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Surface critical behaviour of semi-infinite systems with cubic anisotropy at the ordinary transition

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Abstract

The critical behaviour at the ordinary transition in semi-infinite n-component anisotropic cubic models is investigated by applying the field theoretic approach in $d = 3$ dimensions up to the two-loop approximation. Numerical estimates of the resulting two-loop series expansions for the critical exponents of the ordinary transition are computed by means of Padé resummation techniques. For $n < n_c$ the system belongs to the universality class of the isotropic n-component model, while for $n > n_c$ the cubic fixed point becomes stable, where $n_c < 3$ is the marginal spin dimensionality of the cubic model. The obtained results indicate that the surface critical behaviour of the semi-infinite systems with cubic anisotropy is characterized by a new set of surface critical exponents for $n > n_c$.

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1. Introduction

The investigation of the critical behaviour of real systems is an important task of condensed matter theory. The critical behaviour in systems such as polymers, easy-axis ferromagnets, superconductors, as well as superfluid ^{4}He, Heisenberg ferromagnets and quark–gluon plasma is described by the isotropic $O(n)$ model with $n = 0, 1, 2, 3$ and 4, respectively, and has been analysed in the framework of different theoretical and numerical approaches.

Investigation of the critical behaviour of real cubic crystals has been one of the topics of extensive theoretical work during the last three decades. In crystals, due to their crystalline structure, some kind of anisotropy is always present. One of the simplest examples is cubic anisotropy. A typical model of the critical behaviour of such systems is the model with a cubic term $\frac{v_0}{4!}\sum_{i=1}^{n}\phi_i^4$ added to the usual $O(n)$ symmetric $\frac{u_0}{4!}\left(\sum_{i=1}^{n}|\phi_i|^2\right)^2$ term [1–3]. This n-component cubic model is a particular case of an mn-component model [4, 5] with cubic anisotropy at $m = 1$ (cf appendix A for details). The model exhibits several types of continuous and first-order phase transitions depending on the number of spin components n, space dimensionality d and the sign of the cubic coupling constant v_0. The cubic models are widely applied to the study of magnetic and structural phase transitions. In the limiting case of $n \to 0$ (and $m = 1$), it describes the critical behaviour of random Ising-like systems [6]. The case $m \to 0$ and $n \to 0$ formally describes the critical behaviour of long flexible polymer chains in good solvents as a model of self-avoiding walks (SAW) on a regular lattice, with short range correlated quenched disorder. As has been shown by Harris [7] and Kim [8], the short range correlated (or random uncorrelated pointlike) disorder is irrelevant for such a model. The case $m = 1$ and $n \to \infty$ corresponds to the Ising model with equilibrium magnetic impurities [9].

Depending on the sign of the cubic coupling constant v_0, two types of order are possible: along the diagonals the type $(1, 1, \ldots, 1)$ of a hypercube in n dimensions for $v_0 > 0$ or along the easy axes of the type $(1, 0, \ldots, 0)$ for $v_0 < 0$. In the latter case the system can undergo a first order phase transition, as was confirmed in experiments [10]. In the present work we are concerned with the case $v_0 > 0$.

The presence of a surface leads to the appearance of additional complications. The source of these problems is connected with both the loss of translational invariance and the presence of boundaries. General reviews on surface critical phenomena are given in [11–13]. The simplest model of critical phenomena in systems with a single planar surface is the semi-infinite model [11]. As is known [14, 11, 12], the phase diagram of such a model is richer than that of its bulk correspondent. In the general case of the pure semi-infinite model with continuous $O(n)$ symmetries, there are surface- and bulk-disordered phases (SD and BD, respectively), as well as either the surface-ordered, bulk-disordered phase (SO and BD, respectively) and a surface-ordered, bulk-ordered phase (SO and BO). The surface phase can actually occur, if $d > 2$ ($d \geqslant 2$) and $n = 1$ ($n = 0$) or $d > 3$ and $n > 2$. The boundaries between the phases are the lines of surface, ordinary and extraordinary transitions which meet at a multicritical point $\left(m_0^2, c_0\right) = \left(m_{0c}^2, c_{\mathrm{sp}}^*\right)$, representing the special transition and called the special point. Each of the above mentioned transitions is characterized by its own fixed point. The constant c_0 is related to the surface enhancement, which measures the enhancement of the interactions at the surface. The coupling m_0 is defined in equation (2.1). In the case $n = 2$ and $d = 3$, surface transitions of the Kosterlitz–Thouless type are present. We do not consider this type of transition and extraordinary ones, because they have a different nature from the special and ordinary transitions.

In general, there are different surface universality classes, defining the critical behaviour in the vicinity of the system boundaries, at temperatures close to the bulk critical point ($\tau = (T - T_c)/T_c \to 0$). Each bulk universality class divides into several distinct surface universality classes. Three surface universality classes, called respectively ordinary ($c_0 \to \infty$), special ($c_0 = c_{\mathrm{sp}}^*$) and extraordinary ($c_0 \to -\infty$), are known [12, 13, 15].

In order to investigate the critical behaviour of real cubic crystals we must take into account that two types of anisotropy can be present for such systems. The first one is bulk anisotropy, which can be included into the consideration with the help of the above mentioned cubic term. The other one is surface anisotropy which arises as a consequence of the presence of bulk cubic anisotropy (see appendix B for details). In the present paper we are interested in the investigation of the critical behaviour only at the ordinary transition, where the surface orders simultaneously with the bulk. In this case, as was found by Diehl and Eisenriegler [16, 17], surface anisotropy is irrelevant.

