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# Boundary critical behaviour at $m$ -axial Lifshitz points: the special transition for the case of a surface plane parallel to the modulation axes

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## Abstract

The critical behaviour of  $d$ -dimensional semi-infinite systems with  $n$ -component order parameter  $\phi$  is studied at an  $m$ -axial bulk Lifshitz point whose wave-vector instability is isotropic in an  $m$ -dimensional subspace of  $\mathbb{R}^d$ . Field-theoretic renormalization group methods are utilized to examine the special surface transition in the case where the  $m$  potential modulation axes, with  $0 \leq m \leq d - 1$ , are parallel to the surface. The resulting scaling laws for the surface critical indices are given. The surface critical exponent  $\eta_{\parallel}^{\text{sp}}$ , the surface crossover exponent  $\Phi$  and related ones are determined to first order in  $\epsilon = 4 + \frac{m}{2} - d$ . Unlike the bulk critical exponents and the surface critical exponents of the ordinary transition,  $\Phi$  is  $m$  dependent already at first order in  $\epsilon$ . The  $O(\epsilon)$  term of  $\eta_{\parallel}^{\text{sp}}$  is found to vanish, which implies that the difference of  $\beta_1^{\text{sp}}$  and the bulk exponent  $\beta$  is of order  $\epsilon^2$ .

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## 1. Introduction

As is well known, systems in critical or near-critical states are sensitive to the presence of boundaries such as surfaces or walls: the long-distance behaviour of their local densities and correlation functions gets modified near boundaries. During the past decades impressive progress has been made in our understanding of such boundary critical phenomena (Binder 1983, Diehl 1986, Cardy 1987, Pleimling 2004). A prototype class of systems from whose study considerable insight into general aspects of boundary critical phenomena has emerged is provided by the semi-infinite  $n$ -vector  $\phi^4$  models. At bulk criticality, these models exhibit a variety of physically distinct continuous surface transitions in sufficiently

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high space dimensions  $d$ , called ordinary, special, extraordinary and normal. A simplifying feature they have is that the scale invariance they display at criticality is of *isotropic* nature: distances along arbitrary directions must be scaled with the same power of the length-rescaling factor  $\ell$ . Furthermore, the correlation lengths  $\xi(e)$  defined through the exponential decay  $\sim \exp(-R/\xi(e))$  of the pair correlation function  $\langle \phi(\mathbf{x})\phi(\mathbf{x} + R\mathbf{e}) \rangle$  along a given direction specified by a unit vector  $\mathbf{e}$  all diverge  $\sim |T - T_{b,c}|^{-\nu}$  with the same critical index  $\nu$ , as the critical bulk temperature  $T = T_{c,b}$  is approached via a phase with unbroken  $O(n)$  symmetry. This leaves little room for dependence of boundary critical behaviour on the orientation of the surface with respect to crystal axes. We are aware of only one established scenario for such orientation dependence (Schmid 1993, Diehl *et al* 1997, Leidl and Diehl 1998, Leidl *et al* 1998): bcc binary alloys and antiferromagnets in the presence of weak magnetic fields may map upon coarse graining onto semi-infinite  $\phi^4$  models with or without ordering boundary fields  $h_1$ , depending on whether their surface's orientation breaks the symmetry  $\phi \rightarrow -\phi$  or not. If so, they may belong to basins of attraction of distinct fixed points, such as the normal and ordinary one, so that their boundary critical behaviour is different.

In the present paper, we shall be concerned with boundary critical behaviour at  $m$ -axial bulk *Lifshitz points* (LP) (Hornreich 1980, Selke 1992, Diehl 2002). An LP is a multicritical point at which a disordered, a homogeneous ordered and a modulated ordered phase meet. A characteristic feature of the scale invariance that systems exhibit at such points is its *anisotropic* nature: the coordinates  $x_\alpha, \alpha = 1, \dots, m$ , along any of the  $m$  potential modulation axes scale as a nontrivial power  $(x_\beta)^\theta$  of the  $d - m$  remaining orthogonal ones,  $x_\beta, \beta = m + 1, \dots, d$ . This entails that the orientation of the surface with respect to the modulation axes matters. Two principal surface orientations, parallel and perpendicular, can be distinguished for which the surface normal is directed along an  $\alpha$  or  $\beta$  axis, respectively. The boundary critical behaviour that occurs at a given type of surface transition (ordinary, special, etc) for either parallel or perpendicular surface orientation is expected to correspond to two *distinct* universality classes. Results obtained via mean-field theory (Gumbs 1986, Binder and Frisch 1991, Frisch *et al* 2000) and Monte Carlo simulations (Pleimling 2002) for the ordinary and special transitions of ANNNI models with free surfaces of both types of orientation are in conformity with this expectation.

These findings indicate that systems exhibiting anisotropic scale invariance have potentially richer boundary critical behaviour. Since systems of this kind are abundant in nature—anisotropic scale invariant states exist both in and out of equilibrium—a careful understanding of their boundary critical behaviour is certainly of interest.

Focusing on the case of parallel surface orientation, we have recently introduced an appropriate semi-infinite extension of a standard  $n$ -vector  $\phi^4$  model describing universality classes of *bulk* critical behaviour at  $m$ -axial LP points (Diehl *et al* 2003a, 2003b). We argued that this extension represents the *surface* universality classes of the ordinary, special and extraordinary transitions for this kind of surface orientation (Diehl 1986, 1997). A renormalization group (RG) analysis for dimensions  $d = d^*(m) - \epsilon$  below the upper critical dimension  $d^*(m) = 4 + m/2$  lent support to this claim, giving fixed points we could identify as describing the corresponding surface universality classes. However, this identification was tentative: since of all, only the ordinary transition was analysed in some detail; second, this was done by relying on the asymptotic validity of the Dirichlet boundary condition, bypassing thereby the need to determine the precise location of the ordinary fixed point in the space of surface interaction constants.

The purpose of the present paper is to complement our previous work (Diehl *et al* 2003a, 2003b) by a detailed analysis of the *special* transition. The asymptotic (Robin-type) boundary

condition that the theory satisfies at this transition involves the fixed-point value  $\lambda_+^*$  of a dimensionless surface variable  $\lambda$ , a number which depends on the order of the loop expansion. A trick analogous to that employed in the analysis of the ordinary transition by which the computation of  $\lambda_+^*$  can be avoided does not exist. This entails a *qualitative* difference between the analysis of the  $m > 0$  special transition described below and that of its  $m = 0$  counterpart at bulk *critical* points (Diehl and Dietrich 1981, 1983): in the latter case, the variable  $\lambda$  is missing, and the fixed-point value of the sole remaining renormalized surface interaction constant (the surface enhancement  $c$ ) is zero to all orders in perturbation theory. Unlike the  $m > 0$  case, projection onto the hyper-plane of critical renormalized surface variables is trivial.

We shall determine the surface correlation index  $\eta_{\parallel}^{\text{sp}}$  and the surface crossover exponent  $\Phi$  to first order in  $\epsilon$ . Our RG analysis reveals that below the upper critical dimension, all other surface critical exponents of the special transition can be expressed in terms of these two independent surface critical exponents, along with bulk critical indices. While this is just as in the  $m = 0$  case of the special transition at bulk critical points (Diehl and Dietrich 1981, 1983, Diehl 1986), our result that the  $O(\epsilon)$  contribution to  $\eta_{\parallel}^{\text{sp}}$  vanishes if  $m > 0$  (though not for  $m = 0$ ) is a remarkable difference. Another unusual feature of our results is that the crossover exponent  $\Phi$  starts to depend on  $m$  already at *linear* order in  $\epsilon$ . By contrast, the  $\epsilon$  expansions of both the bulk critical exponents as well as the surface critical exponents of the ordinary transition display first  $m$ -dependent deviations from their  $m = 0$  analogues only at quadratic order in  $\epsilon$ .

The remainder of this paper is organized as follows. In the next section, we define our model and briefly recapitulate the relevant background knowledge required in what follows. Section 3 deals with the RG analysis of the special transition. We derive the scaling forms of the multi-point cumulants involving order parameter fields  $\phi$  on and off the boundary, give some of the implied scaling laws, and present our  $\epsilon$ -expansion results. The latter are utilized to estimate the values of the surface critical exponents  $\eta_{\parallel}^{\text{sp}}$  and  $\beta_1^{\text{sp}}$ , as well as the surface crossover exponent for the uniaxial scalar case in three dimensions, i.e. the ANNNI model. In section 4, RG improved perturbation theory is employed to investigate the surface susceptibility  $\chi_{11}$ . Making an explicit one-loop calculation, we verify the predicted scaling behaviour, corroborating thereby our identification of the special transition. A short discussion and concluding remarks follow in the final section. Finally, there are two appendices explaining computational details.

## 2. Model and background

Following Diehl *et al* (2003a, 2003b), we consider a model defined by the Hamiltonian

$$\mathcal{H} = \int_{\mathfrak{V}} \mathcal{L}_b(\mathbf{x}) \, dV + \int_{\mathfrak{B}} \mathcal{L}_1(\mathbf{x}) \, dA, \quad (1)$$

with the bulk density

$$\mathcal{L}_b(\mathbf{x}) = \frac{\mathring{c}}{2} \left( \sum_{\alpha=1}^m \partial_{\alpha}^2 \phi \right)^2 + \frac{1}{2} \sum_{\beta=m+1}^d (\partial_{\beta} \phi)^2 + \frac{\mathring{\rho}}{2} \sum_{\alpha=1}^m (\partial_{\alpha} \phi)^2 + \frac{\mathring{t}}{2} \phi^2 + \frac{\mathring{u}}{4!} |\phi|^4 \quad (2)$$

and the surface density

$$\mathcal{L}_1(\mathbf{x}) = \frac{\mathring{c}}{2} \phi^2 + \frac{\mathring{\lambda}}{2} \sum_{\alpha=1}^m (\partial_{\alpha} \phi)^2, \quad (3)$$

where the volume and surface integrals  $\int_{\mathfrak{V}} dV$  and  $\int_{\mathfrak{B}} dA$  extend over the half-space  $\mathfrak{V} = \{\mathbf{x} = (\mathbf{r}, z) \mid \mathbf{r} \in \mathbb{R}^{d-1}, 0 \leq z < \infty\}$  and the boundary plane  $\mathfrak{B} = \{(\mathbf{r}, 0) \mid \mathbf{r} \in \mathbb{R}^{d-1}\}$

(‘the surface’), respectively, and the notation  $\partial_\alpha = \partial/\partial x_\alpha$  and  $\partial_\beta = \partial/\partial x_\beta$ , with  $1 \leq \alpha \leq m$  and  $m < \beta \leq d$ , is used. The order parameter is an  $n$ -vector  $\phi = (\phi_a, a = 1, \dots, n)$ .

