

Critical behavior of semi-infinite random systems at the special surface transition

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We use a three-dimensional massive field theory up to the two-loop approximation to study the critical behavior of semi-infinite quenched random Ising-like systems at the special surface transition. Besides, we extend up to the next-to leading order, the previous first-order results of the $\sqrt{\epsilon}$ expansion obtained by Ohno and Okabe [Phys. Rev. B **46**, 5917 (1992)]. The numerical estimates for surface critical exponents in both cases are computed by means of the Padé analysis. Moreover, in the case of the massive field theory we perform Padé-Borel resummation of the resulting two-loop series expansions for surface critical exponents. The most reliable estimates for critical exponents of semi-infinite systems with quenched bulk randomness at the special surface transition, which we can obtain in the frames of the present approximation scheme, are $\eta_{\parallel} = -0.238$, $\Delta_1 = 1.098$, $\eta_{\perp} = -0.104$, $\beta_1 = 0.258$, $\gamma_{11} = 0.839$, $\gamma_1 = 1.426$, $\delta_1 = 6.521$, and $\delta_{11} = 4.249$. These values are different from critical exponents for pure semi-infinite Ising-like systems and show that in a system with quenched bulk randomness the plane boundary is characterized by a new set of critical exponents at the special surface transition.

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I. INTRODUCTION

Investigation of the critical behavior of real physical systems is of considerable theoretical and experimental interest. Real physical systems are usually characterized by the presence of different kinds of defects and impurities that may be localized inside the bulk or at the boundary.

Historically, the systematic investigation of the quenched disordered systems was initiated in the seminal works by Harris, Lubensky [1,2], and Khmel'nitskii [3]. The study of the Ising-like systems among the whole class of $O(n)$ symmetric n -vector models in d dimensions is of special interest, because they satisfy the Harris criterion [4], which states that the presence of randomness is relevant for such pure systems that have a positive specific heat exponent α . The introduction of the bulk dilution into a system shifts the critical temperature of the bulk phase transition and drives the system to another "random" fixed point in which unconventional scaling behavior is observed. It has been confirmed by the Wilson's renormalization group and ϵ expansions [1–3,5–7], a three-dimensional massive field theory [8–10], experiments [12–14], and Monte Carlo simulations [15,16] that the critical behavior of three-dimensional disordered Ising-like systems is characterized by a new set of critical exponents [17]. The Ising model at $d=2$ is a marginal case because in this case $\alpha=0$ and the corresponding logarithmic corrections to the power law singularities of the pure model take place, as was confirmed in a series of papers [18–23].

The presence of a surface leads to the appearance of additional problems in critical phenomena. The most general review of critical behavior at surfaces and the list of related references are given in Refs. [24–26]. It is well known [24–

28] that each surface universality class is defined by the bulk universality class and specific properties of a given boundary. At the present time three surface universality classes, called ordinary, special, and extraordinary, are known [25,26]. They correspond to the respective surface transitions that occur at the bulk critical point $m_0^2 = m_{0c}^2$ [29] and are characterized by different fixed points

$$c_0^{*,ord} = +\infty, \quad c_0^{*,sp} = c_0^{sp}, \quad c_0^{*,extr} = -\infty. \quad (1.1)$$

Here c_0 is so called "bare surface enhancement," which measures the enhancement of the interactions at the surface, and $(m_0^2, c_0) = (m_{0c}^2, c_0^{sp})$ is a multicritical point, called special point.

The influence of quenched surface disorder on the surface critical behavior was investigated by analytic calculations [30,31] and Monte Carlo simulations [23,32]. General irrelevance-relevance criterion of the Harris-type for short-range as well as for long-range correlated quenched surface disorder was derived [30]. In the case of special transition it has been demonstrated [30,33] that the fixed point describing the surface critical behavior of three-dimensional pure systems is stable with respect to short-range correlated quenched surface disorder. Thus, the weak short-range quenched surface disorder is irrelevant for three-dimensional systems, but long-range correlated enhancement disorder could become relevant in $d \leq 4$ dimensions. Another interesting example is the case of random field quenched surface disorder at the special transition of an Ising-like critical system. In this case the disorder also becomes relevant for $d \leq 4$ dimensions [30].

What happens with the surface critical behavior, when the quenched disorder is introduced in the bulk? The answer for this question could be found in our recent paper [34], where we quantitatively confirm the previous general expectation by Ohno and Okabe [35] that the introduction of quenched bulk randomness in semi-infinite systems bounded by a

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plane surface affects the surface critical behavior of these systems. From the results obtained in the frames of the massive field theory directly in $d=3$ dimensions up to the two-loop approximation, we have found that the critical exponents of quenched dilute semi-infinite systems at the ordinary transition [34] differ from the surface critical exponents of the pure semi-infinite systems [33]. Besides, we have shown that to order ϵ , the $\sqrt{\epsilon}$ expansion for surface critical exponents η_{\parallel} and η_{\perp} gave negative value of the correlation function critical exponent η for the random bulk Ising system according to the scaling relation $\eta=2\eta_{\perp}-\eta_{\parallel}$. It confirms the well known fact that the second order of the $\sqrt{\epsilon}$ expansion is not enough to give correct positive value of bulk critical exponent η [6,7,36–40]. The obtained results [34] have shown that these kinds of deficiencies do not appear in the calculations using the massive field-theoretic approach directly in $d=3$ dimensions [41].

All these have stimulated us to study the critical behavior at the special surface transition occurring in quenched bulk dilute semi-infinite systems bounded with a plane surface. It should be mentioned that the problem of investigation of the critical behavior at the special surface transition is very important from such point of view that at some conditions it may be reduced to the problem of the adsorption of θ polymers on a wall [42,43].

Two main analytic methods have been used for the investigation of the critical behavior of the systems with quenched randomness. One of them is the renormalization-group (RG) approach introduced by Harris and Lubensky [1]. This approach involves applying the RG transformation to the random system directly and subsequent averaging over disorder. Ohno and Okabe [35] employed this method to analyze the influence of randomness on the surface critical behavior at $d=4-\epsilon$ dimensions in the frames of $\sqrt{\epsilon}$ expansion.