The theory of critical behaviour of individual surface universality classes is very well developed for pure isotropic systems [13, 15, 18–21], systems with quenched surface-enhancement disorder [22–24] and systems with a random quenched bulk disorder for both the ordinary and the special surface transitions [25, 26]. General irrelevance–relevance criteria of the Harris type for systems with quenched short-range correlated surface-bond disorder were predicted in [22] and confirmed by Monte Carlo calculations [23, 27]. Moreover, it was established that the surface critical behaviour of semi-infinite systems with quenched bulk disorder is characterized by the new set of surface critical exponents in comparison with the case of pure systems [25, 26].

The remainder of this paper is organized as follows. Section 2 contains the description of the model and further useful background. In section 3 the renormalization group approach is described. Section 4 contains the calculations of the surface renormalization factor $Z_{\partial\varphi}$ and surface critical exponent $\eta_{\partial\varphi}$ by applying the field theoretic approach directly in $d = 3$ dimensions, up to the two-loop order. The numerical estimates of the resulting two-loop series expansions for the critical exponents of the ordinary transition are presented in section 5. The calculations are performed by means of the Padé resummation techniques for the cases $n = 3, 4, 8$ and for the case of $n \to \infty$, which corresponds to the Ising model with equilibrium magnetic impurities. Section 6 contains concluding remarks. Appendix A contains the effective Hamiltonian of an mn-component model with cubic anisotropy. Appendix B contains the Landau–Ginzburg–Wilson functional for semi-infinite systems of spins with cubic anisotropy while appendix C contains the standard surface scaling relations for the case $d = 3$.

2. The model

The effective Landau–Ginzburg–Wilson Hamiltonian of the n-vector model with cubic anisotropy in the semi-infinite space is given by (see appendix B)

$$H(\vec{\phi}) = \int_0^\infty \mathrm{d}z \int \mathrm{d}^{d-1}r \left[\frac{1}{2}\, |\nabla\vec{\phi}|^2 + \frac{m_0^2}{2}\, |\vec{\phi}|^2 + \frac{v_0}{4!} \sum_{i=1}^{n} |\phi_i|^4 + \frac{u_0}{4!} \left(\sum_{i=1}^{n} |\phi_i|^2 \right)^2 \right] \tag{2.1}$$

where $\vec{\phi}(\mathbf{x}) = \{\phi_i(\mathbf{x})\}$ is an n-vector field with the components $\phi_i(\mathbf{x})$, $i = 1, \ldots, n$. Here m_0^2 is the 'bare mass', representing a linear measure of the temperature difference from the critical point value. The parameters u_0 and v_0 are the usual 'bare' coupling constants $u_0 > 0$ and $v_0 > 0$. It should be mentioned that the d-dimensional spatial integration is extended over a half-space $\mathbb{R}_+^d \equiv \{\mathbf{x}{=}(\mathbf{r}, z) \in \mathbb{R}^d$, with $\mathbf{r} \in \mathbb{R}^{d-1}$ and $z \geqslant 0\}$, bounded by a planar free surface at $z = 0$. The fields $\phi_i(\mathbf{r}, z)$ satisfy the Dirichlet boundary condition $\phi_i(\mathbf{r}, z) = 0$ at $z = 0$ in the case of ordinary transition, and the Neumann boundary condition $\partial_n\phi_i(\mathbf{r}, z) = 0$ at $z = 0$ in the case of special transition [15, 19]. The model defined in (2.1) is translationally invariant in directions parallel to the external surface, $z = 0$. Thus, we shall use a mixed representation, i.e. Fourier representation in $d - 1$ dimensions and real-space representation in the z direction. Therefore, since then the fields $\phi_i(\mathbf{r}, z)$ vanish identically on a surface and the gradient terms $\sim(\partial_n\phi_i)^2$ are irrelevant [16, 17] (cf also appendix B), no specific surface term will appear in the case of the ordinary transition, when the Dirichlet boundary conditions on the surface are assumed.

The added cubic term breaks the $O(n)$ invariance of the model, leaving a discrete cubic symmetry. The model (2.1) has four fixed points: the trivial Gaussian, the Ising one in which the n components are decoupled, the isotropic ($O(n)$-symmetric) and the cubic fixed points. The Gaussian and Ising fixed points are never stable for any number of components n. For isotropic systems, the $O(n)$-symmetric fixed point is stable for $n < n_c$, whereas for $n > n_c$ it becomes unstable. Here n_c is the marginal spin dimensionality of the cubic model, at which the isotropic and cubic fixed points change stability, i.e. for $n > n_c$, the cubic fixed point becomes stable. The $O(n)$-symmetric fixed point is tricritical. At $n = n_c$, the two fixed points should coincide, and logarithmic corrections to the $O(n)$-symmetric critical exponents are present. The calculation of the critical marginal spin dimensionality n_c is the crucial point in studing the critical behaviour in three-dimensional cubic crystals. Different results for n_c have been published in a series of works in which different methods have been used. In the framework of the field-theoretical RG analysis the one-loop and three-loop approximations at $\epsilon = 1$ lead to the conclusion that n_c should lie between 3 and 4 [34, 35], and the cubic ferromagnets are described by the Heisenberg model. On the other hand, by using the field theoretic approach directly in $d = 3$ dimensions up to the three-loop approximation, it has been found that $n_c = 2.9$ [36, 37]. Similar conclusions were obtained in [38], where it was found that $n_c = 2.3$. The calculations performed by Newman and Riedel [39] with the help of the scaling-field method, developed by Goldner and Riedel [40] for Wilson's exact momentum-space RG equations, have given, for $d = 3$, the value $n_c = 3.4$. Field-theoretical analysis, based on the four-loop series in three dimensions [41, 42], and results of the five-loop [42–44] and six-loop [45] $\epsilon = 4 - d$ expansions suggest that $n_c \leqslant 3$. Recently, a very precise six-loop result for the marginal spin dimensionality of the cubic model, $n_c = 2.89(4)$, was obtained in the framework of the 3D field-theoretic approach [46]. Thus, it was finally established that the critical behaviour of the cubic ferromagnets is not described by the isotropic Heisenberg Hamiltonian, but by the cubic model, at the cubic fixed point. However, it was found that the difference between the values of the bulk critical exponents at the cubic and the isotropic fixed points is very small, i.e. it is hard to determine this difference experimentally. Nevertheless, the recently obtained results stimulated us to perform the analysis of the *surface critical behaviour* of the semi-infinite n-component anisotropic cubic model, and to determine the corresponding surface critical exponents.

