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LETTER TO THE EDITOR

Surface critical behaviour at m -axial Lifshitz points: continuum models, boundary conditions and two-loop renormalization group results

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Abstract

The critical behaviour of semi-infinite d -dimensional systems with short-range interactions and an $O(n)$ invariant Hamiltonian is investigated at an m -axial Lifshitz point with an isotropic wave-vector instability in an m -dimensional subspace of \mathbb{R}^d parallel to the surface. Continuum $|\phi|^4$ models representing the associated universality classes of surface critical behaviour are constructed. In the boundary parts of their Hamiltonians quadratic derivative terms (involving a dimensionless coupling constant λ) must be included in addition to the familiar ones $\propto \phi^2$. Beyond one-loop order the infrared-stable fixed points describing the ordinary, special and extraordinary transitions in $d = 4 + \frac{m}{2} - \epsilon$ dimensions (with $\epsilon > 0$) are located at $\lambda = \lambda^* = O(\epsilon)$. At second order in ϵ , the surface critical exponents of both the ordinary and the special transitions start to deviate from their $m = 0$ analogues. Results to order ϵ^2 are presented for the surface critical exponent β_1^{ord} of the ordinary transition. The scaling dimension of the surface energy density is shown to be given exactly by $d + m(\theta - 1)$, where $\theta = \nu_{14}/\nu_{12}$ is the bulk anisotropy exponent.

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Lifshitz points, i.e. multicritical points at which a disordered, a homogeneous ordered and a modulated ordered phase meet, have been known since the end of the 1970s [1–4]. Appropriate n -vector $|\phi|^4$ -models representing universality classes of m -axial Lifshitz points were introduced at the same time; the simplest ones have a Hamiltonian $\mathcal{H} = \int d^d x \mathcal{L}_b(\mathbf{x})$ with density

$$\mathcal{L}_b = \frac{\delta}{2}(\Delta_\alpha \phi)^2 + \frac{1}{2}(\nabla_\beta \phi)^2 + \frac{\rho}{2}(\nabla_\alpha \phi)^2 + \frac{\tau}{2}\phi^2 + \frac{\dot{u}}{4!}|\phi|^4 \quad (1)$$

where the position vector $\mathbf{x} \equiv (\mathbf{x}_\alpha, \mathbf{x}_\beta)$ has m - and $(d - m)$ -dimensional components \mathbf{x}_α and \mathbf{x}_β , respectively, ∇_α and ∇_β denote the corresponding gradients and Δ_α means the Laplacian ∇_α^2 .

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Although the possibility of studying the universality classes of these models in a systematic manner by means of expansions in d and m about general points on the line of upper critical dimensions $d^*(m) = 4 + m/2$ ($0 \leq m \leq 8$) had been realized already in 1975 [1], the enormous technical difficulties one encounters beyond one-loop order [5–8] had prevented a successful implementation of this programme until recently when a full two-loop renormalization group (RG) analysis was performed and the $\epsilon = d^*(m) - d$ expansions of all critical exponents were determined to order ϵ^2 [9–12].

Here we are concerned with the effects of *surfaces* on the critical behaviour at such m -axial Lifshitz points. The only previous studies of this problem we are aware of are restricted to the uniaxial ($m = 1$) Ising ($n = 1$) case and use either the mean-field approximation [13–15] or Monte Carlo simulations [16] for the ANNNI model. Let us consider semi-infinite systems with a boundary plane \mathfrak{B} at $z = 0$, where $z \geq 0$ is the Cartesian coordinate along the inner normal on \mathfrak{B} . Since \mathbf{x}_α and \mathbf{x}_β scale differently, two distinct basic orientations of the surface plane exist which we call parallel and perpendicular, depending on whether \mathbf{n} is orthogonal to the α or the β subspace. We restrict ourselves here to the case of parallel surface orientation; the case of perpendicular orientation requires separate considerations and a distinct analysis [17].

