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Correlation functions near modulated and rough surfaces

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In a system with long-ranged correlations, the behavior of correlation functions is sensitive to the presence of a boundary. We show that surface deformations strongly modify this behavior as compared to a flat surface. The modified near surface correlations can be measured by scattering probes. To determine these correlations, we develop a perturbative calculation in the deformations in height from a flat surface. Detailed results are given for a regularly patterned surface, as well as for a self-affinely rough surface with roughness exponent ζ. By combining this perturbative calculation in height deformations with the field-theoretic renormalization-group approach, we also estimate the values of critical exponents governing the behavior of the decay of correlation functions near a self-affinely rough surface. We find that for the interacting theory, a large enough ζ can lead to a different surface critical behavior. We also provide scaling relations between roughness induced critical exponents for thermodynamic surface quantities.

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I. INTRODUCTION

In a material with long-ranged correlations, such as a liquid crystal or a superfluid, any local perturbation has influence over large distances. As a result, local properties, such as magnetization density, as well as correlation functions are modified on approaching a surface. *Critical* behavior near surfaces or defects, which is quite different from the bulk, has been extensively studied by means of the field-theoretic renormalization-group approach [1–4]. In this case, the local order parameter Φ is perturbed near the surface up to a distance set by the diverging bulk correlation length $\xi \sim |T - T_c|^{-\nu}$, where T_c is the bulk critical temperature. Theoretical predictions for surface criticality have been tested experimentally [5–9] and in simulations [10,11]. In particular, the grazing incidence of x rays and neutrons [3] has become a standard tool for probing critical behavior near surfaces and interfaces [5–8]. For instance, the decay of the two-point correlation function has been measured close to the surface of a Fe_3Al crystal near its continuous order-disorder transition by the method of grazing incidence of x rays [5]. The phenomenon of critical adsorption near columnar defects [4] has apparently been observed by small angle scattering of light in a NH_4Br crystal near a continuous structural phase transition [12].

Most theoretical investigations so far have been restricted to *flat* surfaces. This is justified to a certain degree, since microscopic deviations from this idealized picture such as terraces of monoatomic height do not change the universal surface critical behavior [13,14]. However, for deviations on mesoscopic length scales, new phenomena are expected. Such deviations can be divided into two classes.

(i) Advanced experimental methods of nanoscience such as x ray [15], guided growth [16], and nanosphere lithography [17], allow one to endow surfaces with specific, regular geometrical patterns down to the nanometer scale. These structures hold much promise for applications towards nanochips [18] or optoelectronic devices [19]. The surface modulations also offer a wide range of possible applications in fluid environments. For instance, at temperatures between the wetting temperature T_w of the corresponding planar substrate and the critical temperature T_c of the bulk fluid, one can manipulate the adsorption properties of the fluid on the substrate by endowing the surface with periodic patterns of various shapes [20,21].

(ii) Surfaces or interfaces can be naturally rough, e.g., due to growth, fracture, or erosion. One possibility is that the substrate has a *fractal* surface, so that the surface area S grows as a power of the projected area, i.e., $S \sim L^{d_f}$ where L is a characteristic length and d_f is the fractal dimension of the surface. Recently, the scaling behavior of correlation functions in a critical system in two dimensions near the fractal boundary of a random walk, for which $d_f = 4/3$, has been studied by methods of quantum gravity [22] and conformal invariance [23]. Another possibility is that the substrate has a *self-affine* surface, for which the surface area is proportional to the projected area. In this case the height fluctuations are characterized by a roughness exponent ζ with $0 < \zeta < 1$, so that $(\delta h)^2 \sim L^{2\zeta}$, where δh is a typical height fluctuation over a distance L. Self-affine scaling is predicted by many numerical and analytical models of surface growth [24,25], and is also observed in a number of experiments [26]. A liquid-vapor interface, which exhibits rippled configurations due to the occurrence of capillary waves, is another realization of a self-affine rough surface [27]. An example where such an interface confines a critical system is given by the interface between liquid ^{4}He near the normalfluid-superfluid transition and its noncritical vapor, which occurs in a recently used experimental setup in which the Casimir force in a critical system is measured [28] (see also Ref. [29]).