Let us introduce the  $(N + M)$ -point cumulants involving  $N$  fields  $\phi_{a_i}(\mathbf{x}_i)$  off the surface and  $M$  boundary fields  $\phi_{b_j}^{\mathfrak{B}}(\mathbf{r}_j)$ ,

$$G^{(N,M)}(\mathbf{x}; \mathbf{r}) \equiv \left\langle \left[ \prod_{i=1}^N \phi_{a_i}(\mathbf{x}_i) \right] \left[ \prod_{j=1}^M \phi_{b_j}^{\mathfrak{B}}(\mathbf{r}_j) \right] \right\rangle^{\text{cum}}, \quad (4)$$

where  $\mathbf{x}$  and  $\mathbf{r}$  are shorthands for the sets of all points  $\mathbf{x}_i$  and  $\mathbf{r}_j$  off or on the boundary, respectively. From previous work (Diehl *et al* 2003a, 2003b) we know that the ultraviolet (uv) singularities of these functions can be absorbed for  $d \leq d^*(m)$  by means of the following re-parametrizations,

$$\begin{aligned} \phi &= Z_\phi^{1/2} \phi_{\text{ren}}, & \hat{\sigma} &= Z_\sigma \sigma, & \hat{u} \hat{\sigma}^{-m/4} F_{m,\epsilon} &= \mu^\epsilon Z_u u, \\ \hat{\tau} - \hat{\tau}_{\text{LP}} &= \mu^2 Z_\tau [\tau + A_\tau \rho^2], & (\hat{\rho} - \hat{\rho}_{\text{LP}}) \hat{\sigma}^{-1/2} &= \mu Z_\rho \rho, \end{aligned} \quad (5)$$

$$\begin{aligned} \phi^{\mathfrak{B}} &= (Z_\phi Z_1)^{1/2} \phi_{\text{ren}}^{\mathfrak{B}}, & \hat{\lambda} \hat{\sigma}^{-1/2} &= \lambda + P_\lambda(u, \lambda, \epsilon), \\ \hat{c} - \hat{c}_{\text{sp}} &= \mu Z_c [c + A_c(u, \lambda, \epsilon) \rho], \end{aligned} \quad (6)$$

where

$$F_{m,\epsilon} = \frac{\Gamma(1 + \epsilon/2) \Gamma^2(1 - \epsilon/2) \Gamma(m/4)}{(4\pi)^{(8+m-2\epsilon)/4} \Gamma(2 - \epsilon) \Gamma(m/2)} \quad (7)$$

is a convenient normalization constant. Further,  $\hat{\tau}_{\text{LP}}$  and  $\hat{\rho}_{\text{LP}}$  are the critical bare values of the LP; in our renormalization scheme based on dimensional regularization and the  $\epsilon$ -expansion, these fluctuation-induced shifts vanish. The same applies to  $\hat{c}_{\text{sp}}$ , the critical value of the bare surface enhancement  $\hat{c}$  at which the special transition occurs.

The bulk renormalization factors  $Z_{\phi,\tau,\rho,u} = Z_{\phi,\tau,\rho,u}(u, \epsilon)$  are power series in  $u$ , the renormalized coupling constant, and Laurent series in  $\epsilon$ ; since we employ the scheme of minimal subtraction of uv poles, their regular part at  $\epsilon = 0$  is exactly 1. The boundary renormalization factors  $Z_{1,c} = Z_{1,c}(u, \lambda, \epsilon)$  have a similar form, except that the series coefficients depend on  $\lambda$ . Finally,  $P_\lambda$  and  $A_c$  are renormalization functions of the form

$$P_\lambda(u, \lambda, \epsilon) = \sum_{i,j=1}^{\infty} P_\lambda^{(i,-j)}(\lambda) u^i \epsilon^{-j} = \sum_{i,j=1}^{\infty} \sum_{k=0}^{\infty} P_\lambda^{(i,-j;k)} u^i \epsilon^{-j} \lambda^k. \quad (8)$$

Two important features should be appreciated: first, although the  $O(u)$  term of  $P(u, \lambda, \epsilon)$  is proportional to  $\lambda$ , its  $O(u^2)$  contribution is not, and hence does *not* vanish for  $\lambda = 0$ . Thus  $P(u, \lambda = 0, \epsilon) \neq 0$ , i.e. a nonzero value of the bare interaction constant  $\hat{\lambda}$  gets generated by the  $\phi^4$  interaction (Diehl *et al* 2003a). Second, the renormalization of  $\hat{\tau}$  and  $\hat{c}$  mixes the corresponding renormalized quantities  $\tau$  and  $c$  with  $\rho^2$  and  $\rho$ , respectively. The consequences (worked out in Diehl *et al* (2003a) and below) should be no surprise: the role of the scaling fields  $\tau$  and  $c$  of the Gaussian theory is taken over by combinations of the form

$$g_\tau(\tau, \rho, u) = \tau + C_\rho^\tau(u) \rho^2, \quad g_c(c, \rho, u, \lambda) = c + C_\rho^c(u, \lambda) \rho. \quad (9)$$

To become more specific, it is necessary to recall the RG equations of the renormalized cumulants  $G_{\text{ren}}^{(N,M)} = Z_\phi^{-(N+M)/2} Z_1^{-M/2} G^{(N,M)}$ . They read

$$\left[ \mu \partial_\mu + \sum_{\wp=u,\sigma,\tau,\rho,c,\lambda} \beta_\wp \partial_\wp + \frac{N+M}{2} \eta_\phi + \frac{M}{2} \eta_1 \right] G_{\text{ren}}^{(N,M)} = 0. \quad (10)$$

The beta functions, defined by  $\beta_{\wp} \equiv \mu \partial_{\mu}|_0 \wp$ , where  $\partial_{\mu}|_0$  denotes a derivative at fixed bare interaction constants, can be expressed in terms of the exponent functions  $\eta_{\wp, \phi, 1} \equiv \mu \partial_{\mu}|_0 \ln Z_{\wp, \phi, 1}$  and  $P_{\lambda}$  as

$$\begin{aligned}\beta_u(u, \epsilon) &= -u[\epsilon + \eta_u(u)], \\ \beta_{\sigma}(u, \sigma) &= -\sigma \eta_{\sigma}(u), \\ \beta_{\tau}(u, \tau, \rho) &= -\tau[2 + \eta_{\tau}(u)] - \rho^2 b_{\tau}(u), \\ \beta_{\rho}(u, \rho) &= -\rho[1 + \eta_{\rho}(u)], \\ \beta_c(u, \lambda, \rho, c) &= -c[1 + \eta_c(u, \lambda)] - \rho b_c(u, \lambda),\end{aligned}\tag{11}$$

and

$$\beta_{\lambda}(u, \lambda) = \frac{-\beta_u(u, \epsilon) \partial_u P_{\lambda}(u, \lambda, \epsilon)}{1 + \partial_{\lambda} P_{\lambda}(u, \lambda, \epsilon)},\tag{12}$$

where the contributions involving  $b_{\tau}$  and  $b_c$  are produced by the terms proportional to  $A_{\tau}$  and  $A_c$  in equations (5) and (6), respectively.

Explicit two-loop results for the bulk quantities  $Z_{\phi, \sigma, \tau, u}$ ,  $\beta_u$  and  $\eta_{\phi, \sigma, \tau, \rho}$  can be found in Shpot and Diehl (2001); see also Diehl and Shpot (2000). The bulk function  $A_{\tau}$  is given to order  $u$  in equation (17) of Diehl *et al* (2003a), where also the renormalization functions  $Z_1$ ,  $Z_c$  and  $P_{\lambda}$  of the semi-infinite system were obtained to the same order in  $u$  for general values of  $\lambda \geq 0$ ; see its equations (21)–(23). The remaining surface counter-term  $A_c$  is computed in appendix A; we obtain

$$A_c(u, \lambda, \epsilon) = \frac{n+2}{3} \frac{u}{2\epsilon} \left[ \frac{1 - i_1(\lambda; m) - \lambda i_1'(\lambda; m)}{2\lambda} - \frac{\sqrt{\pi} \Gamma[(m+2)/4]}{2\Gamma(m/4)} \right] + O(u^2).\tag{13}$$

Utilizing these results gives the beta function

$$\beta_{\lambda}(u, \lambda) = -\frac{n+2}{6} i_1(\lambda; m) \lambda u + 2u^2 P_{\lambda}^{(2, -1)}(\lambda) + O(u^3)\tag{14}$$

and the exponent functions

$$\eta_1(u, \lambda) = -\frac{n+2}{6} i_1(\lambda; m) u + O(u^2)\tag{15}$$

and

$$\eta_c(u, \lambda) = -\frac{n+2}{6} [1 + \lambda i_1'(\lambda; m)] u + O(u^2).\tag{16}$$

Here  $i_1(\lambda; m)$  and  $i_1'(\lambda; m)$  are integrals defined through

$$i_1(\lambda; m) \equiv i_1(\lambda, \epsilon = 0; m),\tag{17}$$

$$i_1'(\lambda; m) \equiv i_1'(\lambda, \epsilon = 0; m),\tag{18}$$

$$i_1'(\lambda, \epsilon; m) \equiv \partial i_1(\lambda, \epsilon; m) / \partial \lambda,\tag{19}$$

$$i_1(\lambda, \epsilon; m) \equiv \left\langle \frac{1 - \lambda t}{1 + \lambda t} \right\rangle_{\epsilon, m},\tag{20}$$

where we have introduced the convenient notation  $\langle f(t) \rangle_{\epsilon, m}$  for the normalized average

$$\langle f(t) \rangle_{\epsilon, m} \equiv \frac{1}{\mathcal{N}_{\epsilon, m}} \int_0^1 dt f(t) t^{(m-2)/2} (1-t^2)^{(2-2\epsilon-m)/4}\tag{21}$$

over  $t$ . The normalization factor is given by

$$\mathcal{N}_{\epsilon,m} \equiv \int_0^1 dt t^{(m-2)/2} (1-t^2)^{(2-2\epsilon-m)/4} = \frac{1}{2} B[m/4, (6-2\epsilon-m)/4] \quad (22)$$

where  $B(a, b)$  is the Euler beta function. This choice of  $\mathcal{N}_{\epsilon,m}$  ensures that

$$i_1(0, \epsilon; m) = 1. \quad (23)$$

The  $t$ -integral required for  $i_1(\lambda; m)$  converges for  $0 < m < 6$ . Since the normalization factor varies as  $1/\mathcal{N}_{0,m} \sim (6-m)$  for  $m \rightarrow 6$ , the integral's singularity  $\sim (6-m)^{-1}$  gets cancelled to produce the finite limiting value

$$i_1(\lambda; 6-) \equiv \lim_{m \rightarrow 6-} i_1(\lambda; m) = \frac{1-\lambda}{1+\lambda}. \quad (24)$$

