{B}}(\partial_n\delta\phi)\left[\frac{\partial\mathcal{L}_1^\perp}{\partial(\partial_n\phi)} - \frac{\partial\mathcal{L}_b}{\partial\left(\partial_n^2\phi\right)} - \sum_{\alpha=1}^{m-1}\partial_\alpha\frac{\partial\mathcal{L}_1^\perp}{\partial(\partial_n\partial_\alpha\phi)}\right].\end{aligned} \tag{10}$$

Equating the expression in curly brackets to zero gives us the classical field equation

$$\left[\mathring{\sigma}(\partial_\alpha\partial_\alpha)^2 - \mathring{\rho}\partial_\alpha\partial_\alpha - \partial_\beta\partial_\beta + \mathring{\tau} + \frac{\mathring{u}}{6}\phi^2\right]\phi = \mathbf{0}. \tag{11}$$

Doing the same with the expressions in square brackets of the surface integrals $\int_{\mathfrak{B}}\delta\phi[\cdots]$ and $\int_{\mathfrak{B}}\delta\partial_n\phi[\cdots]$ yields the boundary conditions

$$\left\{\mathring{\sigma}\partial_n^3 + (\mathring{b} - \mathring{\rho})\partial_n + \mathring{c}_\perp - [\mathring{\lambda}_\parallel + (\mathring{f} - \mathring{\sigma})\partial_n]\sum_{\alpha=1}^{m-1}\partial_\alpha^2\right\}\phi = 0 \tag{12}$$

and

$$\left\{-\mathring{\sigma}\partial_n^2 + \mathring{\lambda}_\perp\partial_n + \mathring{b} - (\mathring{f} + \mathring{\sigma})\sum_{\alpha=1}^{m-1}\partial_\alpha^2\right\}\phi = 0, \tag{13}$$

respectively.

These boundary conditions hold in Landau theory. Yet, they remain valid inside of averages, for the same reason that the classical equation (11) does so. To show this, one can make a shift $\phi \to \phi + \mathbf{\Phi}$ in the functional integral defining the generating functional $\mathcal{Z}[\boldsymbol{J}] \propto \int\mathcal{D}\phi\exp\left(-\mathcal{H} + \int_{\mathfrak{V}}\boldsymbol{J}\cdot\phi\right)$ of multi-point correlation functions $\langle\phi\cdots\phi\rangle$. For a $\mathbf{\Phi}$ independent of ϕ, the functional measure ϕ does not change, and one arrives at the equation

$$\left\langle\delta\mathcal{H} - \int_{\mathfrak{V}}\boldsymbol{J}\cdot\mathbf{\Phi}\right\rangle_{\boldsymbol{J}} = 0, \tag{14}$$

where $\mathbf{\Phi}$ must be substituted for $\delta\phi$ in $\delta\mathcal{H}$. Here $\langle\cdot\rangle_{\boldsymbol{J}}$ indicates a normalized average in the presence of the source $\boldsymbol{J}$, i.e. with the weight $\exp\left(-\mathcal{H} + \int_{\mathfrak{V}}\boldsymbol{J}\cdot\phi\right)$. From the result (14) the validity of equations (11)–(13) inside of averages can be derived in a well-known fashion by setting the source to zero, either directly or after taking functional derivatives with respect to it, and exploiting the arbitrariness of $\mathbf{\Phi}$ at and away from the boundary. As usual, the source term yields extra contributions located at coinciding points to correlation functions generated by functional differentiation of equation (14). Corresponding fluctuation corrections would result from additional surface source terms such as $\int_{\mathfrak{B}} \boldsymbol{J}_1 \cdot \boldsymbol{\phi}$.

It is now easy to understand why the surface operators given in equation (9) do not have to be included in the Hamiltonian: these monomials involve $\partial_n^2\phi$ and $\partial_n^3\phi$. We can solve the boundary conditions (13) and (12) for these operators and substitute the solutions into the monomials. The expressions that result for the surface operators $\mathcal{O}_1$, $\mathcal{O}_2$ and $\mathcal{O}_3$ are linear combinations of the surface operators retained in the surface density (8).[7] Thus, the effect of the boundary operators $\mathcal{O}_1$, $\mathcal{O}_2$ and $\mathcal{O}_3$ can be absorbed by a redefinition of the surface variables of the surface density (8). That is, they are redundant and may be discarded.

3. Free propagator at the Lifshitz point

We now turn to the calculation of the free propagator $G(\boldsymbol{x}, \boldsymbol{x}')$ at the LP. To this end we split the position vector into components parallel and perpendicular to the surface, writing $\boldsymbol{x} = (\boldsymbol{r}, z)$. We choose z to be x_m. The component $\boldsymbol{r}$ then involves the $m-1$ α-components $(x_1, \ldots, x_{m-1}) \equiv \boldsymbol{r}_<$ and the $d-m$ β-coordinates $(x_\beta) = (x_{m+1}, \ldots, x_d) \equiv \boldsymbol{r}_>$. For the wavevector conjugate to $\boldsymbol{r} = (\boldsymbol{r}_<, \boldsymbol{r}_>)$ we use analogous conventions, writing $\boldsymbol{p} = (\boldsymbol{p}_<, \boldsymbol{p}_>)$.

From equation (11) one easily concludes that the partial Fourier transform $\hat{G}(\boldsymbol{p}; z, z')$, defined by

$$G(\boldsymbol{x}, \boldsymbol{x}') = \int_{\boldsymbol{p}} \hat{G}(\boldsymbol{p}; z, z')\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \qquad \text{with } \int_{\boldsymbol{p}} \equiv \int_{\mathbb{R}^{d-1}} \frac{\mathrm{d}^{d-1}p}{(2\pi)^{d-1}}, \tag{15}$$

obeys the equation

$$\left[\mathring{\sigma}\left(p_<^2 - \partial_z^2\right)^2 + p_>^2 + \mathring{\rho}\left(p_<^2 - \partial_z^2\right) + \mathring{\tau}\right]\hat{G}(\boldsymbol{p}; z, z') = \delta(z - z'), \tag{16}$$

provided the order parameter profile $\langle\boldsymbol{\phi}(\boldsymbol{x})\rangle$ vanishes (as it does in the disordered phase). This equation must be solved subject to the boundary conditions