In a previous paper [30], we showed that the shape of the surface has a distinct influence on the properties of an adjacent medium with long-range correlations. Here we demonstrate this in more detail for two-point correlation functions near a critical point of the medium, for both cases (i) and (ii) outlined above. Apart from Appendix B, we choose the Dirichlet boundary condition $\Phi = 0$ at the surface, which represents the so-called *ordinary* surface universality class in case of a flat surface, and is usually appropriate for magnets, binary alloys near a continuous order-disorder transition, and ^{4}He near the normalfluid-superfluid transition [1,2]. In Ref. [31], the influence of surface roughness on the fluctuation properties of wetting films, and on the demagnetizing factor of a thin magnetic film, have been studied.

In order to study the effects of the surface shape, we develop a perturbative expansion of two-point correlation functions in the deformations of the height profile. The method is the path integral approach used previously to calculate free energies [32], and in the context of the dynamic [33] and static [34] Casimir effect. Initially for a Gaussian field, the calculations are carried out to second order in the deformations. The first order results can also be derived by means of the stress tensor in conjunction with a different type of short distance expansion (see Appendix B), and hold quite generally for any critical system bounded by a surface with either (a) Dirichlet boundary conditions $\Phi=0$, or (b) boundary conditions that break the symmetry of the order parameter near the surface. In the latter case, the leading singular behavior can be obtained by setting $\Phi=\infty$ at the surface, corresponding to the *extraordinary* or *normal* surface universality class, describing *critical adsorption* of a binary liquid mixture on the surface of a substrate or the interface between the critical liquid and its noncritical vapor [1,2,9]. The second order results are particularly useful for cases in which the first order contributions vanish (see below).

The diffuse scattering of x rays and neutrons at grazing incidence due to the modified correlations appears in addition to what would be observed if the surface was separating two homogeneous media [35]. The modified correlations may thus provide an additional and indirect means of characterizing the surface profile. This may be of value when other techniques are not possible, as in the case of the interior surface of a glass, or an internal crack, whereas scattering from a critical fluid or binary alloy coating the surface may be feasible. Already at the first order, the two-point correlation functions track the profile from the substrate, with a modulation that decreases with the distance of the two points from the surface. This leads to explicit predictions for the structure factor, as a function of the lateral wave vector transfer, for a modulated surface.

For self-affinely rough surfaces, second order calculations are necessary, as the first order results vanish on average. In this context, the surface roughness is an example of quenched randomness. For a massless Gaussian field, we find the expected result that self-affine roughness leads to subleading corrections to the decay of two-point correlation functions, which at a scale r are smaller by a factor of $r^{-2(1-\zeta)}$ than the leading contribution coming from a flat surface. Typical critical systems, however, are described by a non-Gaussian (interacting) field theory. In this case, the correlations are calculated perturbatively in a double expansion in the deformations and in the strength of the interaction, and the results interpreted with the aid of the renormalization group (RG) in $4-\varepsilon$ dimensions. We find that the subleading corrections now fall off with a slower power as compared to the Gaussian case and, surprisingly, for a sufficiently large ζ even *dominate*, giving rise to a different surface critical behavior. However, for the *XY* model in two dimensions, below the Kosterlitz-Thouless temperature, we again find that the surface correlations fall off with the simple relative factor of $r^{-2(1-\zeta)}$ as compared to a flat surface (line).

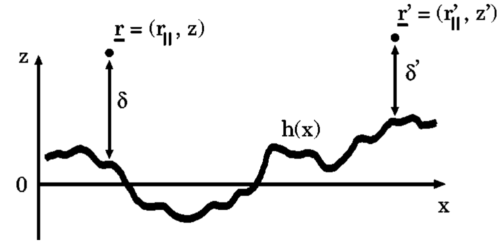

FIG. 1. Position vectors $\underline{r}=(\mathbf{r}_{\|},z)$ and $\underline{r}'=(\mathbf{r}'_{\|},z')$ of the two-point correlation function in the critical system located above and bounded by a deformed surface. The surface profile is described by the height function $h(\mathbf{x})$, and the vertical distances of $\underline{r}$ and $\underline{r}'$ from the surface are given by $\delta=z-h(\mathbf{r}_{\|})$ and $\delta'=z'-h(\mathbf{r}'_{\|})$, respectively.

The results for correlation functions can also be related to thermodynamic quantities. To this end, we introduce distinct fields h_b and h_s in the bulk and close to the surface, respectively, and propose a scaling ansatz for the leading singular part of the surface free energy per projected area $f_s^{(\mathrm{sing})}$. By taking suitable derivatives of $f_s^{(\mathrm{sing})}$ with respect to h_b and h_s, we then obtain scaling relations for a variety of critical exponents related to thermodynamic surface quantities.