For general values  $m \in (0, 6)$ , the integral  $i_1(\lambda; m)$  can be expressed in terms of hypergeometric functions  ${}_2F_1$  and elementary ones. Term-wise integration of the integrand's Taylor series in  $\lambda$  or evaluation via Mathematica<sup>2</sup> leads to

$$i_1(\lambda; m) = {}_2F_1\left(1, \frac{m}{4}; \frac{3}{2}; \lambda^2\right) - 1 + \frac{\sqrt{\pi} \Gamma[(m-2)/4]}{\Gamma(m/4)\lambda} [1 - (1-\lambda^2)^{(2-m)/4}], \quad (25)$$

which simplifies considerably if  $m = 2$  or  $m = 6$ , giving

$$i_1(\lambda; 2) = 2\lambda^{-1} \ln(1+\lambda) - 1 \quad (26)$$

and

$$i_1(\lambda; 4) = \frac{\pi}{\lambda} - \frac{2 \arccos(\lambda)}{\lambda \sqrt{1-\lambda^2}} - 1, \quad (27)$$

respectively. Explicit plots of the functions  $-\lambda i_1(\lambda; m)$  for  $m = 1, 2, \dots, 6$  are displayed in figure 1 of Diehl *et al* (2003a).

Setting the relevant bulk variables  $\tau$  and  $\rho$  to zero and the coupling constant  $u$  to the nontrivial zero of  $\beta_u$  for  $\epsilon > 0$ , namely<sup>3</sup>

$$u^* = \frac{2\epsilon}{3} \frac{9}{n+8} + O(\epsilon^2), \quad (28)$$

we can analyse the RG flow and determine the fixed points in the  $c\lambda$  plane. This yields the schematic flow picture shown in figure 1 (Diehl *et al* 2003a).

The fixed points

$$\begin{aligned} \mathcal{P}_{\text{ord}}^*: & \quad (c_{\text{ord}}^* = \infty, \quad \lambda = \lambda_+^*), \\ \mathcal{P}_{\text{sp}}^*: & \quad (c_{\text{sp}}^* = 0, \quad \lambda = \lambda_+^*), \\ \mathcal{P}_{\text{ex}}^*: & \quad (c_{\text{ex}}^* = -\infty, \quad \lambda = \lambda_+^*), \end{aligned} \quad (29)$$

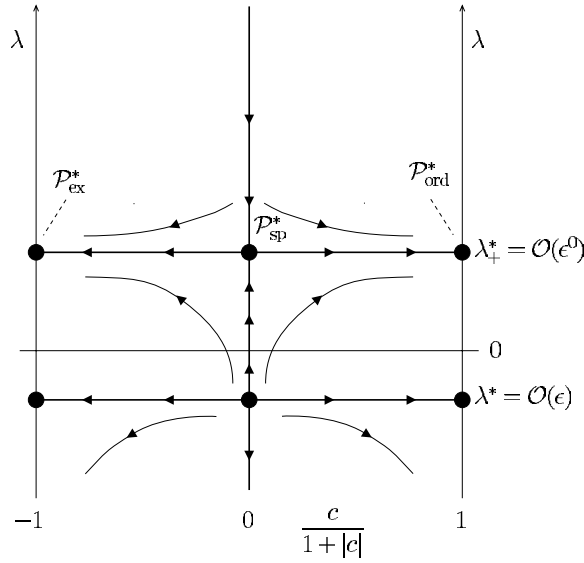
located at the positive value

$$\lambda_+^*(m) = \lambda_0(m) + \frac{72 P_\lambda^{(2,-1)}(\lambda_0)\epsilon}{(n+2)(n+8)\lambda_0 i_1'(\lambda_0; m)} + O(\epsilon^2), \quad (30)$$

should describe the ordinary, special and extraordinary transitions, respectively. Here  $\lambda_0 = \lambda_0(m)$  are the real positive zeros of the functions  $i_1(\lambda; m)$ ; for later use we list their

<sup>2</sup> Mathematica, version 4.1, a product of Wolfram Research.

<sup>3</sup> The expansion of  $u^*$  to  $O(\epsilon^2)$  can be found in equations (60) of Shpot and Diehl (2001) or equation (42) of Diehl *et al* (2003a). It will not be needed in the following because our subsequent analysis is based on one-loop results for the surface RG functions  $\beta_c$  and  $\eta_{1,c}$ .



**Figure 1.** Schematic picture of the RG flow in the  $c\lambda$  plane at  $\rho = \tau = 0$  and  $u = u^*$ , showing the fixed points  $\mathcal{P}_{\text{ord}}^*$ ,  $\mathcal{P}_{\text{sp}}^*$  and  $\mathcal{P}_{\text{ex}}^*$  specified in equation (29).

**Table 1.** Zeros  $\lambda_0(m)$ , derivatives  $i_1'(\lambda; m)$  and coefficients  $1 + \lambda_0 i_1'(\lambda_0; m)$  appearing in the  $O(\epsilon)$  terms of  $\eta_c^*$ ; see equation (60). In the second column the exact limiting values for  $m \rightarrow 0$  are listed. The values for  $m = 1, \dots, 5$  are approximate numerical numbers; those for  $m = 6$  are exact.

$m$	0	1	2	3	4	5	6
$\lambda_0(m)$	$\infty$	6.209 21	2.512 86	1.701 76	1.342 77	1.136 29	1
$-i_1'[\lambda_0(m); m]$	0	0.055 05	0.171 38	0.273 32	0.359 49	0.434 00	$\frac{1}{2}$
$1 + \lambda_0(m)i_1'[\lambda_0(m); m]$	1	0.658 16	0.569 34	0.534 88	0.517 29	0.506 85	$\frac{1}{2}$

values in table 1. We have included the limiting values for  $m \rightarrow 0$ . Of course, for  $m = 0$ , the variable  $\lambda$  becomes meaningless. However, considering  $m$  as a continuous variable, we can ask what happens to the RG flow, the zero  $\lambda_0(m)$  and the critical exponents as  $m \rightarrow 0$ . Utilizing either the integral representation (17) of  $i_1(\lambda; m)$  or the explicit form (25) one easily verifies that  $\lim_{m \rightarrow 0} i_1(\lambda; m) = 1$  for arbitrary fixed  $\lambda \geq 0$ . Hence the root  $\lambda_0(m)$  must approach infinity in this limit. To obtain its limiting behaviour, one can work out the asymptotic expansion of  $i_1$  for  $\lambda \rightarrow \infty$  at fixed  $m < 2$ . A straightforward analysis yields

$$i_1(\lambda; m) \underset{\lambda \rightarrow \infty}{=} -1 + \lambda^{-m/2} \frac{2\pi^{3/2} \csc(m\pi/2)}{\Gamma(m/4)\Gamma[6-m)/4]} + O(\lambda^{-1}), \tag{31}$$

which implies the small- $m$  form

$$\lambda_0(m) \underset{m \rightarrow 0}{\approx} e \times 2^{(2-m)/m}. \tag{32}$$

An evident consequence of these two equations is that the product  $\lambda_0(m)i_1'[\lambda_0(m); m]$  (which will be needed below) vanishes for  $m \rightarrow 0$ .



### 3. RG analysis of the special transition

In order to analyse the asymptotic behaviour described by the special fixed point  $\mathcal{P}_{\text{sp}}^*$ , we must determine the relevant bulk and scaling fields that can be constructed from  $\tau$ ,  $\rho$  and  $c$ . Following Diehl *et al* (2003a), we choose the coefficient  $C_{\rho^2}^\tau(u)$  in equation (9) such that the running variable  $\bar{g}_\tau(\ell)$  into which  $g_\tau$  transforms under a scale change  $\mu \rightarrow \mu\ell$  satisfies

$$\ell \frac{d}{d\ell} \bar{g}_\tau(\ell) = -[2 + \eta_\tau(\bar{u})] \bar{g}_\tau(\ell), \quad \bar{g}_\tau(1) = g_\tau, \quad (33)$$

where the asterisk on functions of  $u$  means their value at  $u = u^*$ .

Upon taking into account the flow equations

$$\ell \frac{d}{d\ell} \bar{\wp}(\ell) = \beta_\wp[\bar{u}(\ell), \dots], \quad \bar{\wp}(1) = \wp, \quad \wp = u, \sigma, \tau, \rho, c, \lambda, \quad (34)$$

one easily derives the condition

$$b_\tau(\bar{u}) = [\eta_\tau(\bar{u}) - 2\eta_\rho(\bar{u}) + \beta_u(\bar{u}, \epsilon) \partial_{\bar{u}}] C_{\rho^2}^\tau(\bar{u}), \quad (35)$$

which is easily solved for  $\bar{u}$  near  $u^*$  to obtain

$$C_{\rho^2}^\tau(\bar{u}) = \frac{b_\tau^*}{\eta_\tau^* - 2\eta_\rho^*} + O(\bar{u} - u^*). \quad (36)$$

We fix the coefficient  $C_\rho^c$  of the scaling field  $g_c$  in a similar fashion. Requiring that

$$\ell \frac{d}{d\ell} \bar{g}_c(\ell) = -[1 + \eta_c(\bar{u}, \bar{\lambda})] \bar{g}_c(\ell), \quad \bar{g}_c(1) = g_c, \quad (37)$$

we arrive at the condition

$$b_c(\bar{u}, \bar{\lambda}) = [\eta_c(\bar{u}, \bar{\lambda}) - \eta_\rho(\bar{u}) + \beta_u(\bar{u}, \epsilon) \partial_{\bar{u}} + \beta_\lambda(\bar{u}, \bar{\lambda}) \partial_{\bar{\lambda}}] C_\rho^c(\bar{u}, \bar{\lambda}), \quad (38)$$

which in turn yields

$$C_\rho^c(\bar{u}, \bar{\lambda}) = \frac{b_c^*}{\eta_c^* - \eta_\rho^*} + O(\bar{u} - u^*, \bar{\lambda} - \lambda_+^*) \quad (39)$$

for  $(u, \lambda)$  sufficiently close to the fixed-point values  $(u^*, \lambda_+^*)$ , where the asterisk on functions of  $u$  and  $\lambda$  indicates their values for  $(u, \lambda) = (u^*, \lambda_+^*)$ , i.e. at the fixed point  $\mathcal{P}_{\text{sp}}^*$ .