Another technique introduced by Grinstein and Luther [5] involves first removing the randomness by averaging, and subsequent employing the renormalization group. They considered an mn -vector model and showed that analytic continuation of this model to $n=0$ is equivalent to a model of a random m -component spin system. An elegant derivation of this equivalence has been given by Emery [44]. We mainly use this technique to treat randomness.

The present paper is dedicated to the investigation of the critical behavior at the special surface transition in semi-infinite, quenched dilute Ising-like systems at the bulk “random” critical point directly in $d=3$ dimensions using the massive field theory up to the two-loop approximation. Besides, we extend up to the next-to leading order of the $\sqrt{\epsilon}$ expansion, the previous first-order results obtained by Ohno and Okabe [35]. The numerical estimates for critical exponents of the special surface transition in both cases are calculated using extensive Padé analyses. Moreover, in the case of the massive field theory we perform Padé-Borel resummations of the resulting two-loop series expansions and obtain quite reasonable and reliable numerical estimates for surface critical exponents. The obtained results confirm that in the case of quenched bulk randomness in semi-infinite systems the new set of the surface critical exponent appears.

II. MODEL

In the previous work [34], we presented an effective Landau-Ginzburg-Wilson Hamiltonian with cubic anisotropy defined in semi-infinite space for description of critical behavior of quenched dilute semi-infinite Ising-like systems at the ordinary transition in the replica limit $n \rightarrow 0$. The critical behavior at the special surface transition has its own peculiarities. In the general case effective Hamiltonian for such systems must involve terms to describe surface interactions [24,25,27,45,30]. Thus, the common form of the effective Hamiltonian to describe the critical behavior of quenched dilute semi-infinite Ising-like systems in the replica limit $n \rightarrow 0$ can be written as

$$H(\vec{\phi}) = \int_0^{\infty} dz \int d^{d-1}r \left[\frac{1}{2} |\nabla \vec{\phi}|^2 + \frac{1}{2} m_0^2 |\vec{\phi}|^2 + \frac{1}{4!} v_0 \sum_{i=1}^n \phi_i^4 + \frac{1}{4!} u_0 (|\vec{\phi}|^2)^2 \right] + \frac{1}{2} \int d^{d-1}r c_0 \vec{\phi}^2. \quad (2.1)$$

It should be mentioned that here $\vec{\phi}$ is an n -vector field with the components $\phi_i, i=1, \dots, n$ defined on a half-space $\mathbb{R}_+^d \equiv \{\mathbf{x}=(\mathbf{r}, z) \in \mathbb{R}^d | \mathbf{r} \in \mathbb{R}^{d-1}, z \geq 0\}$ bounded by a plane free surface at $z=0$. The fields $\phi(\mathbf{r}, z)$ satisfy the Neumann boundary condition [27,45], so that we have $\partial_z \phi(\mathbf{r}, z) = 0$ at $z=0$. This Hamiltonian takes into account surface interaction in the form of an additional term $\frac{1}{2} \int d^{d-1}r c_0 \vec{\phi}^2$. The model defined by Eq. (2.1) is restricted to translations parallel to the boundary surface. Thus, only parallel Fourier transformations in $d-1$ dimensions take place.

III. RENORMALIZATION OF THE CORRELATION FUNCTION

The correlation function of the model of Eq. (2.1), which involves N fields $\phi(\mathbf{x}_i)$ at distinct points \mathbf{x}_i ($1 \leq i \leq N$) in the bulk and M fields $\phi(\mathbf{r}_j, z=0) \equiv \phi_s(\mathbf{r}_j)$ at distinct surface points with parallel coordinates \mathbf{r}_j ($1 \leq j \leq M$), has the form

$$G^{(N,M)}(\{\mathbf{x}_i\} \{ \mathbf{r}_j \}) = \left\langle \prod_{i=1}^N \phi(\mathbf{x}_i) \prod_{j=1}^M \phi_s(\mathbf{r}_j) \right\rangle. \quad (3.1)$$

The corresponding full free propagator in the $\mathbf{p}z$ representation is given by

$$G(\mathbf{p}, z, z') = \frac{1}{2\kappa_0} \left[e^{-\kappa_0 |z-z'|} - \frac{c_0 - \kappa_0}{c_0 + \kappa_0} e^{-\kappa_0(z+z')} \right], \quad (3.2)$$

where $\kappa_0 = \sqrt{p^2 + m_0^2}$ with p being the value of parallel momentum \mathbf{p} associated with $d-1$ translationally invariant directions in the system. The first term in Eq. (3.2) corresponds to usual free bulk propagator in coordinate space, between the points $\mathbf{x}=(\mathbf{r}, z)$ and $\mathbf{x}'=(0, z')$, and the second one, so called “surface” term, depends on the distance between the point \mathbf{x} and its “mirror image” $\hat{\mathbf{x}}'=(0, -z')$.

The formulation of the randomness problem introduced by Grinstein and Luther indicates that the renormalization

process for the random systems is similar to that for the “pure” case [25,33]. As it is known, in the theory of semi-infinite systems the bulk field $\phi(\mathbf{x})$ and the surface field $\phi_s(\mathbf{r})$ should be reparametrized by different uv -finite renormalization factors $Z_\phi(u,v)$ and $Z_1(u,v)$,

$$\phi(x) = Z_\phi^{1/2} \phi_R(x) \quad \text{and} \quad \phi_s(r) = Z_\phi^{1/2} Z_1^{1/2} \phi_{s,R}(r).$$

The renormalized correlation function involving N bulk and M surface fields with $(N,M) \neq (0,2)$ can be written as

$$\begin{aligned} G_R^{(N,M)}(0; m, u, v, c) \\ = Z_\phi^{-(N+M)/2} Z_1^{-M/2} G^{(N,M)}(0; m_0, u_0, v_0, c_0). \end{aligned} \quad (3.3)$$

In order to obtain the critical exponent η_{\parallel}^{sp} that characterizes surface correlations at special transition, it is sufficient to consider a two-point correlation function of surface fields $G^{(0,2)}(p) = \langle \varphi(p, z=0) \varphi(-p, z'=0) \rangle$.