3. Renormalization

The fundamental two-point correlation function of the free static theory corresponding to (2.1) is defined by the Dirichlet propagator:

$$\langle \varphi_i(r, z)\varphi_j(0, z')\rangle_0 = G_D(r; z, z')\delta_{ij}. \tag{3.1}$$

In the mixed pz representation the Dirichlet propagator is

$$G_D(p; z, z') = \frac{1}{2\kappa_0}[\mathrm{e}^{-\kappa_0|z-z'|} - \mathrm{e}^{-\kappa_0(z+z')}] \tag{3.2}$$

where the standard notation is used and $\kappa_0 = \sqrt{p^2 + m_0^2}$. The propagator vanishes identically when at least one of its z coordinates is zero, because we have assumed the Dirichlet boundary conditions. Consequently, all the correlation functions involving at least one field at the surface vanish. This property holds for both the free and the renormalized theories [12].

In fact the critical surface singularities at the ordinary transition can be extracted by studying the nontrivial (in this case) correlation function involving the (*inner*) normal derivatives of the fields at the boundary, $\partial_n\phi(r)$ [49, 15, 19]. Actually, in order to obtain the characteristic exponent $\eta_\parallel^{\mathrm{ord}}$ of surface correlations, it is sufficient to consider a correlation function with two normal derivatives of boundary fields, i.e.

$$\mathcal{G}_2(p) = \left\langle \frac{\partial}{\partial z}\varphi(p, z)\bigg|_{z=0} \frac{\partial}{\partial z'}\varphi(-p, z')\bigg|_{z'=0}\right\rangle \tag{3.3}$$

where the fields $\varphi(p, z)$ are the Fourier transforms of the fields $\varphi(r, z)$ in $(d-1)$ dimensions parallel to surface space. $\mathcal{G}_2(p)$ is a parallel Fourier transform of the corresponding two-point function $\mathcal{G}_2(r)$ in direct space. At the critical point $\mathcal{G}_2(p)$ behaves as $p^{-1+\eta_\parallel^{\mathrm{ord}}}$. It reproduces the leading critical behaviour of a two-point function $G_2(p) = \langle\varphi(p, z)\varphi(-p, z')\rangle$ in the vicinity of the boundary plane. The surface critical exponent $\eta_\parallel^{\mathrm{ord}}$ is provided by the scaling dimension of the boundary operator $\partial_n\varphi(r)$.

The surface correlation function exponent $\eta_\parallel^{\mathrm{ord}}$ in semi-infinite systems with cubic anisotropy differs from its corresponding value for the isotropic semi-infinite system. The remaining surface critical exponents of the ordinary transition can be determined through the surface scaling laws [12] (see appendix C).

In the present formulation of the problem, the renormalization process for the cubic anisotropic system is essentially the same as that in the isotropic case [12, 21]. Explicitly, the renormalized bulk field and its normal derivative at the surface should be reparametrized by different uv-finite renormalization factors $Z_\varphi(u, v)$ and $Z_{\partial\varphi}(u, v)$

$$\varphi_R(x)=Z_\varphi^{-\frac{1}{2}}\varphi(x) \qquad \text{and} \qquad (\partial_n\varphi(r))_R=Z_{\partial\varphi}^{-\frac{1}{2}}\partial_n\varphi(r) \tag{3.4}$$

and renormalized correlation functions involving N bulk fields and M normal derivatives are

$$\mathcal{G}_R^{(N,M)}(p; m, u, v) = Z_\varphi^{-\frac{N}{2}} Z_{\partial\varphi}^{-\frac{M}{2}} \mathcal{G}^{(N,M)}(p; m_0, u_0, v_0) \tag{3.5}$$

for $(N, M) \neq (0, 2)$. In order to remove the ultraviolet (uv) singularities of the correlation function $\mathcal{G}^{(0,2)}$ with two surface operators $(N, M) = (0, 2)$ in the vicinity of the surface, an additional, *additive* renormalization (zero-momentum subtraction) is required, so that

$$\mathcal{G}_R^{(0,2)}(p) = Z_{\partial\varphi}^{-1}[\mathcal{G}^{(0,2)}(p) - \mathcal{G}^{(0,2)}(p=0)]. \tag{3.6}$$

The typical bulk uv singularities, which are present in the correlation function $\mathcal{G}^{(0,2)}$, are subtracted via the standard mass renormalization of the massive infinite-volume theory. It also relates to coupling constants, for which standard vertex renormalization of coupling constants takes place.