For semi-infinite $|\phi|^4$ models with an $O(n)$ symmetric Hamiltonian three distinct types of surface transitions occurring at the bulk critical point can be distinguished [18, 19]: the ordinary, special and extraordinary transitions². Analogues of these surface transitions should exist also for the m -axial bulk Lifshitz points described by Hamiltonians with the bulk density (1) (see footnote 1). For the uniaxial Ising case $m = n = 1$ in $d = 3$ dimensions, Pleimling's Monte Carlo results [16] and the mean field analysis of [15] lend support to this expectation. Our goal is to pave the ground for systematic field theory analyses of these transitions.

To this end we need an appropriate semi-infinite extension of the bulk model with the density (1). For the short-range interaction case we are concerned with, it is justified to choose a Hamiltonian of the form (with $\mathbb{R}_+^d \equiv \mathbb{R}^{d-1} \times [0, \infty)$)

$$\mathcal{H} = \int_{\mathfrak{B}=\mathbb{R}_+^d} \mathcal{L}_b(\mathbf{x}) dV + \int_{\mathfrak{B}} \mathcal{L}_1(\mathbf{x}) dA \quad (2)$$

where $\mathcal{L}_1(\mathbf{x})$ depends on $\phi(\mathbf{x})$ and its derivatives. We must now (i) find out which contributions have to be retained in \mathcal{L}_1 , (ii) determine the boundary conditions they imply, (iii) clarify the renormalization of the field theory and set up a RG approach in $d^*(m) - \epsilon$ dimensions and (iv) derive the fixed-point structure, identifying potential fixed points describing the ordinary, special and extraordinary transitions.

In the case of a critical point (corresponding to the choice $m = 0$), it is sufficient to include a term $\propto \phi^2$ in \mathcal{L}_1 ; other $O(n)$ (or \mathbb{Z}_2) invariant contributions can be shown to be redundant or irrelevant [18, 19]. However, in the ($m \neq 0$) case of a Lifshitz point, this is not sufficient; we must take

$$\mathcal{L}_1(\mathbf{x}) = \frac{\mathring{c}}{2} \phi^2 + \frac{\mathring{\lambda}}{2} (\nabla_\alpha \phi)^2. \quad (3)$$

Power counting tells us that $\mathring{\lambda} \mathring{c}^{-1/2}$ is dimensionless. Hence it is scale invariant at the Gaussian fixed point and potentially infrared relevant for $\epsilon > 0$. All other contributions, notably terms $\propto (\nabla_\beta \phi)^2$, $\propto \phi \nabla_\alpha \phi$ or $\propto \phi \nabla_\beta \phi$, can be ruled out by symmetry or shown to be irrelevant or redundant [17]. The field theory defined by equations (1)–(3) satisfies the boundary conditions (valid in an operator sense [18, 19])

$$\partial_n \phi = (\mathring{c} - \mathring{\lambda} \Delta_\alpha) \phi. \quad (4)$$

² The occurrence of the extraordinary and special transitions requires that the surface dimension $d - 1$ is sufficiently high so that long-range surface order is possible in the presence of a disordered bulk.

This carries over to the free propagator $G(\mathbf{x}, \mathbf{x}')$, whose Fourier transform, \hat{G} , with respect to the $d - 1$ coordinates parallel to the surface reads, in the disordered phase,

$$\hat{G}(\mathbf{p}; z, z') = \frac{1}{2\kappa_p} \left[e^{-\kappa_p|z-z'|} - \frac{\hat{c} + \hat{\lambda}|\mathbf{p}_\alpha|^2 - \kappa_p}{\hat{c} + \hat{\lambda}|\mathbf{p}_\alpha|^2 + \kappa_p} e^{-\kappa_p(z+z')} \right] \quad (5)$$

with

$$\kappa_p = \sqrt{\hat{t} + \hat{\rho}|\mathbf{p}_\alpha|^2 + |\mathbf{p}_\beta|^2 + \hat{\sigma}|\mathbf{p}_\alpha|^4} \quad (6)$$

where \mathbf{p}_α is the m -dimensional α component of the wave vector $\mathbf{p} \in \mathbb{R}^{d-1}$. The back transform of the part depending on $|z - z'|$ is the free bulk propagator $G_b(\mathbf{x} - \mathbf{x}')$. At the Gaussian Lifshitz point $\hat{t} = \hat{\rho} = \hat{u} = 0$, it takes the scaling form

$$G_b(\mathbf{x}) = |\mathbf{x}_\beta|^{-2+\epsilon} \hat{\sigma}^{-m/4} \Phi_{m,d}(\hat{\sigma}^{-1/4}|\mathbf{x}_\alpha||\mathbf{x}_\beta|^{-1/2}). \quad (7)$$