$$\left\{\mathring{\sigma}\,\partial_z^3 + \left[\mathring{b} + (\mathring{f} - \mathring{\sigma})p_<^2 - \mathring{\rho}\right]\partial_z + \mathring{c}_\perp + \mathring{\lambda}_\parallel p_<^2\right\}\hat{G}(\boldsymbol{p}; z = 0, z') = 0, \tag{17}$$

$$\left[-\mathring{\sigma}\,\partial_z^2 + \mathring{\lambda}_\perp \partial_z + \mathring{b} + (\mathring{f} + \mathring{\sigma})p_<^2\right]\hat{G}(\boldsymbol{p}; z = 0, z') = 0, \tag{18}$$

and the requirement that the correct bulk propagator $\hat{G}_{\mathrm{b}}(\boldsymbol{p}, z - z')$ is obtained as $z, z' \to \infty$ at fixed $z - z'$. Furthermore, in order that the highest derivative, ∂_z^4, produces the δ-function in equation (16), both $\hat{G}(\boldsymbol{p}; z, z')$ and its bulk counterpart must satisfy the jump condition

$$\left[\mathring{\sigma}\,\partial_z^3 \hat{G}(\boldsymbol{p}; z, z')\right]_{z=z'-0}^{z=z'+0} = 1. \tag{19}$$

Further, $\hat{G}(\boldsymbol{p}; z, z')$ must be symmetric under exchange of z and z' because $G(\boldsymbol{x}, \boldsymbol{x}')$ is the inverse of a symmetric integral kernel $A(\boldsymbol{x}, \boldsymbol{x}')$ associated with the Gaussian part $\int_{\mathfrak{V}} \mathrm{d}^d x \int_{\mathfrak{V}} \mathrm{d}^d x' \boldsymbol{\phi}(\boldsymbol{x}) A(\boldsymbol{x}, \boldsymbol{x}')\boldsymbol{\phi}(\boldsymbol{x}')/2$ of the Hamiltonian (including boundary terms).

To simplify our analysis, we restrict ourselves to the LP, setting $\mathring{\rho} = \mathring{\tau} = 0$. It is also convenient to set the variable $\mathring{\sigma}$ (whose renormalized counterpart σ changes under RG transformations) temporarily to unity. The dependence on it can be re-introduced whenever needed by elementary dimensional considerations. For instance, for the free propagator these lead to the relation

$$\hat{G}(\boldsymbol{p}_<, \boldsymbol{p}_>; z, z'|\mathring{\sigma}) = \mathring{\sigma}^{-1/4}\hat{G}(\mathring{\sigma}^{1/4}\boldsymbol{p}_<, \boldsymbol{p}_>; \mathring{\sigma}^{-1/4}z, \mathring{\sigma}^{-1/4}z'|1). \tag{20}$$

[7] In expressions such as $\boldsymbol{\phi} \cdot \sum_{\alpha=1}^{m-1} \partial_\alpha^2 \boldsymbol{\phi}$ and $\partial_n \boldsymbol{\phi} \cdot \sum_{\alpha=1}^{m-1} \partial_\alpha^2 \boldsymbol{\phi}$, the derivatives ∂_α evidently can be made to act as $(-\overleftarrow{\partial}_\alpha)$ to the left, by means of integrations by parts.

The bulk propagator at the LP can be computed in a straightforward fashion. One obtains

$$\hat{G}_{\mathrm{b}}(\boldsymbol{p}, z) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{\mathrm{e}^{\mathrm{i}kz}}{\left(k^2 + p_<^2\right)^2 + p_>^2} \tag{21}$$

$$= \frac{\mathrm{e}^{-\kappa_+|z|}}{4\kappa_+\kappa_-\left(\kappa_+^2 + \kappa_-^2\right)} [\kappa_- \cos(\kappa_-|z|) + \kappa_+ \sin(\kappa_-|z|)], \tag{22}$$

where we have written the roots of the denominator of the required Fourier integral as $\pm\kappa_- \pm \mathrm{i}\kappa_+$, with

$$\kappa_\pm = \tfrac{1}{\sqrt{2}} \sqrt{\sqrt{p_<^4 + p_>^2} \pm p_<^2}. \tag{23}$$

In terms of the linearly independent solutions

$$W_j(\boldsymbol{p}, z) = \begin{cases} \mathrm{e}^{-\kappa_+ z} \cos(\kappa_- z) & \text{for } j = 1, \\ \mathrm{e}^{-\kappa_+ z} \sin(\kappa_- z) & \text{for } j = 2, \\ \mathrm{e}^{\kappa_+ z} \cos(\kappa_- z) & \text{for } j = 3, \\ \mathrm{e}^{\kappa_+ z} \sin(\kappa_- z) & \text{for } j = 4, \end{cases} \tag{24}$$

of the homogeneous counterpart of equation (16) with $\mathring{\rho} = \mathring{\tau} = 0$ and $\mathring{\sigma} = 1$, the free propagator of the semi-infinite system can be expressed as

$$\hat{G}(\boldsymbol{p}; z, z') = \theta(z - z') \sum_{j=1}^{2} W_j(\boldsymbol{p}, z) V_j(\boldsymbol{p}, z') + (z \leftrightarrow z') \tag{25}$$

where

$$V_j(\boldsymbol{p}, z') = \sum_{k=1}^{4} C_{jk} W_k(\boldsymbol{p}, z'). \tag{26}$$

The coefficients C_{jk} are chosen such that $V_{j=1,2}(\boldsymbol{p}, z)$ satisfy the two boundary conditions (17) and (18) with $\mathring{\rho} = 0$ and $\mathring{\sigma} = 1$, that $\hat{G}(\boldsymbol{p}; z, z')$ and its first and second derivatives with respect to z are continuous at $z = z'$, and the jump condition (19) is fulfilled (again with $\mathring{\sigma} = 1$).