The surface renormalization factor $Z_{\partial\varphi}(u, v)$ can be conveniently obtained from the consideration of the boundary two-point function $\mathcal{G}^{(0,2)}$,

$$Z_{\partial\varphi} = -\lim_{p\to 0}\frac{m}{p}\frac{\partial}{\partial p}\mathcal{G}^{(0,2)}(p). \tag{3.7}$$

A standard RG argument involving an inhomogeneous Callan–Symanzik equation yields the anomalous dimension of the operator $\partial_n\varphi(r)$

$$\eta_{\partial\varphi} = m\frac{\partial}{\partial m}\ln Z_{\partial\varphi}\bigg|_{FP} = \beta_u(u, v)\,\frac{\partial \ln Z_{\partial\varphi}(u, v)}{\partial u} + \beta_v(u, v)\frac{\partial \ln Z_{\partial\varphi}(u, v)}{\partial v}\bigg|_{FP}. \tag{3.8}$$

'*FP*' indicates here that the above value should be calculated at the infrared-stable cubic fixed point of the underlying bulk theory, $(u, v) = (u^*, v^*)$. The surface critical exponent $\eta_\parallel^{\mathrm{ord}}$ at the ordinary transition is then given by

$$\eta_\parallel^{\mathrm{ord}} = 2 + \eta_{\partial\varphi}. \tag{3.9}$$

4. Perturbation theory up to two-loop approximation

After performing the mass and additive renormalization of the correlation function $\mathcal{G}^{(0,2)}(p)$ and carrying out the integration of Feynman integrals by analogy with [21, 25], we obtain for the renormalization factor

$$Z_{\partial\varphi}(\bar{u}_0, \bar{v}_0) = 1 + \frac{\bar{t}_1^{(0)}}{4} + \bar{t}_2^{(0)}C \tag{4.1}$$

where the constant C follows from the two-loop (melon-like diagrams) contribution to the correlation function and has the value

$$C \simeq \tfrac{107}{162} - \tfrac{7}{3}\ln\tfrac{4}{3} - 0.094\,299 \simeq -0.105\,063. \tag{4.2}$$

The coefficients $\bar{t}_1^{(0)}$ and $\bar{t}_2^{(0)}$ are the weighting factors belonging to one- and two-loop (melon-like) diagrams in the Feynman diagrammatic expansion of the correlation function $\mathcal{G}^{(0,2)}(p)$, and are equal to

$$-\frac{\bar{t}_1^{(0)}}{2} \qquad \text{with} \qquad \bar{t}_1^{(0)} = \frac{n+2}{3}\bar{u}_0 + \bar{v}_0 \tag{4.3}$$

$$\frac{\bar{t}_2^{(0)}}{6} \qquad \text{with} \qquad \bar{t}_2^{(0)} = \frac{n+2}{3}\bar{u}_0^2 + \bar{v}_0^2 + 2\bar{v}_0\bar{u}_0. \tag{4.4}$$

The factors $\bar{t}_1^{(0)}$ and $\bar{t}_2^{(0)}$ follow from the standard symmetry properties of the Hamiltonian (2.1). Here the renormalization factor $Z_{\partial\varphi}$ is expressed as a second-order series expansion in powers of *bare* dimensionless parameters $\bar{u}_0 = u_0/(8\pi m)$ and $\bar{v}_0 = v_0/(8\pi m)$. As is usual in *super* renormalizable theories, the renormalization factor expressed in terms of unrenormalized coupling constants is finite.

As a next step, the vertex renormalizations should be carried out. To the present accuracy, they are

$$\bar{u}_0 = \bar{u}\left(1 + \frac{n+8}{6}\bar{u} + \bar{v}\right) \tag{4.5}$$

$$\bar{v}_0 = \bar{v}\left(1 + \frac{3}{2}\bar{v} + 2\bar{u}\right). \tag{4.6}$$

As known, the vertex renormalization at $d = 3$ is a finite reparametrization. All relevant singularities have been removed already after the mass renormalization and taking into account the special bubble-graph combinations emerging in the theory with *Dirichlet* propagators. Thus we obtain a modified series expansion up to two-loop approximation

$$Z_{\partial\varphi}(\bar{u},\bar{v}) = 1 + \frac{n+2}{12}\bar{u} + \frac{\bar{v}}{4} + \frac{n+2}{3}\left(C + \frac{n+8}{24}\right)\bar{u}^2 + \left(C + \frac{3}{8}\right)\bar{v}^2 + 2\left(C + \frac{n+8}{24}\right)\bar{u}\bar{v}. \tag{4.7}$$

Combining the renormalization factor $Z_{\partial\varphi}(\bar{u},\bar{v})$ together with the one-loop pieces of the beta functions $\beta_{\bar{u}}(\bar{u},\bar{v}) = -\bar{u}\big(1 - \frac{n+8}{6}\bar{u} - \bar{v}\big)$ and $\beta_{\bar{v}}(\bar{u},\bar{v}) = -\bar{v}\big(1 - \frac{3}{2}\bar{v} - 2\bar{u}\big)$ and inserting them into equation (3.8), we obtain the desired series expansion for $\eta_{\partial\varphi}$,

$$\eta_{\parallel}(u,v) = 2 - \frac{n+2}{2(n+8)}u - \frac{v}{6} - 24\frac{(n+2)}{(n+8)^2}\mathcal{C}(n)u^2 - \frac{8}{9}\mathcal{C}(1)v^2 - \frac{16}{n+8}\mathcal{C}(n)uv \tag{4.8}$$

where $\mathcal{C}(n)$ is a function of the order-parameter components number n, and is defined as

$$\mathcal{C}(n) = C + \frac{n+14}{96} \tag{4.9}$$

whereas the renormalized coupling constants u and v, normalized in a standard fashion, are $u{=}\frac{n+8}{6}\bar{u}$ and $v{=}\frac{3}{2}\bar{v}$.