Here the scaling function $\Phi_{m,d}(\nu)$ is a generalization of a generalized hypergeometric function (a Fox–Wright ${}_1\psi_1$ function, cf equations (10)–(13) of [10]). In the special cases $\hat{c} = \hat{\lambda} = 0$ or $\hat{c} \rightarrow \infty$ at arbitrary $\hat{\lambda} \geq 0$, $G(\mathbf{x}, \mathbf{x}')$ reduces to the Neumann or Dirichlet propagator, respectively, whose $z + z'$ dependent parts reduce to $\pm G_b(\mathbf{x} - \mathbf{x}' + 2z' \mathbf{n})$.

Utilizing these results, and employing dimensional regularization in conjunction with minimal subtraction of poles, we have performed a two-loop RG analysis of the model (1)–(3) in $d^*(m) - \epsilon$ dimensions.

Its main results are as follows. To renormalize the multi-point correlation functions $G^{(N,M)}$ involving N fields ϕ off and M fields $\phi^{\mathfrak{B}} \equiv \phi(\mathbf{x} \in \mathfrak{B})$ on the boundary, the ‘bulk’ re-parametrizations known from [9, 10],


$$\begin{aligned} \phi &= Z_\phi^{1/2} \phi_{\text{ren}} & \hat{\sigma} &= Z_\sigma \sigma & \hat{t} - \hat{t}_{\text{LP}} &= \mu^2 Z_t \tau \\ (\hat{\rho} - \hat{\rho}_{\text{LP}}) \hat{\sigma}^{-1/2} &= \mu Z_\rho \rho & \hat{u} \hat{\sigma}^{-m/4} F_{m,\epsilon} &= \mu^\epsilon Z_u u \end{aligned} \quad (8)$$

must be complemented by ‘surface’ re-parametrizations of the form

$$\phi^{\mathfrak{B}} = (Z_\phi Z_1)^{1/2} \phi_{\text{ren}}^{\mathfrak{B}} \quad \hat{c} - \hat{c}_{\text{sp}} = \mu Z_c c \quad \hat{\lambda} \hat{\sigma}^{-1/2} = \lambda + P_\lambda(u, \lambda, \epsilon) \quad (9)$$

where the surface renormalization factors Z_1 and Z_c depend on u and λ . The function

$$P_\lambda(u, \lambda, \epsilon) = \sum_{i,j=1}^{\infty} P_\lambda^{(i,-j)}(\lambda) u^i \epsilon^{-j} = \sum_{i,j=1}^{\infty} \sum_{k=0}^{\infty} P_\lambda^{(i,-j;k)} u^i \epsilon^{-j} \lambda^k \quad (10)$$

does not vanish at $\lambda = 0$; although the one-loop coefficient $P_\lambda^{(1,-1)}(\lambda)$ vanishes at $\lambda = 0$, the graph  of $\langle \phi \phi^{\mathfrak{B}} \rangle$ yields a nonzero $P_\lambda^{(2,-1;0)}$. Thus a contribution $\propto (\nabla_\alpha \phi)^2$ to \mathcal{L}_1 gets generated under the RG even if it was originally absent.