It is convenient to split off the known bulk propagator, writing

$$\hat{G}(\boldsymbol{p}; z, z') = \hat{G}_{\mathrm{b}}(\boldsymbol{p}; z, z') + \hat{G}_{\mathrm{s}}(\boldsymbol{p}; z, z'). \tag{27}$$

Here $\hat{G}_{\mathrm{s}}$, the part due to the surface, is (at least) four times differentiable in z and z', and does not contribute to the jump of $\partial_z^3 \hat{G}$ at $z = z'$, which originates entirely from $\hat{G}_{\mathrm{b}}$. Thus, the jump condition (19) is taken care of. We can decompose $\hat{G}_{\mathrm{b}}$ in the same way as we did for $\hat{G}$ in equations (25) and (26), with corresponding coefficients $C_{jk}^{(\mathrm{b})}$. Evidently, only $C_{jj'+2}^{(\mathrm{b})}$ with $j, j' = 1, 2$ are nonzero and can be read off from equation (21), but $C_{jj'}^{(\mathrm{b})} = 0$. Since $\hat{G}_{\mathrm{s}}$ must not have exponentially increasing parts, four of the coefficients C_{jk}, namely $C_{jk} = C_{jk}^{(\mathrm{b})}$ with $k = 3, 4$, follow immediately from our result (21) for $\hat{G}_{\mathrm{b}}$:

$$C_{13} = C_{24} = \frac{1}{4\kappa_+\left(\kappa_+^2 + \kappa_-^2\right)} = -\frac{\kappa_-}{\kappa_+} C_{14} = \frac{\kappa_-}{\kappa_+} C_{23}. \tag{28}$$

The remaining four coefficients must be determined from the two boundary conditions (17) and (18) for V_1 and V_2.

A straightforward calculation yields

$$C_{11} = \frac{C_{13}}{D}\big[B_+ + p_>^2 + 8\kappa_+^4 + L - C\big],$$
$$C_{12} = C_{21} = \frac{C_{23}}{D}\big[B_- - p_>^2 + L - C\big], \tag{29}$$
$$C_{22} = \frac{C_{13}}{\kappa_-^2 D}\big[B_\kappa + p_>^2\kappa_-^2 - \kappa_-^2 L - C_\kappa\big],$$

where we introduced the short-hand notations

$$\begin{aligned} &\mathring{b}_{p_<} \equiv \mathring{b} + \mathring{f}p_<^2, && \mathring{c}_{p_<} \equiv \mathring{c}_\perp + \mathring{\lambda}_\| p_<^2, \\ &B_+ = \mathring{b}_{p_<}\big(\mathring{b}_{p_<} + 4\kappa_+^2\big), && B_- = \mathring{b}_{p_<}\big(\mathring{b}_{p_<} - 4\kappa_-^2\big), \quad B_\kappa = \mathring{b}_{p_<}\big[\mathring{b}_{p_<}\big(\kappa_-^2 + 2\kappa_+^2\big) - p_>^2\big], \\ &C = \mathring{c}_{p_<}\big(\mathring{\lambda}_\perp + 2\kappa_+\big), && C_\kappa = \mathring{c}_{p_<}\big[2\kappa_-^2\kappa_+ - \mathring{\lambda}_\perp\big(\kappa_-^2 + 2\kappa_+^2\big)\big], \\ &L = 2\mathring{\lambda}_\perp\kappa_+\big(\kappa_-^2 + \kappa_+^2\big), && D = -B_+ + p_>^2 + L + C. \end{aligned} \tag{30}$$

The resulting lengthy expression for the free propagator for general values of the surface interaction constants will not be used in the rest of the paper. The explicit form of the free propagator that we shall actually utilize is given in the next section, see equation (35).

4. Asymptotic boundary conditions at the ordinary transition

We now turn to the analysis of the ordinary transition. Let us begin by considering first the simpler case of the ordinary transition at a *critical point* (CP), and recall some essentials of its RG analysis. The critical behaviour at this transition is described by a fixed point at which the Dirichlet boundary condition $\phi|_{z=0} = 0$ holds. One can choose this boundary condition from the outset (already for the bare theory) by setting the interaction constant $\mathring{c}$ of the corresponding surface density (3) to the value $\mathring{c}_{\text{ord}} = \infty$ [2, 3, 26, 27]. To obtain the behaviour of N-point correlation functions involving fields ϕ close to the surface, one can employ the boundary operator expansion (BOE) [2, 3, 27]

$$\phi^{\text{ren}}(\boldsymbol{r}, z) \underset{z\to 0}{\approx} C_{\partial_n\phi}(z)(\partial_n\phi)^{\text{ren}}(\boldsymbol{r}), \tag{31}$$

where ϕ^{ren} and $(\partial_n\phi)^{\text{ren}}$ denote renormalized operators. The required independent surface critical exponent β_1^{ord}, which together with the usual bulk critical indices yields the other surface critical exponents of this CP ordinary transition via scaling laws, can be inferred from the scaling dimension $\Delta[\partial_n\phi] = \beta_1^{\text{ord}}/\nu$ of $\partial_n\phi$ or the behaviour

$$C_{\partial_n\phi}(z) \sim z^{(\beta-\beta_1^{\text{ord}})/\nu} \tag{32}$$

of the coefficient function $C_{\partial_n\phi}$.

This CP ordinary transition must be recovered when $\rho > 0$ for appropriate choices of the surface interaction constants. It is therefore reasonable to expect that the Dirichlet boundary condition will prevail when $\rho \to 0$, i.e. at the fixed point describing the LP ordinary transition. To show this and to find the required second boundary condition, note that the surface variables with the largest μ-dimension are $\mathring{c}_\perp$ and $\mathring{b}$. At the trivial Gaussian fixed point, their dimensionless counterparts $c_\perp \equiv \mu^{-3/2}\mathring{c}_\perp$ and $b \equiv \mu^{-1}\mathring{b}$ transform under scale transformations $\mu \to \mu\ell$ as

$$c_\perp \to \bar{c}_\perp(\ell) = \ell^{-3/2}c_\perp \qquad \text{and} \qquad b \to \bar{b}(\ell) = \ell^{-1}b. \tag{33}$$

Since the ordinary transition corresponds to the case where order is suppressed near the surface, we can take $\mathring{c}_\perp$ to be positive. Thus, $\bar{c}_\perp \to +\infty$ in the large length-scale limit $\ell \to 0$. Further, unless fine-tuned, $\mathring{b}$ is not expected to vanish. Equation (33) tells us that $\bar{b}(\ell)/\bar{c}(\ell)$ approaches zero as $\ell \to 0$. The other coupling constants appearing in the boundary conditions (12), (13), (17) and (18) with $\mathring{\rho} = 0$ have μ-dimensions smaller than both $\mathring{c}_\perp$ and $\mathring{b}$. Hence, the ratio of the associated running variables and either $\bar{c}_\perp$ or $\mathring{b}$ also becomes small as $\ell \to 0$. We conclude that both $\phi|_{z=0}$ and $\partial_n\phi$ must become small in this limit in order for these boundary conditions to hold. In other words, the boundary condition (7) should apply in the large length-scale limit. In the following we exploit this idea by choosing them from the outset for the bare theory.