Clearly, the mixing of  $\tau$  and  $c$  with  $\rho$  should vanish as  $m \rightarrow 0$ . This is indeed the case as we see from the explicit  $O(u)$  results

$$b_\tau(u) = \frac{n+2}{3} \frac{mu}{16} + O(u^2) \quad (40)$$

and

$$b_c(u, \lambda) = -\frac{n+2}{3} \left[ \frac{1 - i_1(\lambda; m) - \lambda i_1'(\lambda; m)}{4\lambda} - \frac{\sqrt{\pi} \Gamma[(m+2)/4]}{4\Gamma(m/4)} \right] u + O(u^2), \quad (41)$$

the first of which was obtained in Diehl *et al* (2003a), while the second follows from equation (13). Note that the  $O(u)$  terms of both  $b_\tau$  and  $b_c$  vanish in the limit  $m \rightarrow 0$  quite generally, not only at the fixed point  $\mathcal{P}_{\text{sp}}^*$ .

From equations (33) and (37) we can read off the RG eigenexponents of the scaling fields  $g_\tau$  and  $g_c$ . Writing them as  $1/\nu$  and  $\Phi/\nu$ , respectively, we identify the standard correlation-length exponent

$$\nu = (2 + \eta_\tau^*)^{-1} \quad (42)$$

(denoted by  $\nu_{l2}$  in Shpot and Diehl (2001), Diehl *et al* (2003a)) and the surface crossover exponent

$$\Phi = \nu(1 + \eta_c^*). \quad (43)$$

Let us also introduce the bulk anisotropy exponent

$$\theta = \frac{1}{4}(2 + \eta_\sigma^*), \quad (44)$$

the familiar bulk critical exponents

$$\eta = \eta_\phi^*, \quad \beta = \frac{1}{2}\nu[d - 2 + \eta + m(\theta - 1)], \quad (45)$$

(denoted by  $\eta_{l2}$  and  $\beta_l$ , respectively, in Shpot and Diehl (2001), Diehl *et al* (2003a)), the bulk crossover exponent

$$\varphi = \nu(1 + \eta_\rho^*) \quad (46)$$

as well as the surface critical indices

$$\eta_{\parallel}^{\text{sp}} = \eta + \eta_1^* \quad (47)$$

and

$$\beta_1^{\text{sp}} = \frac{1}{2}\nu[d - 2 + \eta_{\parallel}^{\text{sp}} + m(\theta - 1)] = \beta + \frac{1}{2}\nu\eta_1^* \quad (48)$$

of the special transition.

It is now straightforward to solve the RG equation (10) via characteristics and derive the asymptotic scaling forms of the cumulants  $G^{(N,M)}$  near the special transition. Setting  $\mu = \sigma = 1$  for notational simplicity and neglecting corrections to scaling, we obtain

$$G_{\text{ren}}^{(N,M)}(r_\alpha, r_\beta, z; \rho, g_\tau, u, g_c, \lambda) \approx g_\tau^{N\beta + M\beta_1^{\text{sp}}} \mathcal{G}^{(N,M)}[r_\alpha g_\tau^{\nu\theta}, r_\beta g_\tau^\nu, z g_\tau^\nu; \rho g_\tau^{-\varphi}, g_c g_\tau^{-\Phi}]. \quad (49)$$

The special choice  $N = 0$  and  $M = 1$  shows that our identification (48) of  $\beta_1^{\text{sp}}$  is correct. On the other hand, our definition (47) of  $\eta_{\parallel}^{\text{sp}}$  may need explanation. Noting that the surface cumulant  $G_{\text{ren}}^{(0,2)}(\mathbf{r}, \mathbf{0})$  should have a well-defined limit as  $g_\tau, \sigma$  and  $g_c$  approach zero, we can read from equation (49) that this function decays at the special transition as

$$G_{\text{ren}}^{(0,2)}(\mathbf{r}, \mathbf{0}) \sim \begin{cases} r^{-[d-2+m(\theta-1)+\eta_{\parallel}]} & \text{for } r_\alpha = 0, \\ r^{-[d-2+m(\theta-1)+\eta_{\parallel}]/\theta} & \text{for } r_\beta = 0 \end{cases} \quad (50)$$

in the limit of large separations  $r$  (parallel to the surface). This translates into the small-momentum behaviour

$$\chi_{11}(\mathbf{p}) \sim \begin{cases} p^{\eta_{\parallel}-1}, & \text{for } p_\alpha = 0, \\ p^{(\eta_{\parallel}-1)/\theta}, & \text{for } p_\beta = 0, \end{cases} \quad (51)$$

of the momentum-dependent local surface susceptibility  $\chi_{11}(\mathbf{p}) = \hat{G}^{(0,2)}(\mathbf{p})$  (its Fourier transform), where  $\mathbf{p} = (p_\alpha, p_\beta)$  is the wave-vector conjugate to  $\mathbf{r} = (r_\alpha, r_\beta)$ . We have suppressed the specification ‘sp’ on  $\eta_{\parallel}$  in these two equations because analogous results hold in the case of the ordinary transition, with  $\eta_{\parallel}$  given by  $\eta_{\parallel}^{\text{ord}}$ , its analogue for the ordinary transition (Diehl *et al* 2003a, 2003b). For  $m = 0$ , the above dependences on  $r$  and  $p$  for  $r_\alpha = 0$  and  $p_\alpha = 0$ , respectively, reduce to the familiar power laws for the case of the special transition at a bulk *critical* point (Diehl and Dietrich 1981, 1983). Henceforth we will refer to this surface transition as the ‘critical-point (CP) special transition’, calling its  $m > 0$  analogues we are concerned with here ‘Lifshitz-point (LP) special transitions’.

Note also that the scaling forms (49) can be exploited in a straightforward fashion to generalize the standard scaling laws of the CP case to  $m > 0$ . Consider, for example, the

surface critical exponent  $\eta_{\perp}$  defined through the decay

$$G^{(1,1)}[(\mathbf{r}, z), \mathbf{r}] \sim z^{-[d-2+m(\theta-1)+\eta_{\perp}]} \quad (52)$$

at the LP.<sup>4</sup> Upon introducing the momentum-dependent layer surface susceptibility

$$\chi_1(\mathbf{p}) \equiv \int_0^{\infty} dz \hat{G}^{(1,1)}(\mathbf{p}; z), \quad (53)$$

we find from equation (52) the small-momentum behaviour  $\chi_1(\mathbf{p}) \sim p^{\eta_{\perp}-2}$  or  $\sim p^{(\eta_{\perp}-2)/\theta}$ , depending on whether  $p_{\alpha} = 0$  or  $p_{\beta} = 0$ . The result (49) implies that the familiar scaling law

$$\eta_{\perp} = \frac{1}{2}(\eta + \eta_{\parallel}) \quad (54)$$

holds. Furthermore, let  $\gamma_{11}$ ,  $\gamma_1$ ,  $\beta_s$  and  $\gamma_s$  denote the critical indices that characterize, at  $\rho = c = 0$ , the thermal singularities of the surface susceptibilities  $\chi_{11} \equiv \chi_{11}(\mathbf{0})$  and  $\chi_1 \equiv \chi_1(\mathbf{0})$ , the surface excess order parameter

$$m_s = \int_0^{\infty} [G^{(0,1)}(\mathbf{r}, z) - G^{(0,1)}(\mathbf{r}, \infty)] dz \quad (55)$$

and the surface excess susceptibility  $\chi_s \equiv dm_s/dh|_{h=0}$ , its derivative with respect to a bulk magnetic field  $h$ , via  $\chi_{11}^{\text{sing}} \sim g_{\tau}^{-\gamma_{11}}$ ,  $\chi_1^{\text{sing}} \sim g_{\tau}^{-\gamma_1}$ ,  $m_s \sim g_{\tau}^{\beta_s}$  and  $\chi_s^{\text{sing}} \sim g_{\tau}^{-\gamma_s}$ , respectively. From equations (49) and (52) we see that the scaling laws

$$\gamma_{11} = \nu(1 - \eta_{\parallel}), \quad \gamma_1 = \nu(2 - \eta_{\perp}), \quad (56)$$

and

$$\beta_s = \beta - \nu, \quad \gamma_s = \gamma + \nu, \quad (57)$$

also remain valid for  $m > 0$ .

Finally, let us briefly consider the surface energy density  $\langle [\phi^{\text{SB}}(\mathbf{r})]^2 \rangle$ . In analogy to the CP case (Dietrich and Diehl 1981), the renormalization of this quantity involves further (additive) counter-terms, and the implied RG equation becomes inhomogeneous. We refrain from working out the details here, noting that the form

$$\langle [\phi^{\text{SB}}(\mathbf{r})]^2 \rangle^{\text{sing}} \sim g_{\tau}^{2-\alpha-\nu-\Phi} \quad (g_c = \rho = 0) \quad (58)$$

of its thermal singularity at  $\rho = c = 0$  can be inferred from equation (49).