The rest of the paper is organized as follows. In Sec. II we introduce the geometry, and develop the formalism for the perturbative calculation of correlation functions for a free (Gaussian) field theory. In Secs. III and IV we then consider a regularly patterned surface and a self-affinely rough surface in more detail. In Sec. V we combine the previous results with the RG, and obtain results for surface critical exponents. In Sec. VI we consider the *XY* model. Finally, in Sec. VII, we draw our conclusions and outline some possible extensions of our paper; in particular, we relate our previous results for correlation functions to thermodynamic surface quantities via scaling relations. Some technical details are left for Appendices A–C. In Appendix B, for instance, we introduce a different type of short-distance expansion for the stress tensor.

II. GEOMETRY AND FREE FIELD THEORY

We consider a manifold Ω with the shape of a deformed surface. Each point on the manifold is represented by a vector $X(\mathbf{y})=[X^{\mu}(\mathbf{y});\mu=1,\ldots,d]$; a D-dimensional manifold Ω embedded in d-dimensional space is parametrized by $\mathbf{y}=(y_1,\ldots,y_D)$. In the absence of overhangs and inlets, the surface profile can be described by a single-valued height function $h(\mathbf{y})$, where $\mathbf{y}$ spans a $(D=d-1)$-dimensional base plane (see Fig. 1). The parametrization of the surface is thus $X(\mathbf{y})=(\mathbf{y},h(\mathbf{y}))$. Position vectors $\underline{r}$ are decomposed according to $\underline{r}=(\mathbf{r}_{\|},z)$, where $\mathbf{r}_{\|}$ comprises the $D=d-1$ components parallel to the surface, and z is the distance from the base plane. The vertical distance of $\underline{r}$ from the surface is given by $\delta = z - h(\mathbf{r}_\parallel)$ (see Fig. 1). We denote d-dimensional vectors with underlined letters, and D-dimensional vectors with boldface letters.

Fluctuations in the critical system located above the surface will be described by an n-component order parameter field $\Phi(\underline{r}) = (\Phi_1(\underline{r}),\ldots,\Phi_n(\underline{r}))$. We consider the statistical Boltzmann weight $e^{-\beta\mathcal{H}}$ with standard Hamiltonian [1,2],

$$\beta\mathcal{H}\{\Phi\} = \int_V d^d r \left\{ \frac{1}{2}(\boldsymbol{\nabla}\Phi)^2 + \frac{\tau_0}{2}\Phi^2 + \frac{u_0}{4!}(\Phi^2)^2 \right\}, \tag{2.1}$$

where $\tau_0 \sim T - T_c$ and u_0 is the strength of the Φ^4 interaction. In this section, we study the Gaussian theory, for which $u_0 = 0$. The volume V consists of the space available to the critical system. The above expression must be supplemented by a boundary condition on the surface. We choose the Dirichlet boundary condition $\Phi = 0$, representing the ordinary surface universality class. In this case, for $n = 1$ the order parameter Φ can represent the magnetization in a uniaxial ferromagnet or the deviation of the composition in a binary alloy from the critical composition, for $n = 2$ the magnetization in a XY magnet or the superfluid order parameter of ^{4}He near the normalfluid-superfluid transition, and for $n = 3$ the magnetization in a Heisenberg ferromagnet [1,2].

The Gaussian two-point correlation function (or *propagator*)

$$\langle \Phi_i(\underline{r})\Phi_j(\underline{r}')\rangle = \delta_{ij} G(\underline{r}:\underline{r}'), \quad u_0 = 0, \tag{2.2}$$

where the brackets $\langle\,\rangle$ denote the thermal average according to Eq. (2.1) with $u_0 = 0$, can be calculated using functional integral methods [32,33]. The details of this calculation are left to Appendix A. The result is

$$G(\underline{r};\underline{r}') = G_b(\underline{r};\underline{r}') - \int d^D x \int d^D y \times G_b(\underline{r};\mathbf{x},h(\mathbf{x})) M(\mathbf{x},\mathbf{y}) G_b(\underline{r}';\mathbf{y},h(\mathbf{y})), \tag{2.3}$$

where

$$G_b(\underline{r};\underline{r}') = \int \frac{d^D p}{(2\pi)^D} \exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)] \frac{1}{2p} e^{-p|z-z'|}, \tag{2.4}$$

with $p = |\mathbf{p}|$, is the Gaussian propagator in unbounded bulk, and the kernel $M(\mathbf{x},\mathbf{y})$ is the inverse of the kernel $G_b(\mathbf{x},h(\mathbf{x});\mathbf{y},h(\mathbf{y}))$, i.e.,

$$\int d^D y M(\mathbf{x},\mathbf{y}) G_b(\mathbf{y},h(\mathbf{y});\mathbf{y}',h(\mathbf{y}')) = \delta^D(\mathbf{x}-\mathbf{y}'). \tag{2.5}$$

While the above results [with an appropriately modified bulk propagator in Eq. (2.4)] are generally valid, we focus on the behavior of the correlation functions at the bulk critical point, i.e., for $T = T_c$, where correlations are strongest [36].