Equation (4.8) supplies our result for the critical exponent of the surface correlation function for the model with the effective Hamiltonian of the Landau–Ginzburg–Wilson type with cubic anisotropy in the semi-infinite space (2.1) with general number n of order parameter components.

Knowledge of $\eta_\parallel$ gives the possibility of calculating the other surface critical exponents through the scaling relations. For convenience, from now on we omit the superscript *ord* for the surface critical exponents.

The critical exponents should be calculated for different n ($n = 3, 4, 8$ and $n \to \infty$) at the standard infrared-stable cubic fixed points (FP) of the underlying bulk theory, as is usually accepted in the massive field theory. As was mentioned above, in the cases $n < n_c$ the cubic ferromagnets are described by the Heisenberg isotropic Hamiltonian at the $O(n)$-symmetric fixed point.

In the case of the replica limit $n \to 0$ we obtain from (4.8) the series expansion of $\eta_\parallel^{\mathrm{r}}$ for *semi-infinite random Ising-like* systems. This case was investigated in detail by one of us previously [25].

5. Numerical results

In order to obtain the full set of surface critical exponents for the ordinary transition in systems with cubic anisotropy, we substitute the expansion (4.8) for $\eta_\parallel$ into the standard scaling-law expressions for the surface exponents (see appendix C).

For each of the above mentioned surface critical exponents of the ordinary transition we obtain for $d = 3$ a double series expansion in powers of u and v, truncated at the second order. As is known[3] [61–63], power series expansions of this kind are generally divergent due to a nearly factorial growth of expansion coefficients at large orders of perturbation theory. In order to perform the analysis of these perturbative series expansions and obtain accurate estimates of the surface critical exponents, a powerful resummation procedure must be used. One of the simplest ways is to perform the double Padé analysis [47]. This should work well when the series behaves in lowest orders 'in a convergent fashion'.

The results of our calculations of the surface critical exponents of the ordinary transition for various values of $n = 3, 4, 8, \infty$ at the corresponding cubic fixed points are presented in tables 1–5. Unfortunately, the second-order ($p = 2$) analysis of perturbative series[4] gives the cubic fixed point with coordinates $u_0 = 1.5347$ and $v_0 = -0.0674$ at $n = 3$ for the 3D model. The analysis of the eigenvalues of the stability matrix shows that in the frames of the two-loop approximation the cubic fixed point at $n = 3$ is unstable and the $O(n)$-symmetric fixed point is stable. But the estimates of the marginal spin dimensionality of the cubic model n_c in the frames of three-loop [36, 37], four-loop [41, 42], five-loop [42–44] and six-loop [45] $\epsilon = 4 - d$ expansions and six-loop study at fixed dimensions $d = 3$ [46] show that the cubic ferromagnets are not described by the Heisenberg isotropic model, but by the cubic model at the stable cubic fixed point. Higher precision six-loop field-theoretical analysis [46] gives the value of the marginal spin dimensionality of the cubic model equal to $n_c = 2.89(4)$. In accordance with this we use the cubic fixed point of the higher $p = 3$ order of perturbative series for obtaining the set of surface critical exponents at $n = 3$. For estimation of the reliability of the obtained results we performed calculations at the cubic fixed point of the $p = 6$ order in table 2. We obtained that differences in these two cases are approximatively 0.5% for $\eta_\parallel$, 0.4% for $\eta_\perp$, 0.8% for Δ_1, 0.1% for β_1, 6% for γ_{11}, 0.2% for γ_1, 0.2% for δ_1 and

[3] This is an intuitive picture conveyed from the theory of bulk regular systems. Much less is known about the large-order behaviour of perturbative expansions pertaining to infinite random systems (see [61–63]), especially at large space dimensionalities. At the present time, there are no explicit results on large orders for the surface quantities, even in the absence of disorder.

[4] We applied the formulae of β functions, presented in [65] for the case of the cubic anisotropic model with $m = 1$ and $n = 3$.

Table 1. Surface critical exponents of the ordinary transition for $d = 3$ up to the two-loop order at the cubic fixed point (of order $p = 3$): $u^* = 1.348$, $v^* = 0.074$, at $n = 3$.

exp	$\frac{O_1}{O_2}$	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	f
$\eta_\parallel$	2.27	1.67	2.00	1.681	1.725	1.541	1.594	1.429	1.428	1.429
$\eta_\perp$	2.74	1.91	1.00	0.841	0.863	0.783	0.805	0.749	0.749	0.749
Δ_1	2.32	3.69	0.25	0.409	0.440	0.478	0.504	0.530	0.530	0.530
β_1	−4.39	−2.58	0.75	0.909	0.940	0.873	0.858	0.880	0.880	0.880
γ_{11}	0.00	0.00	−0.50	−0.50	−0.50	−0.433	−0.428	–	–	−0.400
γ_1	3.38	17.70	0.50	0.739	0.814	0.810	0.838	0.839	0.837	0.838
δ_1	1.99	2.53	1.67	1.844	1.865	1.933	1.957	2.023	2.023	2.023
δ_{11}	1.83	2.47	0.33	0.475	0.498	0.552	0.582	0.647	0.647	0.647

Table 2. Surface critical exponents of the ordinary transition for $d = 3$ up to the two-loop order at the cubic fixed point (of order $p = 6$) $u^* = 1.321(18)$, $v^* = 0.096(20)$, at $n = 3$.