The fixed points $\mathcal{P}_{\text{ord}}^*$, $\mathcal{P}_{\text{sp}}^*$ and $\mathcal{P}_{\text{ex}}^*$ describing respectively the ordinary, special and extraordinary transitions must lie in the $c\lambda$ plane at $(\tau, \rho, u) = (0, 0, u^*)$, where u^* is the nontrivial root of the bulk beta function $\beta_u(u) = \mu \partial_\mu |_{0} u$, computed to order $\mathcal{O}(\epsilon^2)$ in [10]. For $u = u^*$, the beta function $\beta_\lambda(u, \lambda) \equiv \mu \partial_\mu |_{0} \lambda$ turns out to have an infrared-stable root at

$$\lambda^* = -2\epsilon P_\lambda^{(2,-1;0)} / P_\lambda^{(1,-1;1)} + \mathcal{O}(\epsilon^2) \quad (11)$$

with a correction-to-scaling exponent

$$\omega_\lambda \equiv (\partial_\lambda \beta_\lambda)(u^*, \lambda^*) = -P_\lambda^{(1,-1;1)} u^* + \mathcal{O}(\epsilon^2) = \frac{n+2}{n+8} \epsilon + \mathcal{O}(\epsilon^2). \quad (12)$$

Thus $\mathcal{P}_{\text{ord}}^*$, $\mathcal{P}_{\text{sp}}^*$ and $\mathcal{P}_{\text{ex}}^*$ are the fixed points at $c = \infty, 0$ and $-\infty$ displayed in figure 1.

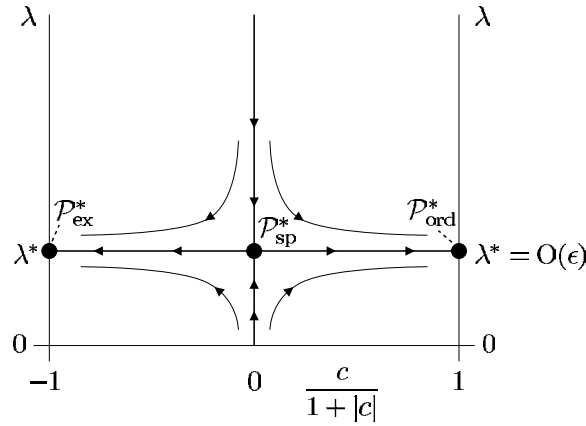


Figure 1. Schematic picture of the RG flow in the $c\lambda$ plane if $m > 0$, showing the fixed points $\mathcal{P}_{\text{ord}}^*$, $\mathcal{P}_{\text{sp}}^*$ and $\mathcal{P}_{\text{ex}}^*$.

Upon exploiting the RG equations implied by the above re-parametrizations (8) and (9) in a standard fashion, one concludes that the critical surface exponents of the special transition can be expressed in terms of bulk exponents and

$$\Delta[\phi^{\text{3B}}] = (d - m - 2 + \eta_{L2} + \eta_1^{*,\text{sp}} + m\theta)/2 = \beta_1^{\text{sp}}/\nu_{L2} \quad (13)$$

and

$$\Delta[\varepsilon^{\text{3B}}] = d - m - 2 + m\theta - \eta_c^{*,\text{sp}} \quad (14)$$

the scaling exponents of $\phi^{\text{3B}}(\mathbf{x})$ and the boundary energy density $\varepsilon^{\text{3B}}(\mathbf{x}) = [\phi^{\text{3B}}(\mathbf{x})]^2/2$, respectively, where the superscript ‘*,sp’ means values taken at $\mathcal{P}_{\text{sp}}^*$. The ϵ expansions of these exponents, like those of the bulk exponents, turn out to be independent of m to order ϵ , but can be shown to be m dependent at $O(\epsilon^2)$ [17]. Thus, $\eta_1^{*,\text{sp}} = -\frac{n+2}{n+8}\epsilon + O(\epsilon^2) = \eta_c^{*,\text{sp}} + O(\epsilon^2)$.³

These statements about the m dependence apply equally well to the surface critical exponents of the ordinary transition. To demonstrate this via explicit $O(\epsilon^2)$ results, note that β_1^{ord} can be expressed quite generally in terms of standard bulk exponents ν_{L2} , η_{L2} (or β_L), θ and a single additional anomalous dimension $\eta_{1,\infty}^*$ as

$$\beta_1^{\text{ord}} = (\nu_{L2}/2)(d - m + \eta_{L2} + m\theta + \eta_{1,\infty}^*) = \beta_L + \nu_{L2}(1 + \eta_{1,\infty}^*/2). \quad (15)$$