Equation (2.3) is difficult to evaluate in general. To proceed, we now consider the height profile $h(\mathbf{x})$ as a small perturbation, and expand $G(\underline{r};\underline{r}')$ in a series $G_0 + G_1 + G_2 + \cdots$ in powers of h up to second order, under the constraint that z and z' are kept fixed. The lowest order result,

$$G_0(\underline{r};\underline{r}') = G_b(\mathbf{r}_\parallel,z;\mathbf{r}'_\parallel,z') - G_b(\mathbf{r}_\parallel,z;\mathbf{r}'_\parallel,-z') \tag{2.6}$$

$$= \int \frac{d^D p}{(2\pi)^D} \exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)] g_0(p;z,z') \tag{2.7}$$

with [see Eq. (2.4)]

$$g_0(p;z,z') = \frac{1}{2p}[e^{-p|z-z'|} - e^{-p(z+z')}] \tag{2.8}$$

corresponds to a flat surface, and can be obtained by the method of images [1,2]. The bulk correlation function $G_b(\underline{r};\underline{r}')$ decays as $r^{-(d-2+\eta)}$ for large separations $r = |\underline{r} - \underline{r}'|$, where the bulk critical exponent η is given by $\eta = 0$ in the Gaussian theory. In contrast, if both points remain close to the surface, $G_0(\underline{r};\underline{r}')$ decays as $r^{-(d-2+\eta_\parallel)}$, where $\eta_\parallel$ is a surface critical exponent given by $\eta_\parallel = 2$ in the Gaussian theory [1,2].

The first order result is given by [37]

$$G_1(\underline{r};\underline{r}') = -4\int d^D x J(\mathbf{r}_\parallel,\mathbf{x};z) h(\mathbf{x}) J(\mathbf{r}'_\parallel,\mathbf{x};z'), \tag{2.9}$$

with

$$J(\mathbf{x},\mathbf{y};z) = \frac{1}{2}\int \frac{d^D p}{(2\pi)^D} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} e^{-pz}. \tag{2.10}$$

Note that $J(\mathbf{x},\mathbf{y};z\to 0^+) = \frac{1}{2}\delta^D(\mathbf{x}-\mathbf{y})$, where $\delta^D(\mathbf{x})$ is the delta function in D dimensions. Already the result at this order tracks the profile $h(\mathbf{x})$ of the surface. For example, for $\rho = |\mathbf{r}_\parallel - \mathbf{r}'_\parallel| \to \infty$ with z and z' fixed, the above results for G_0 and G_1 imply the behavior (see Appendix B)

$$G(\underline{r};\underline{r}') \sim [1 - A(\underline{r}) - A(\underline{r}')]\rho^{-(d-2+\eta_\parallel)}, \tag{2.11}$$

up to terms of order $(h/z)^2$ and $(h/z')^2$. Thus, the leading power law is the same as for a flat surface, but the amplitude is modulated by the surface deformations in the vicinity of $\mathbf{r}_\parallel$ and $\mathbf{r}'_\parallel$ by the dimensionless and universal amplitude,

$$A(\underline{r}) = \frac{\eta_\parallel - \eta}{2}\int d^D x \frac{h(\mathbf{x})}{z}\Delta(\mathbf{x}-\mathbf{r}_\parallel,z), \tag{2.12}$$

where for the present Gaussian case, $\eta_\parallel - \eta = 2$ and $\Delta(\mathbf{x} - \mathbf{r}_\parallel,z) = 2J(\mathbf{x},\mathbf{r}_\parallel;z)$. Equations (2.11) and (2.12) are valid quite generally, and, in particular, also for the boundary condition representing critical adsorption of a binary liquid mixture (see Appendix B). The explicit form of $\Delta(\mathbf{x},z)$, however, depends on the surface universality class considered.