exp	$\frac{O_1}{O_2}$	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	f
$\eta_\parallel$	2.29	1.68	2.00	1.684	1.727	1.545	1.597	1.436	1.435	1.436
$\eta_\perp$	2.76	1.92	1.00	0.842	0.863	0.785	0.806	0.752	0.752	0.752
Δ_1	2.34	3.72	0.25	0.408	0.438	0.476	0.501	0.526	0.526	0.526
β_1	−4.42	−2.60	0.75	0.908	0.938	0.872	0.858	0.879	0.879	0.879
γ_{11}	0.00	0.00	−0.50	−0.50	−0.50	−0.433	−0.428	–	–	−0.424
γ_1	3.41	17.87	0.50	0.737	0.811	0.807	0.834	0.835	0.836	0.836
δ_1	2.01	2.55	1.67	1.842	1.863	1.930	1.953	2.018	2.017	2.018
δ_{11}	1.84	2.48	0.33	0.474	0.497	0.550	0.579	0.642	0.642	0.642

0.8% for δ_{11}. The obtained results indicate that the difference in the methods of β function resummation has no essential influence on the values of the surface critical exponents and that the results obtained in the frames of the two-loop approximation are stable and reliable. The surface critical exponents of the ordinary transition for $n = 4, 8$ and $n \to \infty$ were calculated at the standard infrared-stable cubic FP of the underlying bulk theory, as is usually accepted in the massive field theory[5].

The quantities O_1/O_2 and O_{1i}/O_{2i} represent the ratios of magnitudes of first-order and second-order perturbative corrections appearing in direct and inverse series expansions. The larger (absolute) values of these ratios indicate better apparent convergence of truncated series.

The values $[p/q]$ (where $p, q = 0, 1$) are simply Padé approximants which represent the partial sums of the direct and inverse series expansions up to the first and the second order. The nearly diagonal two-variable rational approximants of the types [11/1] and [1/11] give at $u = 0$ or $v = 0$ the usual [1/1] Padé approximant [47]. As is easy to see from tables 1–5, the values of [11/1] and [1/11] Padé approximants do not differ significantly between themselves. We consider these values as the best we could achieve from the available knowledge about the series expansions in the two-loop approximation scheme. Thus, our final results are presented in the last columns of tables 1–5. Their deviations from the other second-order estimates might serve as a rough measure of the achieved numerical accuracy. As is easy to see, the obtained results indicate good stability of the results calculated in the frames of the two-loop approximation scheme.

[5] The values of ν and η at $n = 4, 8$ and $n \to \infty$ are calculated from formulae presented in [65] for the case of the cubic anisotropic model.

Table 3. Surface critical exponents of the ordinary transition for $d = 3$ up to the two-loop order at the cubic fixed point (of order $p = 2$) $u^* = 1.064$, $v^* = 0.520$, at $n = 4$.

exp	$\frac{O_1}{O_2}$	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	f
$\eta_\parallel$	2.12	1.54	2.00	1.647	1.700	1.481	1.550	1.319	1.314	1.317
$\eta_\perp$	2.51	1.74	1.00	0.824	0.850	0.753	0.783	0.705	0.705	0.705
Δ_1	2.07	3.27	0.25	0.426	0.464	0.511	0.549	0.588	0.589	0.589
β_1	−4.95	−2.64	0.75	0.926	0.964	0.891	0.873	0.898	0.900	0.899
γ_{11}	0.0	0.0	−0.50	−0.50	−0.50	−0.409	−0.400	–	–	0.311
γ_1	2.91	12.61	0.50	0.765	0.860	0.856	0.900	0.899	0.902	0.901
δ_1	1.83	2.34	1.67	1.863	1.889	1.969	2.003	2.105	2.103	2.104
δ_{11}	1.70	2.31	0.33	0.490	0.519	0.583	0.623	0.727	0.724	0.726

Table 4. Surface critical exponents of the ordinary transition for $d = 3$ up to the two-loop order at the cubic fixed point (of order $p = 2$) $u^* = 0.525$, $v^* = 1.146$, at $n = 8$.

exp	$\frac{O_1}{O_2}$	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	f
$\eta_\parallel$	2.13	1.55	2.00	1.645	1.699	1.479	1.548	1.307	1.297	1.302
$\eta_\perp$	2.51	1.74	1.00	0.823	0.849	0.752	0.781	0.702	0.701	0.702
Δ_1	2.05	3.22	0.25	0.427	0.466	0.514	0.553	0.592	0.593	0.593
β_1	−5.45	−2.77	0.75	0.927	0.966	0.895	0.878	0.903	0.905	0.904
γ_{11}	0.0	0.0	−0.50	−0.50	−0.50	−0.393	−0.380	–	–	−0.315
γ_1	2.84	11.57	0.50	0.766	0.863	0.860	0.907	0.902	0.909	0.906
δ_1	1.84	2.34	1.67	1.864	1.890	1.971	2.005	2.113	2.139	2.126
δ_{11}	1.70	2.33	0.33	0.491	0.521	0.584	0.624	0.739	0.732	0.736

Table 5. Surface critical exponents of the ordinary transition for $d = 3$ up to the two-loop order at the cubic fixed point (of order $p = 2$) $u^* = 0.201$, $v^* = 1.508$, for $n \to \infty$.