Let us denote by $\hat{G}_{00}(\boldsymbol{p}; z, z')$ the free propagator that satisfies the boundary conditions

$$\hat{G}_{00}(\boldsymbol{p}; z, z')|_{z=0} = \partial_z \hat{G}_{00}(\boldsymbol{p}; z, z')|_{z=0} = 0. \tag{34}$$

It can be determined in a straightforward manner. One gets

$$\hat{G}_{00}(\boldsymbol{p}; z, z') = \hat{G}_{\mathrm{b}}(\boldsymbol{p}; z - z') - \hat{G}_{\mathrm{b}}(\boldsymbol{p}; z + z') - \frac{\sin(\kappa_- z)\sin(\kappa_- z')}{2\kappa_-^2 \kappa_+}\, \mathrm{e}^{-\kappa_+(z+z')}. \tag{35}$$

Information about correlations near the surface can again be obtained via the BOE. Because of the boundary conditions (7), the leading operator contributing to the BOE of ϕ now is $\partial_n^2\phi$; we have

$$\phi^{\mathrm{ren}}(\boldsymbol{r}, z) \underset{z\to 0}{\approx} C_{\partial_n^2\phi}(z)\big(\partial_n^2\phi\big)^{\mathrm{ren}}(\boldsymbol{r}) \tag{36}$$

instead of equation (31). The renormalized operator will be defined in the next section. Suffice it here to say that its scaling dimension

$$\Delta\big[\partial_n^2\phi\big] = \beta_{\mathrm{L1}}^{(\mathrm{ord},\perp)}\big/\nu_{\mathrm{L2}}, \tag{37}$$

where ν_{L2} is a bulk correlation-length exponent, gives us the surface critical exponent $\beta_{\mathrm{L1}}^{(\mathrm{ord},\perp)}$, and that by analogy with equation (32) we have

$$C_{\partial_n^2\phi}(z) \sim z^{(\beta_{\mathrm{L}} - (\beta_{\mathrm{L1}}^{(\mathrm{ord},\perp)})/(\theta\nu_{\mathrm{L2}})}. \tag{38}$$

5. RG analysis of the ordinary transition

Focusing our attention on the theory with the boundary conditions (7), we introduce the $(N + M)$-point cumulants

$$G^{(N,M)}_{a_1,\ldots,b_M}(\boldsymbol{x}, \boldsymbol{r}) \equiv \left\langle \prod_{i=1}^{N} \phi_{a_i}(\boldsymbol{x}_i) \prod_{j=1}^{M} \partial_n^2 \phi_{b_j}(\boldsymbol{r}_j) \right\rangle^{\mathrm{cum}}. \tag{39}$$

To regularize their ultraviolet (UV) singularities, we employ dimensional regularization. Apart from bulk UV singularities known from studies of bulk critical behaviour [12–14], they have (primitive) UV surface singularities originating from the surface part of the free propagator, i.e. the last two terms on the right-hand side (rhs) of equation (35). We use the reparametrization convention of [14, 16, 17] to absorb the UV bulk singularities, introducing renormalized quantities and renormalization factors via

$$\phi = Z_\phi^{1/2}\phi^{\mathrm{ren}}, \qquad \mathring{\sigma} = Z_\sigma \sigma, \qquad \mathring{u}\mathring{\sigma}^{-m/4} = F_{m,\epsilon}\mu^\epsilon Z_u u, \tag{40}$$

$$\mathring{\tau} - \mathring{\tau}_{\mathrm{LP}} = \mu^2 Z_\tau[\tau + A_\tau \rho^2], \qquad (\mathring{\rho} - \mathring{\rho}_{\mathrm{LP}})\mathring{\sigma}^{-1/2} = \mu Z_\rho \rho, \tag{41}$$

with

$$F_{m,\epsilon} = \frac{\Gamma(1+\epsilon/2)\Gamma^2(1-\epsilon/2)\Gamma(m/4)}{(4\pi)^{(8+m-2\epsilon)/4}\Gamma(2-\epsilon)\Gamma(m/2)}, \tag{42}$$

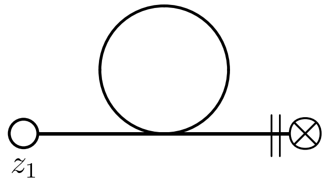

Figure 1. One-loop graph of $\hat{G}^{(1,1)}(\boldsymbol{p}, z_1)$. The stroke indicates the derivative ∂_z. Crossed and open circles indicate points on and off the surface, respectively. Thus, the crossed circle in conjunction with the double stroke on the right represents the surface operator $\partial_n^2 \phi$.

where we have explicitly indicated the dependence on $\mathring{\sigma}$. Two-loop results for the renormalization factors Z_ϕ, Z_σ, Z_ρ and Z_τ can be found in [13]. The renormalization function A_τ was computed to one-loop order in [16]; the result will not be needed in the following.

To absorb the primitive UV surface singularities, additional counter-terms with support on the surface are needed. We introduce a renormalization factor Z_2 and renormalized surface operator $(\partial_n^2\phi)^{\text{ren}}$ via

$$\partial_n^2\phi = [Z_2 Z_\phi]^{1/2}\big(\partial_n^2\phi\big)^{\text{ren}} = Z_2^{1/2}\partial_n^2\phi^{\text{ren}}. \tag{43}$$

Power counting shows that besides the surface counter-term resulting from Z_2, $G^{(0,2)}$ requires an additive renormalization. Let us write the source term of the action needed to generate insertions of the bare surface operator $\partial_n^2\phi$ as $\int_{\mathfrak{B}} \mathrm{d}^{d-1}r\, \boldsymbol{J}_2(\boldsymbol{r})\cdot\partial_n^2\phi(\boldsymbol{r})$. Then the $\boldsymbol{J}_2$-dependent part of the renormalized action can be written as

$$\int_{\mathfrak{B}} \mathrm{d}^{d-1}r\big[Z_2^{-1/2}\boldsymbol{J}_2\cdot\partial_n^2\phi^{\text{ren}} + \mu^{1/2}\sigma^{-5/4}S_2\boldsymbol{J}_2^2\big]. \tag{44}$$