Our two-loop result for $\eta_{1,\infty}^*$ is

$$\eta_{1,\infty}^* = -\frac{n+2}{6}u^*\{1 + u^*[j_1(m) - J_u(m)]\} + O[(u^*)^3]. \quad (16)$$

Here u^* is the fixed-point value whose ϵ expansion to $O(\epsilon^2)$ is given in equation (60) of [10] while $J_u(m)$, defined by equations (49) and (50) of that reference, is one of the four single integrals (j_ϕ , j_σ , j_ρ , j_μ) in terms of which the two-loop series coefficients of the bulk exponents were written there (see its equations (43)–(45) and (50)). Finally,

$$j_1(m) = \frac{2^{10+m}\pi^{6+3m/4}\Gamma(m/2)}{\Gamma(2-m/4)\Gamma^2(m/4)} \int_0^\infty dv v^{m-5} \Phi_{m,d^*}(v) \int_0^v dy y^3 \Phi_{m,d^*}^2(y) \quad (17)$$

³ The implied $O(\epsilon)$ results $\beta_1^{\text{sp}} = \frac{1}{2} - \frac{\epsilon}{4} + O(\epsilon^2)$ and $\Phi = \frac{1}{2} - \frac{n+2}{n+8}\frac{\epsilon}{4} + O(\epsilon^2)$ of β_1^{sp} and the surface crossover exponent Φ may be gleaned from equations (3.156e,b) of [18].

is a similar new integral which can be reduced to a single one. (Upon rewriting $\int_0^\infty dv \int_0^v dy$ as $\int_0^\infty dy \int_y^\infty dv$, the latter v integration can be performed analytically to obtain a combination of hypergeometric functions).

Combining these results yields

$$\eta_{1,\infty}^* = -\frac{n+2}{n+8}\epsilon - \frac{n+2}{16(n+8)^3} \left\{ (n+2) \left[\frac{j_\sigma(m)}{m+2} - 8j_\phi(m) \right] + 64(5n+22)J_u(m) + 96(8+n)[j_1(m) - J_u(m)] \right\} \epsilon^2 + O(\epsilon^3). \tag{18}$$

Just as for the above mentioned four integrals of [10], the values of $j_1(m)$ can be computed analytically for the special choices $m = 2$, $m = 6$ and $m \rightarrow 0$. This yields

$$j_1(0) = \frac{1}{2} \quad j_1(2) = 1 - \frac{\ln 3}{2} \quad j_1(6) = -\frac{2}{3} + 2 \ln \frac{27}{16}. \tag{19}$$

To determine $j_1(m)$ for other values of m we had to resort to numerical means of the kind utilized in [10]. For the uniaxial case $m = 1$, we obtained $j_1(1) = 0.47289(1)$. Note also that in the limit $m \rightarrow 0$, the result (18) reduces to the familiar one for the standard semi-infinite $|\phi|^4$ model, given in equation (IV.35) of [20].

Let us briefly explain how the above results were obtained. Since the fixed point $\mathcal{P}_{\text{ord}}^*$ is located at $c = \infty$, the ordinary transition can be investigated without having to retain the full dependence on c and λ . To see this, note that the free propagator and the regularized bare $G^{(N,M)}$ become independent of λ in the limit $\hat{c} \rightarrow \infty$, and satisfy a Dirichlet boundary condition, which carries over to the renormalized theory. The long-scale behaviour of the $G^{(N,M)}$ with a nonzero number of $\phi^{\mathfrak{B}}$ can be inferred from the theory with $\hat{c} = \infty$ and $\hat{\lambda} = 0$ via the near-boundary behaviour of the operator ϕ . To this end, one considers correlation functions involving an arbitrary number of the operators ϕ and $\partial_n \phi$, and then uses the boundary operator expansion (BOE) $\phi_{\text{ren}}(\mathbf{x}_{\mathfrak{B}} + z\mathbf{n}) \underset{z \rightarrow 0}{\approx} C_{\text{ord}}(z) \partial_n \phi_{\text{ren}}(\mathbf{x}_{\mathfrak{B}})$. The renormalized theory requires in addition to the bulk re-parametrizations, the multiplicative re-parametrization (8),