Next, we turn to the  $\epsilon$ -expansion of the surface critical exponents of the special transition. From equation (15) we see that the  $O(\epsilon)$  contribution to the fixed-point value  $\eta_1^*$  vanishes for all  $m > 0$ , so that

$$\eta_{\parallel}^{\text{sp}} - \eta = \eta_1^* = O(\epsilon^2) \quad (m > 0). \quad (59)$$

On the other hand, substitution of the fixed-point values (28) and (30) into equation (16) yields

$$\frac{\Phi}{\nu} - 1 = \eta_c^* = -\frac{n+2}{n+8} [1 + \lambda_0(m) i_1'(\lambda_0; m)] \epsilon + O(\epsilon^2). \quad (60)$$

Let us see what happens to these results in the limit  $m \rightarrow 0$ . Equation (60) reduces indeed for  $m \rightarrow 0$  to the correct  $O(\epsilon)$  result for the CP case, just as the  $\epsilon$ -expansions of the bulk critical exponents (Diehl and Shpot 2000, Shpot and Diehl 2001) and the surface critical exponents of the LP ordinary transitions (Diehl *et al* 2003a, 2003b) do. On the other hand, the  $O(\epsilon)$  term of the exponent  $\eta_{\parallel}^{\text{sp}}$  of the CP special transition is known to be *nonzero* (Bray and Moore 1977, Diehl and Dietrich 1981, 1983). Consequently, the limits  $m \rightarrow 0$  of

<sup>4</sup> This exponent may be defined more generally through the decay of the pair correlation function  $G^{(2,0)}(\mathbf{x}, \mathbf{x}')$  at criticality as  $\mathbf{x}'$  moves away from the surface along a direction perpendicular (or at least not parallel) to it while  $\mathbf{x}'$  is fixed, similarly as in the CP case (Diehl and Dietrich 1981, 1983, Diehl 1986).

the  $\epsilon$ -expansion (59) of  $\eta_{\parallel}^{\text{sp}}$  (as well as those of related surface exponents such as  $\beta_1^{\text{sp}}$ ) differ from those of their  $m = 0$  counterparts for the CP special transition. Nevertheless, this is no cause for concern. The obvious reason for the apparent discrepancy between the  $m \rightarrow 0$  limit of our result for  $\eta_{\parallel}^{\text{sp}}$  and the established one for  $m = 0$  is that the limits  $\lambda \rightarrow \lambda_+^*(m)$  and  $m \rightarrow 0$  do not commute. Taking the limit  $m \rightarrow 0$  last means to let  $m \rightarrow 0$  while  $\lambda$  follows the root  $\lambda_+^*(m)$  on its way to infinity. Since  $\eta_1[u^*, \lambda_+^*(m)]$  is of order  $\epsilon^2$ , so is its limit  $m \rightarrow 0$ .

However, in order to compare with the CP case, the relevant problem to consider is the following. Given a generic initial value  $\bar{\lambda}(1) \equiv \lambda < \infty$ , what asymptotic behaviour does the RG flow for  $m \rightarrow 0$  yield on large length scales? Noting that the running variable  $\bar{\lambda}(\ell) \rightarrow \infty$ , we see that the appropriate limit of  $\eta_1$  that matters is  $\lim_{\bar{\lambda} \rightarrow \infty} \lim_{m \rightarrow 0} \eta_1(u^*, \bar{\lambda})$ . This implies the replacement of the integral  $i_1(\lambda; m)$  by its  $m \rightarrow 0$  limit  $i_1 \equiv 1$  in our result (15) for  $\eta_1(u, \lambda)$ , whereby it reduces to the correct one-loop expression for the CP case. Upon insertion of its value at  $u = u^*$  into equation (59), the familiar result for the exponent  $\eta_{\parallel}^{\text{sp}}$  of the CP special transition is recovered to order  $\epsilon$ . Thus, extrapolated to  $m = 0$ , the RG flows obtained here yield results in conformity with the CP case, despite the mentioned difference between the  $m \rightarrow 0$  limit of equation (59) and the  $\epsilon$ -expansion of  $\eta_{\parallel}^{\text{sp}}$  for the CP case.

Let us try to use the results (59) and (60) to estimate the values of the associated surface critical exponents of the three-dimensional ANNNI model. Since we know these series expansions merely to first order in  $\epsilon$ , only crude estimates are possible. Clearly, it is desirable to exploit as much as possible the improved knowledge about the bulk critical exponents gained in Diehl and Shpot (2000), Shpot and Diehl (2001). It appears preferable to focus directly on estimates of the differences  $\eta_{\parallel}^{\text{sp}} - \eta$  or  $\beta_1^{\text{sp}} - \beta$  (both of which are proportional to  $\eta_1^*$ ) and the ratio  $\Phi/\nu$ , rather than extrapolating the expansions to  $O(\epsilon)$  of surface critical indices such as  $\eta_{\parallel}^{\text{sp}}$ ,  $\beta_1^{\text{sp}}$  or surface susceptibility exponents and  $\Phi$ .

From the result (59) we conclude that the differences  $\eta_{\parallel}^{\text{sp}} - \eta$  and  $\beta_1^{\text{sp}} - \beta$  are likely to be small. Accepting the best estimate  $\eta \simeq 0.124$  of Shpot and Diehl (2001) for the uniaxial scalar case in  $d = 3$  dimensions, we conclude that  $\eta_{\parallel}^{\text{sp}} \simeq 0.1$ . One way of estimating  $\beta_1^{\text{sp}}$  is to employ the values  $\nu \simeq 0.746$ ,  $\theta = \nu_{1d}/\nu \simeq 0.348/0.746 \simeq 0.47$  of Shpot and Diehl (2001) in equation (48), along with the approximation  $\eta_{\parallel}^{\text{sp}} \simeq \eta \simeq 0.126$ . This gives  $\beta_1^{\text{sp}} \simeq 0.22$ . If the slightly bigger value  $\theta \simeq 0.487$  quoted in Diehl (2002) (and found by direct extrapolation of the  $\epsilon$ -expansion of  $\theta$ ) is utilized instead, one obtains  $\beta_1^{\text{sp}} \simeq 0.23$ . The agreement with Pleimling's Monte Carlo estimate  $\beta_1^{\text{sp}} = 0.23(1)$  is impressive. Another possibility is to start from the second part of equation (48) and utilize the estimate  $\beta_1^{\text{sp}} \simeq \beta$ . The best estimate of Shpot and Diehl (2001) for  $\beta$  was  $\beta \simeq 0.246$ . The most recent Monte Carlo result  $\beta = 0.238 \pm 0.005$  (Pleimling 2002, 2004, Pleimling and Henkel 2001) is in conformity with this and lends support to the approximation  $\beta \simeq \beta_1^{\text{sp}}$ .

Unfortunately, we are not aware of any estimates of the surface crossover exponent  $\Phi$  at  $d = 3$ . If we take again  $m = n = 1$  and boldly set  $\epsilon = 3/2$  in the expansion (60), truncated at  $O(\epsilon)$ , we obtain  $\Phi/\nu \simeq \frac{1}{3} \times 1.65816 \times \frac{3}{2} \simeq 0.83$ . Utilizing once more the value  $\nu \simeq 0.746$  then yields  $\Phi \simeq 0.62$ . We must caution the reader, however, to take these estimates *cum grano salis*: the  $\epsilon$ -expansion to first order does not in general give reliable results. Moreover, in the CP case ( $m = 0$ ), the  $\epsilon^2$  term of the crossover exponent  $\Phi$  is known to have a rather large coefficient (Diehl and Dietrich 1981, 1983), a fact which makes it difficult to obtain precise estimates even from the  $\epsilon$ -expansion to second order. Borel–Padé estimates based on the massive field theory approach at fixed  $d = 3$  (Diehl and Shpot 1994, 1998) give values  $\Phi_{d=3, m=0, n=1} \simeq 0.54$  considerably smaller than the original one ( $\simeq 0.68$ ) found in Diehl and Dietrich (1991, 1983), Diehl (1986) by evaluating the  $\epsilon$ -expansion to second order at

$d = 3$ , though in much better agreement with Monte Carlo results (Landau and Binder 1990, Ruge *et al* 1992, 1993).

In extrapolating our  $\epsilon$ -expansion results for the scalar uniaxial case  $m = n = 1$  to three dimensions, we took it for granted that an LP special transition is possible at  $d = 3$ . Clearly, a transition to a surface phase with long-range order should be possible at temperatures  $T_s$  higher than the line of bulk critical temperatures  $T_c$  if  $m = n = 1$ . Since  $T_s$  can be varied through a change of surface interaction constants, one expects that for appropriately fine-tuned surface enhancement  $T_s$  can become equal to the LP temperature, so that a special LP transition ought to be possible at  $d = 3$ , as also recent Monte Carlo results (Pleimling 2002) indicate.

For other values of  $m$  and  $n$  extrapolations to  $d = 3$  make little sense. Since we precluded in the Hamiltonian (1)–(3) any (bulk and surface) terms breaking its  $O(n)$  symmetry, a bulk-disordered surface phase with long-range order—and hence a special transition of the kind considered above—cannot occur for  $d = 3$  if  $n > 1$  because it would require the breaking of a continuous symmetry in an effectively two-dimensional system.

It is tempting to anticipate the possibility of a special transition for the biaxial scalar case  $m = 2, n = 1$ . However, in the case of a multi-axial LP, one generically expects contributions to the Hamiltonian that break its rotational invariance in the  $(m > 1)$ -dimensional subspace of  $\alpha$ -coordinates, such as bulk terms of cubic symmetry,  $\sum_{\alpha=1}^n (\partial_{\alpha}^2 \phi)^2$ , and similar space anisotropies of further reduced symmetry. According to a recent two-loop RG analysis (Diehl *et al* 2003c), such anisotropies are relevant, at least for small  $\epsilon > 0$ . Unfortunately, no stable new (anisotropic) fixed point could be found. To our knowledge, Monte Carlo investigations of appropriate biaxial generalization of the  $d = 3$  ANNNI model have not yet been carried out. Thus, whenever such anisotropies cannot be ruled out, it is presently unclear whether a biaxial bulk LP exists, in particular in three dimensions. The clarification of this issue is beyond the scope of the present paper. Note also that in order to account for the absence of rotational symmetry in the  $m$ -dimensional subspace, we would have to generalize the surface part  $\mathcal{L}_1$  of the Hamiltonian by allowing its derivative term to become anisotropic as well.