This requires some explanation. The counter-term involving Z_2 absorbs UV singularities $\sim\ln\Lambda$; as usual, the latter manifest themselves as poles at $\epsilon = 0$ in the dimensional regularization scheme we prefer to employ. That such poles indeed occur can be seen from the one-loop graph of $G^{(1,1)}$ shown in figure 1. Its closed loop involves the distribution

$$G_{00}(\boldsymbol{x}, \boldsymbol{x}) = \mathring{\sigma}^{-1/4}\mu^{-3/2}\breve{z}^{-4+2\epsilon}g_\epsilon(m)F_{m,\epsilon}, \tag{45}$$

in which $\breve{z} \equiv \mathring{\sigma}^{-1/4}\mu^{1/2}z$ denotes the dimensionless counterpart of z, while $g_\epsilon(m)$ is a number given by

$$g_\epsilon(m) = F_{m,\epsilon}^{-1}\int_p \hat{G}_{00}(\boldsymbol{p}; 1, 1|\mathring{\sigma} = 1). \tag{46}$$

Since $\breve{z} \geqslant 0$, the power $\breve{z}^{-4+2\epsilon}$ corresponds to the generalized function $\breve{z}_+^{-4+2\epsilon}$ of [28]. Upon substituting its well-known Laurent expansion [28] (see also the appendix of [2]), we obtain

$$G_{00}(\boldsymbol{x}, \boldsymbol{x})/F_{m,\epsilon} = \mathring{\sigma}^{-1/4}\mu^{-3/2}g_0(m)\frac{-1}{6}\frac{\delta'''(\breve{z})}{2\epsilon} + O(\epsilon^0). \tag{47}$$

The quantity $g_\epsilon(m)$ is computed in the appendix for general values of m. Our subsequent results involve its value at $\epsilon = 0$, which is

$$\begin{aligned} g_0(m) = 2 - m - \frac{3}{4-m}\bigg\{&2 - m + \frac{24}{m+2} - \frac{(2\pi)^{1/2}(2m-5)(m-1)\Gamma(m/2)}{8\Gamma[(m+1)/2]} \\ &+ \frac{1}{m}\,{}_2F_1[2, (m-1)/2; (m+2)/2; -1]\bigg\}, \end{aligned} \tag{48}$$

and reduces to

$$g_0(1) = -9 \tag{49}$$

in the uniaxial case $m = 1$.

In accordance with its indicated μ-dimension, the counter-term $\propto S_2$ diverges $\sim\sqrt{\Lambda}$. Its is analogous to the surface counter-term $C_\infty \sim \Lambda$ in equation (3.135) of [2] needed in the CP case to renormalize the corresponding correlation functions $\langle \phi_{a_1} \cdots \phi_{a_N} \partial_n \phi_{b_a} \cdots \partial_n \phi_{b_M} \rangle$ in the cutoff-regularized theory. Just as $C_\infty \sim \Lambda$, the counter-term$\propto S_2$ vanishes in the dimensionally regularized theory. We therefore do not consider it any further.

Suppressing the tensorial indices $a_1, \ldots, b_M$, we denote the renormalized counterparts of the cumulants (39) as

$$G_{\text{ren}}^{(N,M)} = Z_\phi^{-(N+M)/2} Z_2^{-M/2} G^{(N,M)}. \tag{50}$$

A standard way of reasoning yields their RG equations

$$\left[\mu\partial_\mu + \sum_{\wp=u,\sigma,\rho,\tau} \beta_\wp \partial_\wp + \frac{N+M}{2}\eta_\phi + \frac{M}{2}\eta_2\right] G_{\text{ren}}^{(N,M)} = 0, \tag{51}$$

where $\beta_\wp$ are bulk β-functions in the notation of [16, 17]. Both β_ρ and β_τ vanish at the LP and will not be needed in the rest of the paper. The functions $\beta_u(\epsilon, u)$ and $\eta_\sigma(u) \equiv -\beta_\sigma/\sigma$ are known to order u^3 from [13].

As a consequence of these RG equations, we have for the coefficient function $C_{\partial_n^2\phi}(z)$,

$$\left[\mu\partial_\mu + \sum_{\wp=u,\sigma,\rho,\tau} \beta_\wp \partial_\wp - \frac{\eta_2}{2}\right] C_{\partial_n^2\phi}(z) = 0. \tag{52}$$

Solving this at the LP $\rho = \tau = 0$ gives

$$C_{\partial_n^2\phi}(z) \sim (\mu\sigma^{-1/2})^{\eta_2^*/(4\theta)} z^{(\eta_2^*+4\theta)/(2\theta)}, \tag{53}$$

where $\eta_2^* = \eta_2(u^*)$ means the value of η_2 at the infrared-stable fixed point $u^* = O(\epsilon)$. The result can be combined with equation (38) to conclude that

$$\begin{aligned} \beta_{\text{L1}}^{(\text{ord},\perp)} &= (d - m - 2 + \eta_{\text{L2}} + m\theta + \eta_2^* + 4\theta)\nu_{\text{L2}}/2 \\ &= \beta_{\text{L}} + (4\theta + \eta_2^*)\nu_{\text{L2}}/2. \end{aligned} \tag{54}$$

Here $\beta_{\text{L}} = \nu_{\text{L2}}[d - 2 + \eta_{\text{L2}} + m(\theta - 1)]$ is the usual bulk magnetization exponent.

The scaling behaviour of other surface quantities can be derived along similar lines by exploiting the RG equation (51) in conjunction with the BOE (36). In this manner, one can determine how the associated surface critical exponents can be expressed in terms of four independent bulk critical exponents, such as η_{L2}, θ, ν_{L2} and φ, and the surface magnetization index $\beta_{\text{L1}}^{(\text{ord},\perp)}$.

As an example, let us consider the surface susceptibility $\chi_{11}(\boldsymbol{p}) = \hat{G}^{(2,0)}(\boldsymbol{p}; z = 0, z' = 0)$, the Fourier $\boldsymbol{p}$-transform of the response of $\langle \phi|_{z=0} \rangle$ with respect to a surface magnetic field $\boldsymbol{h}_1$. To characterize the asymptotic low-momentum behaviour of this quantity at the LP, we introduce the surface exponent $\eta_\|$ by analogy with the CP case via

$$\chi_{11}^{(\text{sing})}(\boldsymbol{p}) \underset{\boldsymbol{p}\to\boldsymbol{0}}{\sim} \begin{cases} p_<^{(\eta_\| - 1)/\theta} & \text{for } p_> = 0, \\ p_>^{\eta_\| - 1} & \text{for } p_< = 0, \end{cases} \tag{55}$$

where sing means singular part. (At the ordinary transition considered here, χ_{11} does not diverge but approaches a finite value.)