It should be mentioned that the renormalized mass m , coupling constants u , v , and the renormalization factor Z_ϕ are fixed via the standard normalization conditions of the infinite-volume theory [46,5,41,47]. In order to remove short-distance singularities of the correlation function $G^{(0,2)}$ located in the vicinity of the surface, the surface-enhancement shift δc is required. In accordance with this the new normalization condition should be introduced for the definition of the surface-enhancement shift δc and surface renormalization factor Z_1 . We normalize the renormalized surface two-point correlation function in such a manner that at zero external momentum it should coincide with the lowest order perturbation expansion of the surface susceptibility $\chi_{\parallel}(p) = G^{(0,2)}(p)$,

$$G^{(0,2)}(p; m_0, u_0, v_0, c_0) = \frac{1}{c_0 + \sqrt{p^2 + m_0^2}} + O(u_0, v_0) \quad (3.4)$$

and its first derivatives with respect to p^2 . Thus we obtain necessary surface normalization conditions

$$G_R^{(0,2)}(0; m, u, v, c) = \frac{1}{m+c} \quad (3.5)$$

and

$$\left. \frac{\partial G_R^{(0,2)}(p; m, u, v, c)}{\partial p^2} \right|_{p=0} = - \frac{1}{2m(m+c)^2}. \quad (3.6)$$

Equation (3.5) defines the required surface-enhancement shift δc and shows that the surface susceptibility diverges at $m=c=0$. This point corresponds to the multicritical point (m_{0c}^2, c_0^{sp}) at which special transition takes place.

From the normalization condition of Eq. (3.6) and expression for renormalized correlation function of Eq. (3.3), we can define the renormalization factor $Z_{\parallel} = Z_1 Z_\phi$ by

$$Z_{\parallel} = 2m \left. \frac{\partial}{\partial p^2} [G^{(0,2)}(p)]^{-1} \right|_{p^2=0} = \lim_{p \rightarrow 0} \frac{m}{p} \frac{\partial}{\partial p} [G^{(0,2)}(p)]^{-1}. \quad (3.7)$$

The renormalization Z factors in the critical region have the scaling behavior

$$\begin{aligned} Z_\phi &\propto m^\eta, \\ Z_1^{sp} &\propto m^{\eta_1^{sp}}, \end{aligned} \quad (3.8)$$

where m is identified as the inverse bulk correlation length $\xi^{-1} \propto t^\nu$, $t = (T - T_c)/T_c$. Here η is the standard bulk correlation exponent and exponent η_1^{sp} is specific for our *quenched* random semi-infinite system. The exponents η and η_1^{sp} arise from RG arguments of an inhomogeneous Callan-Symanzik equation for correlation functions $G_R^{(0,2)}$, Eq. (3.3), [48,33]

$$\eta_\phi = m \left. \frac{\partial}{\partial m} \ln Z_\phi \right|_{FP}, \quad \eta_1^{sp} = m \left. \frac{\partial}{\partial m} \ln Z_1 \right|_{FP}. \quad (3.9)$$

The simple scaling dimensional analysis of $G_R^{(0,2)}$ and mass dependence of Z factors, Eq. (3.8), defines the surface correlation exponent η_{\parallel}^{sp} via

$$\eta_{\parallel}^{sp} = \eta_1^{sp} + \eta. \quad (3.10)$$

From Eqs. (3.7), (3.9), and (3.10), we obtain for surface correlation exponent η_{\parallel}^{sp} ,

$$\begin{aligned} \eta_{\parallel}^{sp} &= m \left. \frac{\partial}{\partial m} \ln Z_{\parallel} \right|_{FP} \\ &= \beta_u(u, v) \frac{\partial \ln Z_{\parallel}(u, v)}{\partial u} \\ &\quad + \beta_v(u, v) \frac{\partial \ln Z_{\parallel}(u, v)}{\partial v} \Big|_{FP}. \end{aligned} \quad (3.11)$$

Above equations should be calculated at the infrared-stable random fixed point (FP) of the underlying bulk theory. The other critical exponents of the special surface transition can be determined via the set of surface scaling relations [25].

IV. THE PERTURBATION SERIES UP TO TWO LOOPS

In the preceding section we showed that the surface critical exponent η_{\parallel}^{sp} can be obtained from Eq. (3.11), where renormalization factor Z_{\parallel} is defined by Eq. (3.7). By analogy with infinite-volume theory, we considered the inverse surface correlation function $[G^{(0,2)}(p; m_0, u_0, v_0, c_0)]^{-1}$ in order to avoid the dependence of external lines on the external momentum p and the surface enhancement c_0 in each external propagator. Thus we considered the Feynman diagram expansion of the unrenormalized surface correlation function $[G^{(0,2)}(p)]^{-1}$ in terms of the free propagator of Eq. (3.2) up to the two-loop order. It should be mentioned that here, by

analogy with Refs. [33,49,34] in order to avoid the usual bulk and surface uv singularities, which are present in correlation function $[G^{(0,2)}(p; m_0 u_0, v_0, c_0)]^{-1}$, we performed the mass- and surface-enhancement renormalizations. After carrying out the integration of Feynman integrals, which arise in the calculation of the correlation function $[G^{(0,2)}(p; m_0 u_0, v_0, c_0)]^{-1}$, we obtained

$$Z_{\parallel}^{-1}(\bar{u}_0, \bar{v}_0) = 1 - \frac{\bar{t}_1^{(0)}}{4} + \frac{\bar{t}_1^{(0)2}}{4} \left[\frac{1}{2} - \ln 2 + \ln^2 2 \right] + \bar{t}_2^{(0)} A, \quad (4.1)$$

where the constant $A \approx 0.202428$ arose from the two-loop contribution. The corresponding weighting factors $\bar{t}_1^{(0)} = [(n+2)/3]\bar{u}_0 + \bar{v}_0$ and $\bar{t}_2^{(0)} = [(n+2)/3]\bar{u}_0^2 + \bar{v}_0^2 + 2\bar{u}_0\bar{v}_0$ arise from the standard symmetry factors of the effective Hamiltonian of Eq. (2.1) (see Ref. [34]). Thus the renormalization factor Z_{\parallel} is expressed as a second-order series expansion in powers of *bare* dimensionless parameters $\bar{u}_0 = u_0/8\pi m$ and $\bar{v}_0 = v_0/8\pi m$.