#### 4. RG improved perturbation theory

In the previous section we exploited the RG equations (10) to deduce the scaling forms (49) of the  $(N + M)$ -point cumulants (4). A tacit assumption underlying this derivation is that the renormalized cumulants  $G_{\text{ren}}^{(N,M)}$  are well behaved at the fixed point  $\mathcal{P}_{\text{sp}}^*$ . More precisely, these functions were assumed to approach for  $\epsilon > 0$  finite and nonzero limits, as  $\lambda$  and  $u$  approach their respective fixed-point values  $\lambda_+^*$  and  $u^*$ . This can and should be checked within the framework of RG improved perturbation theory. Furthermore, other conditions exist to which this statement applies just as much. For example, consistency of the scaling forms for  $g_{\tau} \neq 0$  with their counterparts for  $g_{\tau} = 0$  imposes constraints on the asymptotic  $g_{\tau}$ -dependence of the scaling function for  $g_{\tau} \rightarrow 0$ . Further constraints concern the dependence on  $g_c$ ; they arise from matching requirements between the  $g_c$ -dependent scaling forms and the asymptotic behaviour at those transitions to which the special transition crosses over, namely the ordinary, surface or extraordinary transition.

Our aim here is the explicit verification of some of these properties by means of RG improved perturbation theory to one-loop order. For the sake of simplicity, we will restrict ourselves to the illustrative case of the (renormalized) surface susceptibility

$\chi_{11}^{(\text{ren})}(\mathbf{p})$ . We begin by considering this quantity at  $\tau = \rho = 0$  for general nonzero momentum  $\mathbf{p} = (p_\alpha, p_\beta) \in \mathbb{R}^{d-1}$  as a function of  $g_c$ . Upon introducing the dimensionless momenta

$$\hat{p} = (p_\beta p_\beta / \mu^2)^{1/2}, \quad \hat{P} = (\sigma^{1/2} p_\alpha p_\alpha / \mu)^{1/2}, \quad (61)$$

we can write its scaling form as

$$\chi_{11}^{(\text{ren})}(\mathbf{p}) \approx \mu^{-1} \hat{p}^{\eta_{\parallel}^{\text{sp}}-1} \Xi(\hat{P} \hat{p}^{-\theta}, g_c \hat{p}^{-\Phi/\nu}) \quad (62)$$

$$= \mu^{-1} \hat{P}^{(\eta_{\parallel}^{\text{sp}}-1)/\theta} \Psi(\hat{P} \hat{p}^{-\theta}, g_c \hat{p}^{-\Phi/\nu}), \quad (63)$$

where the scaling functions  $\Psi$  and  $\Xi$  are related to each other via

$$\Psi(\mathbf{P}, \mathbf{c}) = \mathbf{P}^{(1-\eta_{\parallel}^{\text{sp}})/\theta} \Xi(\mathbf{P}, \mathbf{c}). \quad (64)$$

Consistency with the scaling forms that hold if either  $\hat{p} = 0$  or  $\hat{P} = 0$  requires the limiting behaviour

$$\Xi(\mathbf{P}, \mathbf{c}) \approx \begin{cases} \Xi_0(\mathbf{c}) & \text{for } \mathbf{P} \rightarrow 0, \\ \mathbf{P}^{(\eta_{\parallel}^{\text{sp}}-1)/\theta} \Psi_\infty(\mathbf{c}) & \text{for } \mathbf{P} \rightarrow \infty. \end{cases} \quad (65)$$

Next we consider the limits  $\hat{p} \rightarrow 0$  and  $\hat{P} \rightarrow 0$  for  $g_c > 0$ . The limiting dependences on  $\hat{p}$  and  $\hat{P}$  must be in conformity with the leading infrared singularities  $\sim \hat{p}^{\eta_{\parallel}^{\text{ord}}-1}$  and  $\sim \hat{P}^{(\eta_{\parallel}^{\text{ord}}-1)/\theta}$  at the ordinary transition. Hence we anticipate that  $\Xi$  varies for  $\mathbf{c} \rightarrow \infty$  as

$$\Xi(\mathbf{P}, \mathbf{c}) \underset{\mathbf{c} \rightarrow \infty}{\approx} \mathbf{c}^{-\nu(1-\eta_{\parallel}^{\text{sp}})/\Phi} [X_{11} + Y_1 \mathbf{P}^2 \mathbf{c}^{-2\nu\theta/\Phi} + \dots] + \mathbf{c}^{-\nu(\eta_{\parallel}^{\text{ord}}-\eta_{\parallel}^{\text{sp}})/\Phi} \Xi_\infty(\mathbf{P}) + \dots, \quad (66)$$

where  $X_{11}$  and  $Y_1$  are constants, while  $\Xi_\infty(\mathbf{P})$  behaves as

$$\Xi_\infty(\mathbf{P}) \approx \begin{cases} \Xi_{\infty,0} \equiv \Xi_\infty(0) & \text{for } \mathbf{P} \rightarrow 0, \\ \Xi_{\infty,\infty} \mathbf{P}^{(\eta_{\parallel}^{\text{ord}}-1)/\theta} & \text{for } \mathbf{P} \rightarrow \infty. \end{cases} \quad (67)$$

The latter properties ensure that the term of equation (66) following the square brackets produces the required powers  $\hat{p}^{\eta_{\parallel}^{\text{ord}}-1}$  and  $\hat{P}^{(\eta_{\parallel}^{\text{ord}}-1)/\theta}$ . To understand the terms of equation (66) involving the square brackets, one should recall that  $\chi_{11}$  remains *finite* at the ordinary transition. Thus a momentum-independent contribution to  $\chi_{11}^{(\text{ren})}(\mathbf{0})$  must exist, apart from additional ones with analytic momentum dependence. The contribution  $\propto X_{11}$  accounts for the former; except for a contribution proportional to  $\hat{P}^2$ , terms of the latter analytic kind have been suppressed, along with momentum-dependent subleading corrections.

In appendix B the renormalized function  $\chi_{11}^{(\text{ren})}$  is computed to one-loop order for  $\tau = \rho = 0$  and general values of  $c \geq 0$  and  $\lambda \geq 0$ . The result can be written as

$$\begin{aligned} \frac{\mu}{\chi_{11}^{(\text{ren})}(\mathbf{p})} &= \kappa_p + c + \lambda \hat{P}^2 + \frac{u}{2} \frac{n+2}{3} \left\{ [(\kappa_p + c)i_1 + c(1 + \lambda i_1')] \ln(2\kappa_p) - c\lambda i_1^{(1,1)} \right. \\ &\quad \left. - (\kappa_p + c)i_1^{(0,1)} + 2 \frac{c^2}{\hat{p}} \mathcal{A}(\hat{P}/\sqrt{\hat{p}}, c/\hat{p}, \lambda) + O(\epsilon) \right\} + O(u^2), \end{aligned} \quad (68)$$

where

$$\kappa_p \equiv \sqrt{\hat{p}^2 + \hat{P}^4}, \quad (69)$$

while the function  $\mathcal{A}$  is an average of the form (21):

$$\mathcal{A}(\mathbf{P}, \mathbf{c}, \lambda) \equiv \left\langle \frac{\ln[\mathbf{c}/(1 + \lambda t)\sqrt{1 + \mathbf{P}^4}]}{(1 + \lambda t)^2 [\mathbf{c} - (1 + \lambda t)\sqrt{1 + \mathbf{P}^4}]} \right\rangle_{0,m}. \quad (70)$$

Further,  $i_1^{(0,1)}$  and  $i_1^{(1,1)}$  denote the partial derivatives  $\partial i_1/\partial \epsilon$  and  $\partial^2 i_1/\partial \epsilon \partial \lambda$ , respectively. Just as  $i_1$  and  $i_1'$ , these are to be evaluated at  $\epsilon = 0$  in equation (68).

From the perturbative result (68), the universal scaling function  $\Xi(\mathbf{P}, \mathbf{c})$  must follow up to non-universal metric factors upon setting the coupling constants  $u$  and  $\lambda$  to their fixed-point values (28) and (30)<sup>5</sup>. Recalling the  $O(\epsilon)$  expressions (59) and (60) for  $\eta_{\parallel}^{\text{sp}}$  and  $\Phi/\nu$ , one easily verifies that  $\chi_{11}^{(\text{ren})}$  takes indeed the scaling form (62), where the scaling function is given by

$$\frac{1}{\Xi(\mathbf{P}, \mathbf{c})} = a_n(\epsilon)\sqrt{1+\mathbf{P}^4} + b_n(\epsilon)\mathbf{c} + \lambda_0\mathbf{P}^2 + \frac{n+2}{n+8}\epsilon\{2\mathbf{c}^2\mathcal{A}(\mathbf{P}, \mathbf{c}, \lambda_0) + \mathbf{c}[1 + \lambda_0 i_1'(\lambda_0; m)] \ln[2\sqrt{1+\mathbf{P}^4}]\} + O(\epsilon^2) \quad (71)$$

with

$$a_n(\epsilon) = 1 - \epsilon \frac{n+2}{n+8} i_1^{(0,1)}(\lambda_0, 0; m) \quad (72)$$

and

$$b_n(\epsilon) = 1 - \epsilon \frac{n+2}{n+8} [i_1^{(0,1)}(\lambda_0, 0; m) + \lambda_0 i_1^{(1,1)}(\lambda_0, 0; m)]. \quad (73)$$

Obviously, the limiting forms (65) for small and large  $\mathbf{P}$  hold. Checking the consistency with the critical behaviour at the ordinary transition is less trivial because the  $\epsilon$ -expanded version (71) of the scaling function does not yet contain the anticipated asymptotic power laws (65) and (66) in exponentiated form. To proceed, we consider the behaviour of  $\Xi^{-1}$  as  $\mathbf{c} \rightarrow \infty$ . The leading contributions are of order  $\mathbf{c} \ln \mathbf{c}$ . One finds that the terms  $\propto \ln \sqrt{1+\mathbf{P}^4}$  of this order cancel. The remaining (momentum-independent) terms  $\sim \mathbf{c} \ln \mathbf{c}$  can be combined with part of the contributions  $\sim \mathbf{c}$  to identify the power  $\mathbf{c}^{1-\eta_c^*}$  to  $O(\epsilon)$ . The associated exponent satisfies  $1 - \eta_c^* = \nu(1 - \eta_{\parallel}^{\text{sp}})/\Phi + O(\epsilon^2)$ . Hence this contribution gives rise to the first term in equation (66). For its amplitude  $X_{11}$  we obtain the  $\epsilon$ -expansion

$$X_{11}^{-1} = 1 - \epsilon \frac{n+2}{n+8} \left\{ i_1^{(0,1)}(\lambda_0, 0; m) + \lambda_0 i_1^{(1,1)}(\lambda_0, 0; m) + 2 \left\langle \frac{\ln(1 + \lambda_0 t)}{(1 + \lambda_0 t)^2} \right\rangle_{0,m} - [1 + \lambda_0 i_1'(\lambda_0; m)] \ln 2 \right\} + O(\epsilon^2). \quad (74)$$