To identify $\eta_\parallel$, we apply the BOE (36) to both external legs of $\hat{G}^{(2,0)}(\boldsymbol{p}, z, z')$, and exploit the behaviour (53) of the coefficient function together with the scaling forms of $G^{(2,0)}$ and $G^{(0,2)}$ implied by their RG equations. This gives, for example,

$$\hat{G}^{(2,0)}_{\text{ren}}(\boldsymbol{p}; z, z') \underset{z,z'\to 0}{\sim} p_>{}^{-2+\eta_{\text{L2}}+\theta}\big[\big(zp_>^\theta\big)\big(z'p_>^\theta\big)\big]^{(\eta_2^*+4\theta)/(2\theta)}, \tag{56}$$

which tells us that

$$\eta_\parallel^{(\text{ord},\perp)} = 5\theta - 1 + \eta_{\text{L2}} + \eta_2^*. \tag{57}$$

Other surface exponents, such as the surface susceptibility exponents γ_{11} and γ_1, can be expressed in a similar manner in terms of $\beta_{\text{L1}}^{(\text{ord},\perp)}$ and bulk exponents. In particular, the usual scaling law $\gamma_{11} = \nu_{\text{L2}}(1-\eta_\parallel)$ for the surface susceptibility exponent γ_{11} is found to remain valid, as suspected by Binder and Frisch [21].

Next, we turn to the computation of the still unknown RG function Z_2. Using the result (47), one can determine it to one-loop order in a straightforward fashion. Application of the distribution $-\delta'''(z)$ to the external legs of $\hat{G}^{(0,2)}(\boldsymbol{p})$ and $\hat{G}^{(1,1)}(\boldsymbol{p}; z_1)$ gives

$$\big(-\delta'''(z), \big[\hat{G}_{00}\overleftarrow{\partial}_n^2\big]^2\big) = 6\partial_n^2\hat{G}_{00}\overleftarrow{\partial}_n^2 \tag{58}$$

and

$$\big(-\delta'''(z), \hat{G}_{00}(\boldsymbol{p}; z_1, z)\big[\hat{G}_{00}\overleftarrow{\partial}_n^2\big](\boldsymbol{p}; z, 0)\big) = 3\big[\hat{G}_{00}\overleftarrow{\partial}_n^2\big](z_1, 0), \tag{59}$$

respectively. The implied poles of both $\hat{G}^{(0,2)}_{\text{ren}}(\boldsymbol{p})$ and $\hat{G}^{(1,1)}_{\text{ren}}(\boldsymbol{p}; z_1)$ get cancelled if we choose

$$Z_2 = 1 - g_0(m)\frac{n+2}{3}\frac{u}{4\epsilon} + O(u^2), \tag{60}$$

where we utilized the fact that $Z_\phi = 1 + O(u^2)$. The derivative $-u\partial_u$ of this function's residuum at $\epsilon = 0$ gives us the RG function η_2. Substituting for u its fixed-point value $u^* = 6\epsilon/(n+8) + O(\epsilon^2)$ then yields

$$\eta_2^* = g_0(m)\frac{n+2}{12}u^* + O[(u^*)^2] = g_0(m)\frac{n+2}{n+8}\frac{\epsilon}{2} + O(\epsilon^2). \tag{61}$$

The result can be combined with the known ϵ expansions of the bulk exponents in equation (54) to obtain

$$\begin{aligned}\beta_{\text{L1}}^{(\text{ord},\perp)} &= (\nu_{\text{L2}}/2)[4 - \epsilon + \eta_2^*] + O(\epsilon^2)\\ &= 1 + \frac{\epsilon}{4(n+8)}\left[n - 4 + \frac{n+2}{2}g_m(0)\right] + O(\epsilon^2).\end{aligned} \tag{62}$$

In the uniaxial scalar case $m = n = 1$ of the ANNNI model, this simplifies to

$$\beta_{\text{L1}}^{(\text{ord},\perp)} = 1 - \frac{11}{24}\epsilon + O(\epsilon^2) = \left[1 + \frac{11}{24}\epsilon + O(\epsilon^2)\right]^{-1}. \tag{63}$$

Setting $\epsilon = 3/2$ in the first and second expressions on the rhs (i.e. in the direct series and the [0/1] Padé approximant) yields the $d = 3$ estimates $\beta_{\text{L1}}^{(\text{ord},\perp)} \simeq 0.31$ and 0.59, respectively, which is to be compared with Pleimling's Monte Carlo result 0.62(1) [19]. Though these numbers are encouraging, our present knowledge of the series (63) to just first order in ϵ clearly is insufficient to produce estimates that are competitive in accuracy with this Monte Carlo value. We therefore refrain from giving further extrapolated values for other surface exponents. Experience with the bulk case [13] suggests that much better field-theoretic estimates should become possible once η_2^* is known to $O(\epsilon^2)$. In view of the simplifications entailed by the approach developed here, such a two-loop calculation should not be too difficult.

6. Concluding remarks

In this paper, we have extended previous field-theoretic work on boundary critical behaviour at m-axial LPs [15–17, 22] by studying the critical behaviour at the ordinary transition of a semi-infinite system that is bounded by a surface perpendicular to an α-direction. This geometry was the one considered in the earliest investigations [20, 21] of boundary critical behaviour at LPs. However, to construct an appropriate minimal field-theory model and analyse it in a systematic fashion by means of modern RG method below the upper critical dimension turned out to be quite a challenge, mainly because significantly more potentially relevant (short-range) surface contributions must be considered than in the simpler case where the surface is perpendicular to the β-direction.

Taking up a suggestion made earlier [22], we found a way to by-pass the enormous technical difficulties one is faced with when having to carry along many surface interaction constants. The basic idea is to choose the boundary conditions (7) the theory is expected to satisfy on long length-scales at the ordinary transition from the outset, showing that they *correspond to a fixed point* of the RG. While we have not investigated deviations from this fixed point associated with modification of these boundary conditions (e.g. finite values of the surface couplings $\mathring{c}_\perp$ and $\mathring{b}$), our results are completely consistent with the physically reasonable expectation that these boundary conditions are associated with a stable fixed point of the RG.