After carrying out the vertex renormalizations $\bar{u}_0 = \bar{u}(1 + [(n+8)/6]\bar{u} + \bar{v})$, $\bar{v}_0 = \bar{v}(1 + \frac{3}{2}\bar{v} + 2\bar{u})$, we obtain a modified series expansion of Z_{\parallel} in terms of new renormalized coupling constants \bar{u} and \bar{v} ,

$$Z_{\parallel}^{-1}(\bar{u}, \bar{v}) = 1 - \frac{n+2}{12}\bar{u} - \frac{\bar{v}}{4} + \frac{n+2}{3} B(n)\bar{u}^2 + B(1)\bar{v}^2 + 2B(n)\bar{u}\bar{v}, \quad (4.2)$$

where $B(n) = A - \frac{1}{4} + [(n+2)/12](\ln^2 2 - \ln 2)$ and n is the replica number.

Combining the renormalization factor $Z_{\parallel}(\bar{u}, \bar{v})$ with the one-loop pieces of the β functions $\beta_{\bar{u}}(\bar{u}, \bar{v}) = -\bar{u}(1 - [(n+8)/6]\bar{u} - \bar{v})$, $\beta_{\bar{v}}(\bar{u}, \bar{v}) = -\bar{v}(1 - \frac{3}{2}\bar{v} - 2\bar{u})$ according to Eq. (3.11), we obtain the desired series expansion for η_{\parallel}^{sp} ,

$$\eta_{\parallel}^{sp}(u, v) = -\frac{n+2}{2(n+8)}u - \frac{v}{6} + 12\frac{(n+2)}{(n+8)^2}A(n)u^2 + \frac{4}{9}A(1)v^2 + \frac{8}{n+8}A(n)uv, \quad (4.3)$$

where $A(n)$ is a function of the replica number n , defined as

$$A(n) = 2A + \frac{n-10}{48} + \frac{n+2}{6}(\ln^2 2 - \ln 2), \quad (4.4)$$

and renormalized coupling constants u and v , normalized in a standard fashion $u = [(n+8)/6]\bar{u}$ and $v = \frac{3}{2}\bar{v}$.

In fact, Eq. (4.3) for η_{\parallel}^{sp} provides a result for the *cubic anisotropic* model given by the effective Hamiltonian (2.1) with general number n of order-parameter components. In the case of infinite space, this cubic anisotropic model attracted much attention very recently (see, e.g., Refs. [50–52] and references therein).

In the present paper, we restrict our discussion to the case of *semi-infinite random Ising-like* systems by taking the replica limit $n \rightarrow 0$. Equation (4.3) in such a limit implies

$$\eta_{\parallel}^{sp} = -\frac{u}{8} - \frac{v}{6} + \frac{3}{8}A(0)u^2 + \frac{4}{9}A(1)v^2 + A(0)uv. \quad (4.5)$$

As it is well known, the knowledge of one surface critical exponent gets access via the usual scaling relations [25] to the other surface critical exponents. For convenience, further below we suppress the superscript sp at the critical exponents.

V. CALCULATION OF THE SURFACE CRITICAL EXPONENTS

The present section is devoted to numerical calculation of the critical exponents at the special surface transition. The individual RG series expansions for other critical exponents can be derived from Eq. (4.5) through standard scaling relations [25] (with $d=3$),

$$\eta_{\perp} = \frac{\eta + \eta_{\parallel}}{2},$$

$$\beta_1 = \frac{\nu}{2}(d-2 + \eta_{\parallel}),$$

$$\gamma_{11} = \nu(1 - \eta_{\parallel}),$$

$$\gamma_1 = \nu(2 - \eta_{\perp}), \quad (5.1)$$

$$\Delta_1 = \frac{\nu}{2}(d - \eta_{\parallel}),$$

$$\delta_1 = \frac{\Delta}{\beta_1} = \frac{d+2-\eta}{d-2+\eta_{\parallel}},$$

$$\delta_{11} = \frac{\Delta_1}{\beta_1} = \frac{d-\eta_{\parallel}}{d-2+\eta_{\parallel}}.$$

Each of these critical exponents characterizes certain properties of the system with the surface in the vicinity of the critical point (see Ref. [35]) with ν , η , and $\Delta = \nu(d+2 - \eta)/2$ being the standard bulk exponents; the series expansions for ν and η at $d=3$ are given by [8–10]

$$\nu = \frac{1}{2} \left[1 + \frac{v}{6} + \frac{(n+2)}{2(n+8)}u - \frac{1}{324} \left(\frac{11}{9}v^2 - \frac{2}{n+8} \times (27n-38)uv - \frac{3(n+2)}{(n+8)^2} (27n-38)u^2 \right) \right],$$

$$\eta = \frac{8}{27} \left[\frac{v^2}{27} + \frac{2uv}{3(n+8)} + \frac{(n+2)}{(n+8)^2}u^2 \right]. \quad (5.2)$$

TABLE I. Critical exponents of the special surface transition for $d=3$ up to two-loop order at the random fixed point $u^* = -0.60509$, $v^* = 2.39631$.

exp	$\frac{O_{1i}}{O_{2i}}$	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[11/1]	[1/11]	R^{-1}	$f(\eta_{\parallel}, \nu, \gamma)$
η_{\parallel}	-23.82	0.00	-0.324	-0.245	-0.205	-0.237	-0.244	-0.238	-0.238	-0.238
Δ_1	-3.39	0.75	1.074	1.229	1.083	1.046	1.083	1.090	1.101	1.098
η_{\perp}	-3.35	0.00	-0.162	-0.139	-0.087	-0.102	-0.115	-0.114	-0.116	-0.104
β_1	0.00	0.25	0.25	0.25	0.263	0.263				0.258
γ_{11}	-3.14	0.50	0.824	0.979	0.825	0.783	0.825	0.834	0.845	0.839
γ_1	-2.56	1.00	1.405	1.680	1.410	1.327	1.410	1.421	1.442	1.426
δ_1	-1.41	5.00	6.619	7.394	7.062	5.521	6.205	6.236	6.343	6.521
δ_{11}	-1.40	3.00	4.295	5.279	3.926	3.418	4.032	4.070	4.172	4.249