exp	$\frac{O_1}{O_2}$	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	f
$\eta_\parallel$	2.14	1.56	2.00	1.648	1.701	1.484	1.552	1.312	1.300	1.306
$\eta_\perp$	2.53	1.75	1.00	0.824	0.850	0.755	0.783	0.706	0.704	0.705
Δ_1	2.07	3.26	0.25	0.426	0.463	0.511	0.549	0.585	0.587	0.586
β_1	−5.34	−2.75	0.75	0.926	0.963	0.893	0.876	0.901	0.904	0.903
γ_{11}	0.0	0.0	−0.50	−0.50	−0.50	−0.387	−0.373	–	–	−0.323
γ_1	2.88	11.93	0.50	0.764	0.858	0.856	0.901	0.895	0.902	0.899
δ_1	1.85	2.36	1.67	1.862	1.888	1.968	2.001	2.108	2.105	2.107
δ_{11}	1.71	2.34	0.33	0.490	0.519	0.581	0.621	0.736	0.728	0.732

The results for surface critical exponents of the semi-infinite model with cubic anisotropy, calculated at the cubic fixed point, are different from the results for surface critical exponents of the standard semi-infinite n-component model (see [15, 18, 60, 21])[6].

6. Concluding remarks

We have studied the *ordinary transition* for semi-infinite systems with cubic anisotropy by applying the field theoretic approach directly in $d = 3$ dimensions, up to the two-loop approximation. We have performed a double Padé analysis of the resulting perturbation series

[6] In order to evaluate the difference between surface critical exponents of the semi-infinite model with cubic anisotropy and surface critical exponents of the standard semi-infinite n-component model [15, 18, 60, 21] we performed additional calculations for surface critical exponents on the basis of formulae from [60, 21] in the case of the 3D semi-infinite model with $n = 3$.

for the surface critical exponents of the ordinary transition for various $n = 3, 4, 8, \infty$, in order to find the best numerical estimates. We find that at $n > n_c$, the surface critical exponents of the ordinary transition in semi-infinite systems with cubic anisotropy belong to the cubic universality class.

In order to obtain more precise numerical estimates for the case of 3D cubic crystal with $n = 3$, a further theoretical investigation of the asymptotic surface critical behaviour of semi-infinite cubic systems would be highly desirable within the framework of higher-order RG approximations.

We suggest that the obtained results could stimulate further experimental and numerical investigations of the surface critical behaviour of systems with cubic anisotropy.

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Appendix A. The effective Hamiltonian of an *mn*-component model with cubic anisotropy

The effective Ginzburg–Landau–Wilson Hamiltonian of an *mn*-component model with cubic anisotropy reads as follows [4, 5]

$$H(\vec{\phi}) = \int \mathrm{d}^d x \left[\frac{1}{2} \sum_{i=1}^{n} \left(|\nabla \vec{\phi}^i|^2 + m_0^2 \, |\vec{\phi}^i|^2 \right) + \frac{1}{4!} v_0 \sum_{i=1}^{n} |\vec{\phi}^i|^4 + \frac{1}{4!} u_0 \left(\sum_{i=1}^{n} |\vec{\phi}^i|^2 \right)^2 \right] \tag{A.1}$$

where each vector field $\vec{\phi}^i(x)$ with $i = 1, \ldots, n$ has m-components $\vec{\phi}^i(x) = \left(\phi_1^i, \ldots, \phi_m^i\right)$. Here m_0, u_0, v_0 are the 'bare' mass and coupling constants, respectively.

Appendix B. The Landau–Ginzburg–Wilson functional for the semi-infinite systems with cubic anisotropy

We outline the main steps for deriving the Landau–Ginzburg–Wilson functional for the case of the Heisenberg ferromagnet and discuss briefly the surface term leading to the surface boundary conditions. We perform the calculation for a simple cubic structure and start from the mean-field approximation for the Heisenberg exchange interaction, as the cubic-anisotropy term can be added afterwards. Additionally, we limit ourselves to one-component theory, as the generalization to the n-component version is not important to the essence of the principal argument.

Suppose we have the system of localized spins of magnitude S, described by the Heisenberg Hamiltonian, which in the applied field h takes the form

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z. \tag{B.1}$$

In the mean-field approximation

$$\mathbf{S}_i \cdot \mathbf{S}_j = \langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \langle \mathbf{S}_j \rangle \cdot \mathbf{S}_i - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle \tag{B.2}$$

and for the spin quantization axis taken as the z-axis. We can write the free energy in the form

$$F = -\tilde{N} k_B T \ln \frac{\sinh(\beta h_i (S + 1/2))}{\sinh(\beta h_i/2)} + \frac{1}{2} \sum_{i \neq j} J_{ij} \langle S_i^z \rangle \langle S_j^z \rangle \tag{B.3}$$

where $h_i = \sum_j J_{ij} \langle S_j^z \rangle + h$ is the effective field acting on S_i^z, $\beta = (k_B T)^{-1}$ is the inverse temperature in energy units and $\bar{N}$ is the total number of spins.

The constant term can be rewritten in the first nontrivial order of the continuum-medium approximation as

$$\frac{1}{2} \sum_j J_{ij} \langle S_i^z \rangle \langle S_j^z \rangle \simeq \frac{1}{2} J_0 \langle S^z(\mathbf{x}) \rangle \bigg|_{\mathbf{x}=\mathbf{R}_i} + \frac{1}{2} a_0^2 \langle S^z(\mathbf{x}) \rangle \nabla^2 \langle S^z(\mathbf{x}) \rangle \bigg|_{\mathbf{x}=\mathbf{R}_i} \tag{B.4}$$

where $J_0 = \sum_j J_{ij}$, a_0 is the lattice constant and $i = \mathbf{R}_i$ denotes here the lattice site position.