The benefit of our procedure is twofold: (i) used in conjunction with the BOE, the RG equations we obtained enabled us to derive scaling laws relating the surface critical exponents at this transition to bulk exponents and a single independent surface index, such as $\beta_{L1}^{(\mathrm{ord},\perp)}$. (ii) Owing to the gain in technical simplification, an explicit one-loop calculation could be performed to obtain the ϵ expansion of $\beta_{L1}^{(\mathrm{ord},\perp)}$ and related surface exponents to first order. Of course, one cannot expect to get precise numerical estimates for the critical exponents at $d = 3$ from such an $O(\epsilon)$ result. Nevertheless, the extrapolated values we obtained for $\beta_{L1}^{(\mathrm{ord},\perp)}$ in the case of the three-dimensional semi-infinite ANNNI model by direct extrapolation to $d = 3$ and via a [0/1] Padé approximant agree reasonably well with recent Monte Carlo results [19] (albeit different numbers could be obtained if other scaling-law expressions for $\beta_{L1}^{(\mathrm{ord},\perp)}$ were employed in conjunction with the best estimates of [13] for the required bulk exponents). More reliable field-theoretic estimates should be possible on the basis of $O(\epsilon^2)$ results. The required two-loop calculation appears to be quite manageable.

A more difficult task is to perform an analogous two-loop RG analysis of the corresponding LP special transition. Since this requires the identification of the associated fixed point in the space of surface coupling constants, one cannot avoid retaining the dependence on these variables (see the analysis of the special transition for the case of parallel surface orientation [17] for comparison).

From a more general perspective, the present investigation is, to our knowledge, the first one dealing beyond the classical level with a field theory subject to the two boundary conditions (7). Both our way of investigating this field theory as well as our result that this boundary condition correspond to a stable fixed point of the RG might have applications in other contexts.

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Appendix. Calculation of one-loop integral

Here we compute the number $g_\epsilon(m)$ introduced in equation (46).

Let us denote the bulk propagator in position space as $G_{\mathrm{b}}(\boldsymbol{x}-\boldsymbol{x}')$. Taking into account that $G_{\mathrm{b}}(\mathbf{0})$ vanishes at the LP in dimensional regularization, we obtain from equations (45) and (46) the result

$$g_\epsilon(m)F_{m,\epsilon} = G_{00}(\boldsymbol{x},\boldsymbol{x}|\mathring{\sigma}=1)|_{z=1} = -G_{\mathrm{b}}(\boldsymbol{r}=0,2z|1)|_{z=1} + K_{d-m}K_{m-1}I_\epsilon(m). \tag{A.1}$$

The first term on the rhs follows from equations (7), (A.5) and (A.6) of [13]. It is given by

$$G_{\mathrm{b}}(\mathbf{0},2|1) = 2^{-1-m}\pi^{-(6+m-2\epsilon)/4}\frac{\Gamma(2-\epsilon)}{\Gamma[(m-2+2\epsilon)/4)]}. \tag{A.2}$$

In the second contribution we have split off the factors originating from the angular integrations, with

$$K_d \equiv 2(4\pi)^{-d/2}/\Gamma(d/2). \tag{A.3}$$

In the remaining integral we make the changes of variables $p_> \to P = p_>/p_<^2$ and $p_< \to p = p_</\sqrt{2}$ to obtain

$$\begin{aligned} I_\epsilon(m) &= -\int_0^\infty \mathrm{d}p_>\, p_>^{d-m-1}\int_0^\infty \mathrm{d}p_<\, p_<^{m-2}\frac{\sin^2(\kappa_-)}{2\kappa_-^2\kappa_+}\,\mathrm{e}^{-2\kappa_+} \\ &= -2^\beta\int_0^\infty \mathrm{d}P\,P^\nu\int_0^\infty \mathrm{d}p\,p^{\alpha-1}\frac{\sin^2(pk_-)}{k_-}\,\mathrm{e}^{-2pk_+} \end{aligned} \tag{A.4}$$

with

$$\alpha = 2d-4-m = 4-2\epsilon, \qquad \beta = \frac{\alpha+1}{2}, \qquad \nu = \frac{\alpha-m}{2}. \tag{A.5}$$

We have introduced

$$k_\pm \equiv \left(\sqrt{1+P^2}\pm 1\right)^{1/2}, \tag{A.6}$$

for which

$$k_-k_+ = P, \qquad k_+^2-k_-^2 = 2, \qquad (k_+-\mathrm{i}k_-)^2 = 2(1-\mathrm{i}P). \tag{A.7}$$

Upon integrating by parts with respect to p and using $\sin^2 x = (1-\cos 2x)/2$, we arrive at

$$\begin{aligned} I_\epsilon(m) &= \frac{2^\beta}{\alpha}\int_0^\infty \mathrm{d}P\,P^\nu\left[\int_0^\infty \mathrm{d}p\,p^\alpha\sin(2pk_-)\,\mathrm{e}^{-2pk_+} - \frac{2k_+}{k_-}\int_0^\infty \mathrm{d}p\,p^\alpha\sin^2(pk_-)\,\mathrm{e}^{-2pk_+}\right] \\ &= \frac{2^\beta}{\alpha}\left[-\int_0^\infty \mathrm{d}P\,P^{\nu-1}k_+^2 I_p^{(0)} + \int_0^\infty \mathrm{d}P\,P^\nu I_p^{(1)} + \int_0^\infty \mathrm{d}P\,P^{\nu-1}(\sqrt{1+P^2}+1)I_p^{(2)}\right] \end{aligned} \tag{A.8}$$

with

$$I_p^{(0)} = \int_0^\infty \mathrm{d}p p^\alpha \,\mathrm{e}^{-2pk_+} = 2^{-2\beta}\Gamma(2\beta)k_+^{-2\beta}, \tag{A.9}$$

$$I_p^{(1)} = \int_0^\infty \mathrm{d}p p^\alpha \sin(2pk_-)\,\mathrm{e}^{-2pk_+} = 2^{-3\beta}\frac{\Gamma(2\beta)}{2\mathrm{i}}[(1-\mathrm{i}P)^{-\beta} - (1+\mathrm{i}P)^{-\beta}] \tag{A.10}$$

and

$$I_p^{(2)} = \int_0^\infty \mathrm{d}p p^\alpha \cos(2pk_-)\,\mathrm{e}^{-2pk_+} = 2^{-3\beta}\frac{\Gamma(2\beta)}{2}[(1-\mathrm{i}P)^{-\beta} + (1+\mathrm{i}P)^{-\beta}]. \tag{A.11}$$