For each of the surface critical exponents we obtain from Eq. (5.1) and Eq. (4.3) at $d=3$ a double series expansion in powers of u and v truncated at the second order

$$f(u, v) = \sum_{j, l \geq 0} f_{jl} u^j v^l. \quad (5.3)$$

Since perturbation expansions of this kind are generally divergent [53], the powerful resummation procedure of the series is essential to obtain accurate estimates of the critical exponents. One of the simplest ways is to calculate for each quantity a sequence of rational Padé approximants in two variables from the original series expansions. This should work well when the series behave in lowest orders “in a convergent fashion.” Besides, if the series are alternating in sign [56], we can use more modern Padé-Borel resummation procedures [57] for their analysis. The results of our Padé and Padé-Borel analyses for critical exponents at the special surface transition are represented in Table I.

Since our calculations are performed in the frames of the two-loop approximation, we evaluate the surface critical exponents at the corresponding standard RG random fixed point of the underlying bulk theory [8],

$$u^* = -0.60509, \quad v^* = 2.39631, \quad (5.4)$$

as it is usually accepted in the massive field-theoretical framework.

The values [0/0], [1/0], and [2/0] are simply the direct partial sums up to the zeroth, first, and second orders, respectively. Padé approximants [0/1] and [0/2] represent the partial sums of the inverse series expansions up to the first and second order.

As in Ref. [34], we also consider nearly diagonal two-variable rational approximants of the type

$$[11/1] = \frac{1 + a_1 u + \bar{a}_1 v + a_{11} uv}{1 + b_1 u + \bar{b}_1 v} \quad (5.5)$$

and

$$[1/11] = \frac{1 + a_1 u + \bar{a}_1 v}{1 + b_1 u + \bar{b}_1 v + b_{11} uv}, \quad (5.6)$$

which give the numerical values listed in Table I.

Table I contains the ratios of magnitudes of first-order (O_{1i}) and second-order (O_{2i}) perturbative corrections appearing in inverse series expansions of our critical exponents. The larger (absolute) values of these ratios correspond to the better apparent convergence of truncated series. It is easy to see that the series of inverse expansions for all critical exponents, except β_1 , are alternating in sign and consequently adapted to the above-mentioned Padé-Borel resummation analysis (see Appendix A). Among the direct series the situation is more complicated. The ratios of the first-order (O_1) and the second-order (O_2) perturbative corrections of the direct series expansions for the critical exponents δ_1 , γ_{11} , and γ_1 are positive [58]. This means that the signs of the first- and second-order corrections do not alternate and hence the corresponding series are not suitable to the Padé-Borel resummation technique, since the [11/1] approximant of the Borel transform have a pole in the integration range. But these series are slowly convergent, because the contribution of the second order are considerably less than contribution of the first order. For example, the ratio O_1/O_2 for the critical exponent Δ_1 is equal to 35.1. Thus the above-mentioned series adapted to the Padé analysis. It should be noted, that a very similar situation has been met in the analysis of the perturbation series expansions of the surface critical exponents at the ordinary transition in pure [33] and quenched dilute semi-infinite Ising-like systems [34].

The results of Padé-Borel analysis of the inverse series expansions R^{-1} are given in Table I. These values give numerical estimates of surface critical exponents with a high degree of reliability. As it is easy to see from Table I, the most reliable estimate is obtained from the inverse series expansion for the exponent η_{\parallel} , which represent the best convergence properties. Substituting this value of $\eta_{\parallel} = -0.238$ together with the standard bulk values $\nu = 0.678$ and $\gamma = 0.031$ [8] into the scaling laws of Eq. (5.1), we have obtained the remaining critical exponents that are present in the last column of Table I. The deviations of these estimates from the other estimates of the table might serve as a rough measure of the achieved numerical accuracy.

In order to understand the reliability of the results obtained in the two-loop approximation, we have also calculated some critical exponents from $\eta_{\parallel} = -0.238$ and six-loop

TABLE II. Critical exponents of the special surface transition from the $\sqrt{\epsilon}$ expansion.

exp	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]
η_{\parallel}	0.00	-0.336	-0.252	-0.289	-0.287	-0.295
Δ_1	0.75	0.960	1.016	0.938	0.917	0.940
η_{\perp}	0.00	-0.168	-0.144	-0.149	-0.151	-0.151
β_1	0.25	0.208	0.210	0.197	0.198	0.194
γ_{11}	0.50	0.752	0.838	0.740	0.714	0.741
γ_1	1.00	1.252	1.338	1.224	1.190	1.227
δ_1	5.00	6.682	7.535	7.019	6.729	7.104
δ_{11}	3.00	4.346	5.441	4.608	4.232	4.671

perturbation theory results for bulk critical exponents: $\nu=0.678(10)$ and $\eta=0.030(3)$ [47]. We have obtained $\Delta_1=1.098$, $\eta_{\perp}=-0.104$, $\beta_1=0.258$, $\gamma_{11}=0.839$, $\gamma_1=1.427$, $\delta_1=6.522$, and $\delta_{11}=4.249$, which differ very little from the values in the last column of Table I. This indicates good stability of the results obtained in the frames of the two-loop approximation.