The expansion of the ratio of hyperbolic function in $y = \beta h_i$ can be represented as

$$\frac{\sinh(y(S + 1/2))}{\sinh(y/2)} \simeq (2S + 1) \left[1 + \frac{1}{6} S(S + 1) y^2 + \frac{1}{360} S(3S^3 + 6S^2 + 2S - 1) y^4 \right] + O(y^6). \tag{B.5}$$

Hence, the free energy (per site) to the same approximation after taking the continuum-medium limit reads

$$\begin{aligned} \frac{F}{\tilde{N}} = \frac{F_0}{\tilde{N}} + \int \mathrm{d}^d x \bigg(& \frac{3}{2S(S + 1)} k_B (T - T_c) \phi(\mathbf{x})^2 \\ & + \frac{1}{2} J_0 a_0^2 |\nabla \phi(\mathbf{x})|^2 - \frac{1}{3} S(S + 1) \beta h J_0 \phi(\mathbf{x}) \\ & + \frac{\beta^3}{72} \left(S^2 (S + 1)^2 - \frac{S}{5} (3S^3 + 6S^2 + 2S - 1) \right) (J_0 \phi(\mathbf{x})^4) \bigg) \\ & + o(|\phi|^6) + o(h^2) + o(|\nabla \phi|^4) \end{aligned} \tag{B.6}$$

with $\frac{F_0}{\tilde{N}} = -k_B T \ln(2S + 1)$. The continuous field $\phi(\mathbf{x})$ expresses the limiting value of $\langle S_i^z \rangle$ per volume a_0^d.

Defining the mean-field critical temperature $T_c = \frac{1}{3k_B} J_0 S(S + 1)$ and assuming that we can put $T \simeq T_c$ in the last two terms we obtain the desired free energy functional in the form

$$\frac{F}{\tilde{N}} = \frac{F_0}{\tilde{N}} + \int \mathrm{d}^d x \left(\frac{A_0}{2} |\nabla \phi(\mathbf{x})|^2 + \frac{A_1}{2} (T - T_c) |\phi(\mathbf{x})|^2 + \frac{A_2}{4!} |\phi(\mathbf{x})|^4 - h \phi(\mathbf{x}) \right) \tag{B.7}$$

where the constants are related in an obvious fashion to the coefficients m_0^2 and u_0, when we divide F by the exchange stiffness constant A_0, which contains non-divergent constants at the critical point.

Now, the boundary conditions appear when we derive the Landau–Ginzburg equation in the form of the Euler equation for $\phi(\mathbf{x})$. However, in such a situation specific surface terms appear. There are two types of terms. First is the gradient term $A_0' |\nabla \phi(\mathbf{r}, z = 0)|^2$, since in $J_0 = \sum_j J_{ij}$ the spins above the surface are missing. Second, the geometrical surface term of the form $\frac{1}{2} c_0 \int \mathrm{d}^{d-1} r \phi^2(\mathbf{r}, z = 0)$ may appear where c_0 is the surface enhancement constant. This is because on the surface the role of the bulk cubic anisotropy is taken over by surface anisotropy, which in the first nontrivial order has the form $\frac{1}{2} \sum_{i=1}^n c_0^i \phi_i^2(\mathbf{r}, z = 0)$. In effect, the condition on the surface coming from the Euler variational scheme takes the following form

$$\sum_{i=1}^n \int \mathrm{d}^{d-1} r \left\{ A_0' \vec{n} \cdot \nabla \phi_i(\mathbf{r}, z) + c_0^i \phi_i(\mathbf{r}, z) \right\} \delta \phi_i(\mathbf{r}, z)|_{z=0} = 0 \tag{B.8}$$

where $\delta\phi_i(\mathbf{r}, z = 0)$ is the variation of $\phi_i(\mathbf{r}, z)$ on the surface and $\vec{n}$ is the vector perpendicular to the surface. Therefore, we can choose the boundary conditions in either way, namely

$$(1) \quad \delta\phi_i(\mathbf{r}, z)|_{z=0} = 0 \quad \text{i.e. } \phi_i(\mathbf{r}, z)|_{z=0} = \text{const} = S_0 \tag{B.9}$$

$$(2) \quad \left(\partial_n\phi_i(\mathbf{r}, z) + \frac{c_0^i}{A_0'}\phi_i(\mathbf{r}, z)\right)\Bigg|_{z=0} = 0. \tag{B.10}$$

In this paper we have selected the bc (1) with $S_0 = 0$, which corresponds to the Dirichlet boundary condition. In such a situation, no specific surface term appears in the starting functional (2.1). However, it must be said that it is the concrete experimental situation that determines the type of boundary conditions to be taken into the theoretical analysis.

Appendix C. Scaling relations between the surface critical exponents

The individual RG series expansions for other critical exponents can be derived through standard surface scaling relations [12] with $d = 3$:

$$\begin{aligned} &\eta_\perp = \frac{\eta + \eta_\|}{2} && \beta_1 = \frac{\nu}{2}(d - 2 + \eta_\|) \\ &\gamma_{11} = \nu(1 - \eta_\|) && \gamma_1 = \nu(2 - \eta_\perp) \\ &\Delta_1 = \frac{\nu}{2}(d - \eta_\|) && \delta_1 = \frac{\Delta}{\beta_1} = \frac{d + 2 - \eta}{d - 2 + \eta_\|} \\ &\delta_{11} = \frac{\Delta_1}{\beta_1} = \frac{d - \eta_\|}{d - 2 + \eta_\|}. \end{aligned} \tag{C.1}$$

Each of these critical exponents characterizes certain properties of the cubic anisotropic system near the surface. The values ν, η and $\Delta = \nu(d + 2 - \eta)/2$ are the standard bulk exponents.

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