Turning to the contributions of order  $\ln \mathbf{c}$  and  $\mathbf{c}^0$ , we note that the former can be combined with part of the latter to obtain the term  $\epsilon \frac{n+2}{n+8} \kappa \ln(\mathbf{c}/\kappa)$ , where  $\kappa \equiv \sqrt{1+\mathbf{P}^4}$ , and we employed the fact that  $\langle (1 + \lambda_0)^{-1} \rangle_{0,m} = (i_1(\lambda_0; m) + \langle 1 \rangle_{0,m})/2 = 1/2$ . This logarithm can be cast in the form  $\kappa[(\mathbf{c}/\kappa)^{\epsilon(n+2)/(n+8)} - 1] + O(\epsilon^2)$ . Recalling the  $\epsilon$ -expansion

$$\eta_{\parallel}^{\text{ord}} = 2 - \epsilon \frac{n+2}{n+8} + O(\epsilon^2), \quad (75)$$

one easily verifies that the term  $\kappa(\mathbf{c}/\kappa)^{\epsilon(n+2)/(n+8)}$  produces a contribution to  $\Xi$  consistent with the form of the term of equation (66) after the closing square bracket, with

$$\Xi_{\infty}(\mathbf{P}) = -(1 + \mathbf{P}^4)^{(\eta_{\parallel}^{\text{ord}} - 1)/4\theta} [1 + O(\epsilon)]. \quad (76)$$

Furthermore, the term  $\propto \lambda_0 \mathbf{P}^2$  in equation (71) yields an analytic contribution  $\propto \mathbf{P}^2$ . Its form matches the one  $\propto Y_1$  in equation (66), where the coefficient is given by

$$Y_1 = -\lambda_0 + O(\epsilon). \quad (77)$$

<sup>5</sup> As non-universal factors we have, in this case, the overall amplitude of  $\Xi(\mathbf{P}, \mathbf{c})$  and the two metric factors associated with  $\sigma$  and  $g_c = c$ , respectively.

In summary, we find that our result (71) for the scaling function  $\Xi$  is also in conformity with the limiting forms (66) and (67). This means that the asymptotic momentum singularities one obtains at the ordinary transition from the  $c$ -dependent analysis here, to first order in  $\epsilon$ , agree with those found in Diehl *et al* (2003a) for the case  $\hat{c} = \infty$  with Dirichlet boundary conditions. Although expected, this manifestation of universality is gratifying in that it corroborates our identification of the fixed points  $\mathcal{P}_{\text{sp}}^*$  and  $\mathcal{P}_{\text{ord}}^*$ .

## 5. Summary and conclusions

We have investigated the special surface transition that occurs at an  $m$ -axial bulk LP in the case where the  $m$  (potential) modulation axes are parallel to the surface. Our RG analysis in  $d = 4 + \frac{m}{2} - \epsilon$  dimensions corroborates the observation of Diehl *et al* (2003a, 2003b) that a square gradient term of the form shown in equation (3) must be included in the boundary part  $\mathcal{L}_1$  of the Hamiltonian, in addition to its usual  $\phi^2$  contribution.

The RG fixed point associated with the special transition is located at a nontrivial value  $\lambda_+^* = O(\epsilon^0)$  of the associated renormalized surface coupling constant  $\lambda$ , zero (renormalized) surface enhancement  $c = 0$  (see equation (29)) and the usual fixed-point value  $u^*$  of order  $\epsilon$  of the bulk interaction constant. As a direct consequence of the fact that  $\lambda_+^* = O(\epsilon^0)$ , the surface crossover exponent  $\Phi$  becomes  $m$  dependent already at *first* order in  $\epsilon$ , whereas this happens for the bulk critical indices and the surface critical exponents of the ordinary transition only at *second* order in  $\epsilon$ .

It would be natural to anticipate the same behaviour as that of  $\Phi$  for the surface correlation exponent  $\eta_{\parallel}^{\text{sp}}$ , the second independent surface critical index of the special transition. Yet this is *not* the case because the expansion to order  $\epsilon$  of  $\eta_{\parallel}^{\text{sp}}$  turns out to *vanish*, whereas the contribution of order  $\epsilon$  of its  $m = 0$  analogue is known to be nonzero (Diehl and Dietrich 1981, 1983), as is its  $O(\epsilon^2)$  term. Thus the limit  $m \rightarrow 0$  of the  $\epsilon$ -expansion of  $\eta_{\parallel}^{\text{sp}}$  differs from the established  $m = 0$  result for the CP case. This behaviour is exceptional. For once, the  $\epsilon$ -expansions of all those *bulk* critical indices that retain their physical meaning for  $m = 0$  turn over into their  $m = 0$  counterparts for the CP case in the limit  $m \rightarrow 0$ , as has been explicitly verified to order  $\epsilon^2$  (Shpot and Diehl 2001). Second, the same applies to the surface critical exponents of the *ordinary* transition (Diehl *et al* 2003a, 2003b). Moreover, even our  $O(\epsilon)$  result for  $\Phi$  implied by equation (60) is fully consistent with the  $\epsilon$ -expansion of  $\Phi_{m=0}$  (Diehl and Dietrich 1981, 1983).

As we have seen, the origin of the discrepancy between the  $\epsilon$ -expansions of  $\lim_{m \rightarrow 0} \eta_{\parallel}^{\text{sp}}$  and its  $m = 0$  analogue for the CP case can be traced back to the non-commutativity of the limits  $\lambda \rightarrow \lambda_+^*(m)$  and  $m \rightarrow 0$  of the RG function  $\eta_1(u^*, \lambda)$ . It is gratifying that we could recover the correct  $O(\epsilon)$  term of  $\eta_{\parallel}^{\text{sp}}$  for the CP case by analysing the RG flow directly for  $m \rightarrow 0$ .

The above, not necessarily expected, results are a clear message that further surprises might well be encountered when the surface orientation is taken to be perpendicular. Since in this case the distance  $z$  from the surface scales naively as  $\mu^{-1/2}$  (rather than as the inverse of the momentum scale  $\mu$ ), more surface monomials exist whose coupling constants have nonnegative momentum dimensions for  $\epsilon \geq 0$ , and hence are potentially dangerous. This makes the analysis of multi-critical surface transitions such as the special one even more interesting and challenging.

The series expansions of the surface critical exponents of the LP special transition determined here are restricted to first order in  $\epsilon$ . Unless their knowledge can be combined with information from other sources, one certainly cannot hope to get numerically accurate



estimates of the surface critical exponents at  $d = 3$ . The additional information we could benefit from was the  $\epsilon$ -expansions of the bulk critical exponents to  $O(\epsilon^2)$  and previous field theory and Monte Carlo estimates for  $d = 3$  (Shpot and Diehl 2001, Pleimling and Henkel 2001). Our result (59), which means that  $\beta_1^{\text{sp}} = \beta + O(\epsilon^2)$ , is in accordance with the small difference between the values of  $\beta_1^{\text{sp}}$  and the bulk exponent  $\beta$  obtained in Pleimling (2002) via Monte Carlo simulations of the three-dimensional ANNNI model.

We see no principal obstacle to extending the present analysis to second order in  $\epsilon$ . However, the effort required appears to be considerably greater than was necessary for our—already quite demanding—analysis of the ordinary transition (Diehl *et al* 2003a, 2003b). Furthermore, the residues of some pole terms one must determine seem to be expressible only in terms of multi-dimensional integrals which must be computed by numerical means.

In order to corroborate our identification of the fixed points (29) we also computed the scaling functions (71) of the momentum-dependent local surface susceptibility  $\chi_{11}(\mathbf{p})$  at the Lifshitz point  $\tau = \rho = 0$ , to first order in  $\epsilon$ , and confirmed that the momentum singularities at both the special as well as the ordinary transition have the predicted power-law forms, consistent with our own RG results here and those of Diehl *et al* (2003a) for the ordinary transition.

We close with three remarks:

- (i) There are several worthwhile goals which future Monte Carlo simulations of the ANNNI model might accomplish. An obvious one is obtaining an accurate estimate of the surface crossover exponent  $\Phi$ . A second—equally important and not unrelated—task is a careful check of the predicted scaling behaviour at the special transition. We believe that appropriate (non)linear scaling fields  $g_c, g_\tau$  etc (see equations (9)) should be introduced when performing the required analysis of the data.
- (ii) While mathematically rigorous results on the surface phase diagram of the three-dimensional semi-infinite Ising model can be found in the literature (Fröhlich and Pfister 1987, Pfister and Penrose 1988), we are not aware of similar work on the semi-infinite ANNNI model. Clearly, rigorous results both on bulk and surface phase diagrams involving bulk LP could be very valuable.
- (iii) Finally, let us emphasize the need for careful experimental studies of bulk and surface critical behaviour at LP. Owing to the enormous advances in experimental technology and our better theoretical understanding, tests much more stringent than the (more than 20-year-old) experimental study (Shapira *et al* 1981) of bulk critical behaviour at the uniaxial LP of MnP ought to be possible today. The situation is even worse for *surface* critical behaviour at LP, since experimental investigations do not yet exist apparently.

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## Appendix A. Calculation of $A_c$

In this appendix, we derive the one-loop result (13) for the renormalization function  $A_c$ . To this end, we consider the surface cumulant  $G_{\text{ren}}^{(0,2)}(\mathbf{p})$  for  $\tau = c = 0$  and generic  $\lambda > 0$  and  $\rho > 0$ . The free propagator of the renormalized theory may be gleaned from equation (7)

of Diehl *et al* (2003a) and the re-parametrizations (5) and (6). We express it in terms of the dimensionless momenta  $\hat{p}$  and  $\hat{P}$  introduced in equation (61). For  $\tau = c = 0$ , it then becomes

$$\hat{G}(\mathbf{p}; z_1, z_2) = \frac{1}{2\mu\kappa_p} \left[ e^{-\kappa_p|z_1-z_2|} + \frac{\kappa_p - \lambda\hat{P}^2}{\kappa_p + \lambda\hat{P}^2} e^{-\mu\kappa_p(z_1+z_2)} \right] \quad (\text{A.1})$$

in the  $\mathbf{p}z$  representation, with

$$\kappa_p = \sqrt{\hat{p}^2 + \hat{P}^4 + \rho\hat{P}^2}. \quad (\text{A.2})$$

Upon taking into account all counter-terms that contribute to first order in  $u$ , we obtain

$$\hat{G}_{\text{ren}}^{(0,2)}(\mathbf{p}) = \frac{Z_1^{-1}/\mu}{\kappa_p + (\lambda + P_\lambda)\hat{P}^2} + \int_{0-}^{\infty} dz [\hat{G}(\mathbf{p}; 0, z)]^2 \left[ \frac{\bigcirc}{\mathbf{x}} - A_\tau \mu^2 \rho^2 - A_c \mu \rho \delta(z) \right] + O(u^2), \quad (\text{A.3})$$

where the lower limit  $0-$  of the  $z$  integration serves to ensure that  $\int dz \delta(z) = 1$ .