VI. $\sqrt{\epsilon}$ EXPANSION

As it is mentioned above, there is an alternative method to analyze the influence of randomness on the critical behavior introduced by Harris and Lubensky [1]. This method was used by Ohno and Okabe [35] to study critical behavior of semi-infinite systems with a *Gaussian randomness* in $4-\epsilon$ dimensions in the frames of $\sqrt{\epsilon}$ expansion for obtaining the two-loop approximation for correlation function and deriving corresponding series expansions for the surface critical exponents η_{\parallel} and η_{\perp} . Their results in the case of special surface transition at $n=1$ (see Ref. [35]) with corresponding changes of coupling constant normalizations ($u \rightarrow v/24, w \rightarrow -u/3$) in accordance with our notations are written in the form

$$\eta_{\parallel} = -\frac{u}{3} - \frac{v}{2} + \frac{7}{12}u^2 + \frac{11}{12}v^2 + \frac{7}{4}uv + O(\epsilon^{3/2}),$$

$$\eta_{\perp} = -\frac{u}{6} - \frac{v}{4} + \frac{11}{36}u^2 + \frac{23}{48}v^2 + \frac{11}{12}uv + O(\epsilon^{3/2}). \quad (6.1)$$

Unfortunately, only the first order $\sqrt{\epsilon}$ corrections have been obtained from these equations for the surface critical exponents η_{\parallel} and η_{\perp} in Ref. [35]. In the present paper, we derive the next term in $\sqrt{\epsilon}$ expansion for above-mentioned surface critical exponents using the fixed-point values up to $O(\epsilon)$ [6,7]

$$u^* = -3\sqrt{\frac{6\epsilon}{53}} + 18\frac{110+63\zeta(3)}{53^2}\epsilon,$$

$$v^* = 4\sqrt{\frac{6\epsilon}{53}} - 72\frac{19+21\zeta(3)}{53^2}\epsilon, \quad (6.2)$$

where $\zeta(3) \approx 1.2020569$ is the Riemann ζ function, and the usual geometric factor $K_d = 2^{1-d}\pi^{-d/2}/\Gamma(d/2)$ has been absorbed into the redefinitions of the coupling constants. As a result we obtain

$$\eta_{\parallel} = -\sqrt{\frac{6\epsilon}{53}} + \frac{756\zeta(3)-641}{2 \times 53^2}\epsilon,$$

$$\eta_{\perp} = -\sqrt{\frac{3\epsilon}{106}} + \frac{378\zeta(3)-347}{2 \times 53^2}\epsilon. \quad (6.3)$$

From scaling relations for surface critical exponents and $\sqrt{\epsilon}$ expansions for random bulk exponents ν and η [6,7], we can obtain perturbative series expansions for other surface critical exponents (see Appendix B).

As in the case of the preceding section, we perform a Padé analysis of our $\sqrt{\epsilon}$ expansions at $\epsilon=1$. The numerical values of critical exponents obtained in this way are represented in Table II. It should be noticed that the $\sqrt{\epsilon}$ expansion is not Borel summable [39,40].

The Padé approximants [1/0] for the exponents η_{\parallel} and η_{\perp} reproduce the first-order results obtained by Ohno and Okabe [35]. On the other hand, the other exponents, β_1 , γ_{11} , and γ_1 slightly differ from the previous results [35]

$$\beta_1 = 0.17, \quad \gamma_{11} = 0.78, \quad \gamma_1 = 1.26. \quad (6.4)$$

The reason is that we calculated our [1/0] estimates directly from each $\sqrt{\epsilon}$ expansion, while in Ref. [35] they were obtained from the scaling relations using the above-mentioned numerical values of η_{\parallel} and η_{\perp} (6.3). In addition we performed the analysis of the corresponding series expansions for surface magnetic shift exponent Δ_1 , exponents δ_1 and δ_{11} , which give relations between the surface magnetization and the surface and bulk external magnetic fields, respectively.

Comparing Tables I and II, we find that the values of the first-order approximants, denoted by [1/0] and [0/1] in both cases, are of comparable magnitudes. It can be easily verified that the above first-order approximants of the critical exponents satisfy the scaling relation

$$\eta_{\perp} = (\eta + \eta_{\parallel})/2 \quad (6.5)$$

with the value of the bulk exponent $\eta = -(\epsilon/106) + O(\epsilon^{3/2})$ [2,3,5].

But, on the other hand, the values of the second-order approximants are significantly different in both tables. As was shown previously [36–40], $\sqrt{\epsilon}$ series expansions possess rather irregular structure and are practically unsuitable for subsequent resummation and are ineffective for obtaining reliable numerical estimates. Our results confirm this assumption. If we try to reproduce the numerical value of bulk exponent η [see Eq. (6.5)] from our second-order data of Table II according to the scaling relations of Eq. (6.5), we always obtain negative values. But, this does not agree with the sufficiently precise positive results of massive field-theoretic approach for random bulk systems in three dimensions up to two-loop [8,59], three-loop [60,10,39], and to four-loop [61] order. Besides, very recently the values $\eta = 0.025 \pm 0.01$ and $\eta = 0.030(3)$ were obtained, respectively, in the frames of five-loop [50] and six-loop [47] renormalization-group expansions. This discrepancy is not present in our calculation performed directly at $d=3$ (see Table I). From the surface scaling relation of Eq. (6.5) and the second-order results of Table I we always obtain positive value of critical exponent η , which quite well agree with previous estimates.

VII. SUMMARY

The main aim of the present paper was an investigation of the influence of quenched bulk randomness on the surface critical behavior of semi-infinite Ising-like systems at the special transition. We have calculated the surface critical exponents for such systems using two alternative techniques: by the massive field theory directly at $d=3$ dimensions up to two-loop order, and the $\sqrt{\epsilon}$ expansion at $d=4-\epsilon$ dimensions to the order of $O((\sqrt{\epsilon})^2)$. In the last case we extend up to the next-to leading order, the previous first-order results obtained by Ohno and Okabe [35].