$$\partial_n \phi = [Z_{1,\infty}(u) Z_\phi(u)]^{1/2} \partial_n \phi_{\text{ren}} \tag{20}$$

and an additive surface counter-term subtracting the primitive divergence ($\propto p_\alpha^2$) of $\langle \partial_n \phi \partial_n \phi \rangle$. The resulting RG equations imply scaling and yield the behaviour $C_{\text{ord}}(z) \sim z^{1+\eta_{1,\infty}^*/2}$, where $\eta_{1,\infty}^*$ is the fixed-point value of the exponent function associated with $Z_{1,\infty}$. A straightforward consequence is that the exponents characterizing the leading infrared singularities of the $G^{(N,M)}$ can be expressed in terms of (four independent) bulk critical indices and a single surface one, namely, $\eta_{1,\infty}^*$ or β_1^{ord} . Upon computing $Z_{1,\infty}$ and its exponent function to two-loop order and making extensive use of the results of [9, 10], we arrived at equations (15)–(18).

Let us also note that the scaling dimension of the surface energy density at the ordinary fixed point is given exactly by

$$\Delta^{\text{ord}}[\varepsilon^{\mathfrak{B}}] = d + m(\theta - 1). \tag{21}$$

That is, the leading thermal singularity of $\varepsilon^{\mathfrak{B}}$ has the bulk-free energy form $\sim |\tau|^{2-\alpha_L}$ with $\alpha_L = \nu_{L2}(d - m + m\theta)$. The result can be obtained in a variety of ways, namely (i) by generalizing the analysis given in appendix C of [21], (ii) by showing that the operator with smallest scaling dimension appearing in the BOE of the energy density $\varepsilon(\mathbf{x})$ is the component T_{zz} of the stress–energy tensor (whose scaling dimension is given by (21)) and (iii) by proceeding as in the derivation for the $m = 0$ case given in section III.B of [22].

The results (16) and (18) can be combined with known bulk results [10] to estimate the values of surface critical exponents such as β_1^{ord} for $d = 3$. In the uniaxial Ising case $m = n = 1$, equation (18) becomes

$$\eta_{1,\infty}^*(m = n = 1) = -0.333\bar{3}\epsilon - 0.1804\epsilon^2 + O(\epsilon^3) \tag{22}$$

which gives $\eta_{1,\infty}^* \simeq -0.906$ if we set $\epsilon = 3/2$ (i.e. $d = 3$), truncating the series at order ϵ^2 . Inserting this value together with the bulk estimates $\beta_L \simeq 0.246$, $\nu_{L2} \simeq 0.746$ and $\eta_{L2} \simeq 0.124$ of [10] into equation (15) and the analogous expressions $\gamma_1^{\text{ord}} = \nu_{L2}(1 - \eta_{L2} - \eta_{1,\infty}^*/2)$ and $\gamma_{11}^{\text{ord}} = -\nu_{L2}(1 + \eta_{L2} + \eta_{1,\infty}^*)$ for the surface susceptibility exponents yields

$$\beta_1^{\text{ord}} \simeq 0.65 \quad \gamma_1^{\text{ord}} \simeq 0.99 \quad \gamma_{11}^{\text{ord}} \simeq -0.2 \quad (m = n = 1, d = 3). \quad (23)$$

Owing to the low order ϵ^2 of the available series expansions and the large value $\epsilon = 3/2$ involved, these estimates cannot be trusted to be very precise. (They inherit, in particular, any uncertainty of the inserted bulk exponents.) However, they compare reasonably well with Pleimling's recent Monte Carlo estimates [16] $\beta_1^{\text{ord}} = 0.687(5)$, $\gamma_1^{\text{ord}} = 0.82(4)$ and $\gamma_{11}^{\text{ord}} = -0.29(6)$.

In summary, we have identified the continuum models that represent the universality classes of the considered ordinary, special and extraordinary (surface) transitions at m -axial bulk Lifshitz points, clarified their fixed point structure and presented two-loop RG results. A more detailed account of this work will be presented elsewhere [17].

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