The tadpole graph displayed in this equation yields two contributions: one corresponding to the translation invariant part of  $G$ —its ‘bulk’ part  $G_b$ —and a second one resulting from its remaining ‘surface’ part  $G_s$ . Since

$$G_b(\mathbf{x} - \mathbf{x}) = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{1}{2\mu\kappa_p} = \frac{\mu^{2-\epsilon} F_{m,0}}{\sigma^{m/4}} \frac{m\rho^2}{8\epsilon} + O(\epsilon^0), \quad (\text{A.4})$$

the pole term of  $\bigcirc_b$  (the former) gets cancelled by the subtraction  $\propto A_\tau$  in the square brackets, for our choice of  $A_\tau$ , made in accordance with equation (17) of Diehl *et al* (2003a).

The graph  $\bigcirc_s$  yields pole terms of the form  $\delta'(z)/\epsilon$  and  $\delta(z)/\epsilon$ . To see this, note that upon making the change of variables  $\hat{p} \rightarrow \hat{p}/2\mu z$  and  $\hat{P} \rightarrow \hat{P}/\sqrt{2\mu z}$ , the surface part  $G_s(\mathbf{x}, \mathbf{x})$  can be written as

$$G_s(\mathbf{x}, \mathbf{x}) = \sigma^{-m/4} (2z)^{\epsilon-2} f_\epsilon(\mu z) \quad (\text{A.5})$$

with

$$f_\epsilon(\hat{z}) = \int \frac{d^{d-m-1}\hat{p} d^m \hat{P}}{(2\pi)^{d-1}} \frac{\kappa(\hat{p}, \hat{P}, \hat{z}) - \lambda\hat{P}^2}{\kappa(\hat{p}, \hat{P}, \hat{z}) + \lambda\hat{P}^2} \frac{e^{-\kappa(\hat{p}, \hat{P}, \hat{z})}}{2\kappa(\hat{p}, \hat{P}, \hat{z})}, \quad (\text{A.6})$$

where

$$\kappa(\hat{p}, \hat{P}, \hat{z}) = \sqrt{\hat{p}^2 + \hat{P}^4 + 2\hat{z}\rho\hat{P}^2}. \quad (\text{A.7})$$

The pole terms of the generalized function (A.5) originate from the contributions that behave as  $z^{\epsilon-2}$  and  $z^{\epsilon-1}$  near  $z = 0$ . Utilizing the well-known Laurent expansion  $z^{\epsilon-k} = (-1)^k \delta^{(k)}(z)/k! + O(\epsilon)$  of such generalized functions (Gel'fand and Shilov 1964) gives

$$(2\hat{z})^{\epsilon-2} f_\epsilon(\hat{z}) = -\frac{f_0(0)}{4\epsilon} \delta'(\hat{z}) + \frac{f_0'(0)}{4\epsilon} \delta(\hat{z}) + O(\epsilon). \quad (\text{A.8})$$

The Taylor coefficients  $f(0)$  and  $f'(0)$  can both be expressed in terms of the function  $i_1$  and its derivative  $i_1'$ . A straightforward calculation yields

$$f_0(0) = 2F_{m,0} i_1(\lambda; m) \quad (\text{A.9})$$

and

$$f_0'(0) = -4\rho F_{m,0} \left[ \frac{1 - i_1(\lambda; m) - \lambda i_1'(\lambda; m)}{2\lambda} - \frac{\sqrt{\pi} \Gamma[(m+2)/4]}{2\Gamma(m/4)} \right]. \quad (\text{A.10})$$

The uv singularity of the graph  $\overset{\circ}{\bigcirc}$  implied by the pole term  $\propto \delta(z)$  in equation (A.8) is momentum independent; it must be cancelled by a renormalization of the surface enhancement  $\hat{c}$ . Since we set the renormalized quantity  $c$  to zero, this condition immediately gives the renormalization function  $A_c$  to one-loop order. The result (13) can be read off from the above equations. The pole term  $\propto \delta'(z)$  in equation (A.8) looks like a counter-term of the form  $\int_{\mathfrak{S}^3} \phi \partial_n \phi$ , which we did *not* introduce, knowing that it can be transformed by means of the boundary condition

$$\partial_n \phi = (\hat{c} - \hat{\lambda} \partial_\alpha \partial_\alpha) \phi \quad (\text{A.11})$$

into surface counter-terms we included, such as that  $\propto \int_{\mathfrak{S}^3} (\partial_\alpha \phi)^2$  (Diehl *et al* 2003a). In fact, using the one-loop results

$$Z_1(u, \lambda, \epsilon) - 1 = -\lambda^{-1} P_\lambda(u, \lambda, \epsilon) + O(u^2) = \frac{n+2}{3} \frac{i_1(\lambda; m)u}{2\epsilon} + O(u^2) \quad (\text{A.12})$$

of this paper, one easily convinces oneself that the pole terms produced by the renormalization functions  $Z_1$  and  $P_\lambda$  of the first term in equation (A.3) cancel those originating from the singularity  $\propto \delta'(z)$  of  $G_s(\mathbf{x}, \mathbf{x})$ .

## Appendix B. One-loop calculation of $\chi_{11}(p)$

In this appendix, we outline the computation of the renormalized surface susceptibility  $\chi_{11}^{(\text{ren})}(p)$  to one-loop order for  $\tau = \rho = 0$  and general values  $c \geq 0$  and  $\lambda > 0$ . The contribution of the bulk part  $\overset{\circ}{\bigcirc}$  to the one-loop term vanishes for  $\tau = \rho = 0$  (in dimensional regularization), just as the terms proportional to  $A_\tau$  and  $A_c$  in equation (A.3) do. In the remaining one-loop integral we perform both the integration over  $z$  as well as the angular integrations, obtaining

$$\frac{\mu}{\chi_{11}^{(\text{ren})}(p)} = Z_1[\kappa_p + (\lambda + P_\lambda) \hat{P}^2 + Z_c c] + \frac{u}{2} \frac{n+2}{3} \frac{K_{d-m-1} K_m}{F_{m,\epsilon}} J + O(u^2) \quad (\text{B.1})$$

with

$$J = \int_0^\infty d\hat{p}_1 \hat{p}_1^{d-m-2} \int_0^\infty d\hat{P}_1 \hat{P}_1^{m-1} \frac{\kappa_{p_1} - c - \lambda \hat{P}_1^2}{4\kappa_{p_1} (\kappa_p + \kappa_{p_1}) (\kappa_{p_1} + c + \lambda \hat{P}_1^2)}. \quad (\text{B.2})$$

Here  $\hat{p}$  and  $\hat{P}$  denote again the dimensionless momenta (61), while  $\kappa_p$ , defined by equation (69), is the  $\rho = 0$  analogue of the quantity (A.2). The renormalization factor  $Z_c$  may be gleaned from equation (22) of Diehl *et al* (2003a): expressed in terms of  $i'_1$ , it reads

$$Z_c(u, \lambda, \epsilon) = 1 + \frac{n+2}{3} \frac{[1 + \lambda i'_1(\lambda; m)]u}{2\epsilon} + O(u^2). \quad (\text{B.3})$$

Finally,  $Z_1$  and  $P_\lambda$  are given by equation (A.12).

In the double integral  $J$  we introduce new variables  $s$  and  $t$  via  $\hat{P} = \sqrt{t/s}$  and  $\hat{p} = s^{-1} \sqrt{1-t^2}$ , whereby  $J$  becomes

$$\begin{aligned} J &= \frac{1}{8} \int_0^1 dt t^{(m-2)/2} (1-t^2)^{(2-m-2\epsilon)/4} \int_0^\infty ds \frac{s^{-2+\epsilon} (1-cs-t\lambda)}{(1+s\kappa_p)(1+cs+t\lambda)} \\ &= \frac{\mathcal{N}_{\epsilon,m}}{8} \left\langle \int_0^\infty ds \frac{s^{-2+\epsilon} (1-cs-t\lambda)}{(1+s\kappa_p)(1+cs+t\lambda)} \right\rangle_{\epsilon,m}, \end{aligned} \quad (\text{B.4})$$

where  $\langle \cdot \rangle_{\epsilon, m}$  and  $\mathcal{N}_{\epsilon, m}$  are the average and the normalization factor introduced by equations (21) and (22), respectively. The integral  $\int_0^\infty ds$  can be performed analytically and its Laurent series coefficients of order  $\epsilon^{-1}$  and  $\epsilon^0$  determined. One thus arrives at

$$\frac{u K_{d-m-1} K_m}{2 F_{m, \epsilon}} J = -\frac{u}{2} \left\{ [\epsilon^{-1} - \ln(2\kappa_p)] [\kappa_p i_1(\lambda, \epsilon; m) + 2c \langle (1 + \lambda t)^{-2} \rangle_{\epsilon, m}] + 2c^2 \left\langle \frac{\ln[c/\kappa_p(1 + \lambda t)]}{(1 + \lambda t)^2 [(1 + \lambda t)\kappa_p - c]} \right\rangle_{0, m} + O(\epsilon) \right\}. \quad (\text{B.5})$$

We now substitute this result together with the above expressions for the renormalization functions  $Z_1$ ,  $Z_c$  and  $P_\lambda$  into equation (B.1) and use the fact that the average in the first line of equation (B.5) can be written as

$$\langle (1 + \lambda t)^{-2} \rangle_{\epsilon, m} = \frac{1}{2} [1 + i_1(\lambda, \epsilon; m) + \lambda i_1'(\lambda, \epsilon; m)]. \quad (\text{B.6})$$

The poles in  $\epsilon$  are found to cancel, and one arrives at the result (68).

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