In both cases the resummation of obtained perturbation series expansions for surface critical exponents was performed using Padé analysis. But, the $\sqrt{\epsilon}$ expansions possess rather irregular structure, as was shown in Refs. [39,38,40]. This makes them practically unsuitable for subsequent Padé-Borel resummation and ineffective for getting reliable quantitative numerical estimates. However, in the case of the massive field theory the resulting two-loop series expansions could be resummed by means of a more precise Padé-Borel resummation technique. In the previous sections, we have discussed some merits of using the massive field theory directly in $d=3$ dimensions for obtaining most reliable numerical estimates for critical exponents. Thus, the best estimates for surface critical exponents of semi-infinite systems with quenched bulk disorder at the special transition, which we can obtain in the frames of the present approximation scheme, are

$$\eta_{\parallel} = -0.238, \quad \Delta_1 = 1.098, \quad \eta_{\perp} = -0.104, \quad \beta_1 = 0.258,$$

$$\gamma_{11} = 0.839, \quad \gamma_1 = 1.426, \quad \delta_1 = 6.521, \quad \delta_{11} = 4.249. \quad (7.1)$$

These are evidently different from results obtained for pure semi-infinite Ising-like systems [35,61]

$$\begin{aligned} \eta_{\parallel} &= -0.165, & \Delta_1 &= 0.997, & \eta_{\perp} &= -0.067, & \beta_1 &= 0.263, \\ \gamma_{11} &= 0.734, & \gamma_1 &= 1.302, & \delta_1 &= 5.951, & \delta_{11} &= 3.791, \end{aligned} \quad (7.2)$$

and show that the presence of quenched bulk disorder affects the critical behavior of the boundary surface. So, in the case of special surface transition, similarly as in the case of previously investigated ordinary transition [34], a new set of surface critical exponents appear. It should be mentioned that at the present time the investigation of the crossover phenomenon from ordinary to special surface transition for such kinds of semi-infinite systems with quenched bulk disorder is still an open question. This problem will be the topic of our next publication.

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APPENDIX A

As was mentioned above, the power series expansions of critical exponents [see Eq. (5.3)] are in general not convergent. In order to obtain meaningful and rather accurate numerical estimates we must apply to them sufficiently powerful “resummation” procedure. In the present paper we employ a two-variable resummation technique [8,60,10,61,59] that is a simple generalization of the single-variable Padé-Borel method. The starting point of this calculation is to construct a Borel transform for truncated power series of Eq. (5.3)

$$F(ut, vt) = \sum_{j, l \geq 0} \frac{f_{jl}}{(j+l)!} (ut)^j (vt)^l. \quad (A1)$$

Then we construct the rational approximant $F^B(x, y)$,

$$F^B(u, v) = \frac{1 + a_{10}u + a_{01}v + a_{11}uv}{1 + b_{10}u + b_{01}v}, \quad (A2)$$

which is the extrapolation of the Borel transform (A1). It is clear that at $u=0$ or $v=0$ we obtain from Eq. (A2) the usual [1/1] Padé approximant. The coefficients a_{jl} and b_{jl} are expressed as expansion coefficients of $f(u, v)$ in Eq. (5.3)

$$\begin{aligned} a_{10} &= g_{10} + b_{10}, & b_{10} &= -g_{20}/g_{10}, \\ a_{01} &= g_{01} + b_{01}, & b_{01} &= -g_{02}/g_{01}, \\ a_{11} &= g_{11} + b_{10}g_{01} + b_{01}g_{10}, \end{aligned} \quad (A3)$$

where $g_{jl} = f_{jl}/(j+l)!$. Hence, for the resummed function by means of the Padé-Borel resummation technique we obtain

$$\bar{f}(u, v) = \int_0^{\infty} F^B(ut, vt) e^{-t} dt. \quad (A4)$$

This technique has been applied to the inverse power series expansions of surface critical exponents to find the corresponding Padé-Borel approximants R^{-1} .

APPENDIX B

The perturbation series expansions of other surface critical exponents up to $O((\sqrt{\epsilon})^2)$ order can be obtained from scaling relations of Eq. (5.1) and are given by

$$\begin{aligned}\Delta_1 &= \frac{3}{4} + \frac{5}{8} \sqrt{\frac{6\epsilon}{53}} + \frac{3523 - 3780\zeta(3)}{16 \times 53^2} \epsilon, \\ \beta_1 &= \frac{1}{4} - \frac{1}{8} \sqrt{\frac{6\epsilon}{53}} + \frac{3}{16} \frac{[252\zeta(3) - 461]}{53^2} \epsilon, \\ \gamma_{11} &= \frac{1}{2} + \frac{3}{4} \sqrt{\frac{6\epsilon}{53}} - \frac{2268\zeta(3) - 2453}{8 \times 53^2} \epsilon, \\ \gamma_1 &= 1 + \frac{3}{4} \sqrt{\frac{6\epsilon}{53}} - \frac{3}{4} \frac{[378\zeta(3) - 347]}{53^2} \epsilon, \\ \delta_1 &= 5 + 5 \sqrt{\frac{6\epsilon}{53}} - 3 \frac{[630\zeta(3) - 1073]}{53^2} \epsilon, \\ \delta_{11} &= 3 + 4 \sqrt{\frac{6\epsilon}{53}} - 2 \frac{[756\zeta(3) - 1277]}{53^2} \epsilon. \quad (\text{B1})\end{aligned}$$