The remaining p-integrations can be conveniently performed by means of Maple[8]. After some rearrangements the result becomes

$$\begin{aligned} I_\epsilon(m) = -2^{2\epsilon-5}\Gamma\left(\frac{m-1}{2}\right)\Gamma(4-2\epsilon)\Bigg[&\frac{\Gamma(2-m/2-\epsilon)}{\Gamma(3/2-\epsilon)}\cos\left(\pi\frac{m+2\epsilon}{4}\right) \\ &+ (3-2\epsilon)2^{1-m/2-\epsilon}\frac{\Gamma(1-m/4-\epsilon/2)}{\Gamma(3/2+m/4-\epsilon/2)} \\ &- \frac{1}{2\sqrt{\pi}}\Gamma\left(-\frac{m}{2}\right)\cos\left(\pi\frac{m-2\epsilon}{4}\right)\,{}_2F_1\left(2-\epsilon, \frac{m-2}{2}; \frac{m+2}{2}; -1\right) \\ &+ \frac{m-1}{2}\frac{\Gamma(2-m/2-\epsilon)\Gamma(m/2)}{\Gamma(2-\epsilon)\Gamma(m/2+1/2)}\cos\left(\pi\frac{m+2\epsilon}{4}\right) \\ &\times {}_2F_1\left(2-\frac{m}{2}-\epsilon, -\frac{1}{2}; 1-\frac{m}{2}; -1\right)\Bigg]. \end{aligned} \tag{A.12}$$

For the uniaxial case $m = 1$, the required integration is simple, yielding

$$\begin{aligned} I_\epsilon(1) &= -\sqrt{2}\int_0^\infty \mathrm{d}p p^{1-\epsilon}\sin^2(\sqrt{p/2})\,\mathrm{e}^{-\sqrt{2p}} \\ &= 2^{\epsilon-7/2}\Gamma(4-2\epsilon)[4+2^\epsilon\cos(\pi\epsilon/2)] \end{aligned} \tag{A.13}$$

in conformity with equation (A.12).

Upon substituting expression (A.12) into equation (A.1) and using equation (45) together with the definition (42) of $F_{m,\epsilon}$, one obtains the result for $g_0(m)$ given in equation (48).

References

[1] Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (London: Academic) pp 1–144

[2] Diehl H W 1986 *Phase Transitions and Critical Phenomena* vol 10, ed C Domb and J L Lebowitz (London: Academic) pp 75–267

[3] Diehl H W 1997 *Int. J. Mod. Phys.* B **11** 3503 (*Preprint* cond-mat/9610143)

[4] Pleimling M 2004 *J. Phys. A: Math. Gen.* **37** R79

[5] Hornreich R M 1980 *J. Magn. Magn. Mater.* **15–18** 387

[6] Selke W 1992 *Phase Transitions and Critical Phenomena* vol 15, ed C Domb and J L Lebowitz (London: Academic) pp 1–72

[7] Diehl H W 2002 *Acta Phys. Slovaca* **52** 271
Diehl H W 2002 *Proc. of the 5th International Conference "Renormalization Group 2002", (Tatranska Strba, High Tatra Mountains, Slovakia, 10–16 March)* (*Preprint* cond-mat/0205284)

[8] Hornreich R M, Luban M and Shtrikman S 1975 *Phys. Rev. Lett.* **35** 1678

[9] Sak J and Grest G S 1978 *Phys. Rev.* B **17** 3602

[8] Maple 8, a product of Waterloo Maple Inc.

[10] Mergulhão C Jr and Carneiro C E I 1998 *Phys. Rev.* B **58** 6047
[11] Mergulhão C Jr and Carneiro C E I 1999 *Phys. Rev.* B **59** 954
[12] Diehl H W and Shpot M 2000 *Phys. Rev.* B **62** 338 (*Preprint* cond-mat/0006007)
[13] Shpot M and Diehl H W 2001 *Nucl. Phys.* B **612** 340 (*Preprint* cond-mat/0106105)
[14] Diehl H W, Shpot M and Zia R K P 2003 *Phys. Rev.* B **68** 224415 (*Preprint* cond-mat/0307355)
[15] Diehl H W, Rutkevich S and Gerwinski A 2003 *J. Phys. A: Math. Gen.* **36** L243
[16] Diehl H W, Gerwinski A and Rutkevich S 2003 *Phys. Rev.* B **68** 224428 (*Preprint* cond-mat/0308483)
[17] Diehl H W and Rutkevich S 2004 *J. Phys. A: Math. Gen.* **37** 8575 (*Preprint* cond-mat/0406216)
[18] Frisch H L, Kimball J C and Binder K 2000 *J. Phys.: Condens. Matter* **12** 29
[19] Pleimling M 2002 *Phys. Rev.* B **65** 184406
[20] Gumbs G 1986 *Phys. Rev.* B **33** 6500
[21] Binder K and Frisch H L 1999 *Eur. Phys. J.* B **10** 71
[22] Diehl H W 2005 *Pramana—J. Phys.* **64** 803
Diehl H W 2004 *Proc. of the 22nd International Conference on Statistical Physics (STATPHYS 22) of the International Union of Pure and Applied Physics (IUPAP) (Bangalore, India, 4–9 July 2004)* (*Preprint* cond-mat/0407352)
[23] Krech M and Dietrich S 1992 *Phys. Rev. Lett.* **66** 345
Krech M and Dietrich S 1992 *Phys. Rev. Lett.* **67** 1055 (erratum)
[24] McAvity D M and Osborn H 1993 *Nucl. Phys.* B **394** 728
[25] Chandrasekhar S 1970 *Hydrodynamic and Hydromagnetic Stability* 3rd edn (Oxford: Oxford University Press)
[26] Diehl H W and Dietrich S 1980 *Phys. Lett.* A **80** 408
[27] Diehl H W and Dietrich S 1981 *Z. Phys.* B **42** 65
Diehl H W and Dietrich S 1981 *Z. Phys.* B **43** 281 (erratum)
[28] Gel'fand I M and Shilov G E 1964 *Generalized Functions* vol 1 (New York: Academic) pp 1–423