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- [1] A.B. Harris and T.C. Lubensky, Phys. Rev. Lett. **33**, 1540 (1974).
- [2] T.C. Lubensky, Phys. Rev. B **11**, 3573 (1975).
- [3] D.E. Khmel'nitskii, Zh. Éksp. Teor. Fiz. **68**, 1960 (1975) [Sov. Phys. JETP **41**, 981 (1975)].
- [4] A.B. Harris, J. Phys. C **7**, 1671 (1974).
- [5] G. Grinstein and A. Luther, Phys. Rev. B **13**, 1329 (1976).
- [6] B. Shalaev, Zh. Eksp. Teor. Fiz. **73**, 2301 (1977).
- [7] C. Jayaprakash and H.J. Katz, Phys. Rev. B **16**, 3987 (1977).
- [8] G. Jug, Phys. Rev. B **27**, 609 (1983).
- [9] A.I. Sokolov and B.N. Shalaev, Fiz. Tverd. Tela **23**, 2058 (1981) [Sov. Phys. Solid State **23**, 1200 (1981)]; I.O. Maier, A.I. Sokolov, *ibid.* **26**, 3454 (1984) [*ibid.* **26**, 2076 (1984)]. The three-loop β functions derived and used in these papers are in error. The correct expressions for the RG functions of the relevant anisotropic mn -component model in three dimensions have been obtained, for the first time, in Ref. [10].
- [10] N.A. Shpot, Phys. Lett. A **142**, 474 (1989). The analytical expressions for the relevant three-loop Feynman integrals at $d = 3$ dimensions are listed in Ref. [11].
- [11] C. Bervillier and M. Shpot, Phys. Rev. B **46**, 955 (1992).
- [12] R.J. Birgeneau *et al.*, Phys. Rev. B **27**, 6747 (1983).
- [13] P.W. Mitchell *et al.*, Phys. Rev. B **34**, 4719 (1986).
- [14] D.P. Belanger, e-print cond-mat/0009029.
- [15] D. Chowdhury and D. Stauffer, J. Stat. Phys. **44**, 203 (1986).
- [16] J. Marro, A. Labarta, and J. Tejada, Phys. Rev. B **34**, 347 (1986).
- [17] For a review of critical behavior of infinite systems with bulk randomness and for a more complete list of references, see Refs. [47,50].
- [18] V. Dotsenko, Usp. Fiz. Nauk **165**, 481 (1995).
- [19] B.N. Shalaev, Phys. Rep. **237**, 129 (1994).
- [20] W. Selke, L. N. Shcur, and A. L. Talapov, in *Annual Reviews of Computational Physics*, edited by D. Stauffer (World Scientific, Singapore, 1994), Vol. 1, p. 17.
- [21] V. Dotsenko, M. Picco, and P. Pujol, Nucl. Phys. B **455**, 701 (1995).
- [22] A.W.W. Ludwig, Nucl. Phys. B **330**, 639 (1990).
- [23] F. Iglói, P. Lajkó, W. Selke, and F. Szalma, J. Phys. A **31**, 2801 (1998).
- [24] K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, London, 1983), Vol. 8, pp. 1–144.
- [25] H. W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, London, 1986), Vol. 10, pp. 75–267.
- [26] H.W. Diehl, Int. J. Mod. Phys. B **11**, 3503 (1997).
- [27] H.W. Diehl and S. Dietrich, Z. Phys. B: Condens. Matter **42**, 65 (1981).
- [28] K. Ohno, Y. Okabe, and R. Abe, Phys. Lett. **107A**, 41 (1985).
- [29] The corresponding phase diagram of the semi-infinite systems was represented in Refs. [25,26].
- [30] H.W. Diehl and A. Nüsser, Z. Phys. B: Condens. Matter **79**, 69 (1990); **79**, 79 (1990).
- [31] H.W. Diehl, Eur. Phys. J. B **1**, 401 (1998).
- [32] M. Pleimling and W. Selke, Eur. Phys. J. B **1**, 385 (1998).
- [33] H.W. Diehl and M. Shpot, Nucl. Phys. B **528**, 595 (1998).
- [34] Z.E. Usatenko, M.A. Shpot, and C.-K. Hu, Phys. Rev. E **63**, 056102 (2001).
- [35] K. Ohno and Y. Okabe, Phys. Rev. B **46**, 5917 (1992).
- [36] A.J. Bray, T. McCarthy, M.A. Moore, J.D. Reger, and A.P. Young, Phys. Rev. B **36**, 2212 (1987).
- [37] A.J. McKane, Phys. Rev. B **49**, 12 003 (1994).
- [38] B. Shalaev, S.A. Antonenko, and A.I. Sokolov, Phys. Lett. A **230**, 105 (1997).
- [39] R. Folk, Yu. Holovatch, and T. Yavors'kii, JETP Lett. **69**, 747 (1999).
- [40] R. Folk, Yu. Holovatch, and T. Yavors'kii, Phys. Rev. B **61**, 114 (2000).
- [41] G. Parisi, J. Stat. Phys. **23**, 49 (1980).
- [42] E. Eisenriegler and H.W. Diehl, Phys. Rev. B **37**, 5257 (1988).
- [43] R. Hegger and P. Grassberger, J. Phys. A **27**, 4069 (1994).
- [44] V.J. Emery, Phys. Rev. B **11**, 239 (1975).
- [45] H.W. Diehl, S. Dietrich, and E. Eisenriegler, Phys. Rev. B **27**, 2937 (1983).
- [46] E. Brézin, J. C. Le Guillou, J. Zinn-Justin, in *Phase Transition and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic Press, New York, 1976), Vol. 6 .
- [47] A. Pelissetto and E. Vicari, Phys. Rev. B **62**, 6393 (2000).
- [48] M. Shpot, Condens. Matter Phys. **10**, 143 (1997).

- [49] H.W. Diehl and M. Shpot, Phys. Rev. Lett. **73**, 3431 (1994).
- [50] D.V. Pakhnin and A.I. Sokolov, Phys. Rev. B **61**, 15 130 (2000).
- [51] K.B. Varnashev, Phys. Rev. B **61**, 14 660 (2000).
- [52] J.M. Carmona, A. Pelissetto, and E. Vicari, Phys. Rev. B **61**, 15 136 (2000).
- [53] For this kind of series, the expansion coefficients at large orders of perturbation theory grow nearly factorially. In fact, this is an intuitive picture conveyed from the theory of bulk regular systems. Much less is known about the large-order behavior of perturbative expansions pertaining to infinite random systems (see Refs. [54,37,55]), especially at large space dimensionalities. To our knowledge, there are no explicit results on large orders for surface quantities, even in the absence of any disorder.
- [54] A.J. Bray *et al.*, Phys. Rev. B **36**, 2212 (1987).
- [55] G. Álvarez, V. Martin-Mayor, and J.J. Ruiz-Lorenzo, J. Phys. A **33**, 841 (2000).
- [56] G.A. Baker Jr., B.G. Nickel, and D.I. Meiron, Phys. Rev. B **17**, 1365 (1978).
- [57] G.A. Baker Jr., B.G. Nickel, M.S. Green, and D.I. Meiron, Phys. Rev. Lett. **36**, 1351 (1976).
- [58] For the sake of simplicity, we do not present the ratio O_1/O_2 here.
- [59] Yu. Holovatch and M. Shpot, J. Stat. Phys. **66**, 867 (1992).
- [60] I.O. Mayer and A.I. Sokolov, Fiz. Tverd. Tela **26**, 3454 (1984).
- [61] I.O. Mayer, A.I. Sokolov, and B.N. Shalaev, Ferroelectrics **95**, 93 (1989); I.O. Mayer, J. Phys. A **22**, 2815 (1989).