The second order result reads

$$G_2(\underline{r};\underline{r}')=\int d^Dx\int d^Dy\,h(\mathbf{x})h(\mathbf{y})C(\underline{r},\underline{r}';\mathbf{x},\mathbf{y}) \tag{2.13}$$

with

$$C(\underline{r},\underline{r}';\mathbf{x},\mathbf{y})=-8J(\mathbf{r}_\parallel,\mathbf{x};z)J(\mathbf{r}'_\parallel,\mathbf{y};z')K(\mathbf{x},\mathbf{y};z\to 0^+) \tag{2.14}$$

and

$$K(\mathbf{x},\mathbf{y};z)=\frac{1}{2}\int\frac{d^Dp}{(2\pi)^D}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}pe^{-pz}. \tag{2.15}$$

In a scattering experiment with grazing incidence, one probes the lateral structure factor $S(\mathbf{p},z;\mathbf{p}',z')$ [3,6,35], which is defined by the Fourier transform

$$G(\underline{r};\underline{r}')=\int\frac{d^Dp}{(2\pi)^D}e^{i\mathbf{p}\cdot\mathbf{r}_\parallel}\int\frac{d^Dp'}{(2\pi)^D}e^{i\mathbf{p}'\cdot\mathbf{r}'_\parallel}S(\mathbf{p},z;\mathbf{p}',z'). \tag{2.16}$$

Using the Fourier transform of the height profile

$$h(\mathbf{y})=\int\frac{d^Dk}{(2\pi)^D}e^{i\mathbf{k}\cdot\mathbf{y}}\hat{h}(\mathbf{k}), \tag{2.17}$$

with $\hat{h}(-\mathbf{k})=\hat{h}(\mathbf{k})^*$, we obtain an equivalent expansion $S=S_0+S_1+S_2+\dots$, with

$$S_0=\frac{1}{2p}[e^{-p|z-z'|}-e^{-p(z+z')}](2\pi)^D\delta(\mathbf{p}+\mathbf{p}'), \tag{2.18}$$

$$S_1=-e^{-pz}e^{-p'z'}\hat{h}(\mathbf{p}+\mathbf{p}'), \tag{2.19}$$

$$S_2=-e^{-pz}e^{-p'z'}\int\frac{d^Dk}{(2\pi)^D}|\mathbf{p}-\mathbf{k}|\hat{h}(\mathbf{k})\hat{h}(\mathbf{p}+\mathbf{p}'-\mathbf{k}). \tag{2.20}$$

For a rough surface, the deviations in height from a planar surface have no upper bound. In this case, it is convenient to carry out the expansion in $h(\mathbf{x})$ for fixed vertical distances $\delta=z-h(\mathbf{r}_\parallel)$ and $\delta'=z-h(\mathbf{r}'_\parallel)$, instead of for fixed z and z' (see Fig. 1). This representation facilitates the perturbative analysis of the field theory described by Eq. (2.1) (see Sec. V). Moreover, in view of probing correlation functions lateral to the substrate surface by grazing incidence scattering of x rays and neutrons [3,6,35], this representation is natural, since in these experiments δ and δ' show up as length scales which are set by the finite penetration depth of the x rays.

Writing $G=G_0+G_{\mathrm{I}}+G_{\mathrm{II}}+\dots$ where the subscripts 0, I, II, indicate the corresponding order in $h(\mathbf{x})$ under the constraint that δ and δ' are kept fixed, we find

$$G_0(\underline{r};\underline{r}')=G_b(\mathbf{r}_\parallel,\delta;\mathbf{r}'_\parallel,\delta')-G_b(\mathbf{r}_\parallel,\delta;\mathbf{r}'_\parallel,-\delta'), \tag{2.21}$$

$$\begin{aligned}G_{\mathrm{I}}(\underline{r};\underline{r}')=&-[h(\mathbf{r}_\parallel)-h(\mathbf{r}'_\parallel)]\frac{\partial}{\partial\delta'}G_b(\mathbf{r}_\parallel,\delta;\mathbf{r}'_\parallel,\delta')\\&+2\int d^Dx\,J(\mathbf{r}_\parallel,\mathbf{x};\delta)[h(\mathbf{r}_\parallel)+h(\mathbf{r}'_\parallel)\\&-2h(\mathbf{x})]J(\mathbf{r}'_\parallel,\mathbf{x};\delta'),\end{aligned} \tag{2.22}$$

$$\begin{aligned}G_{\mathrm{II}}(\underline{r};\underline{r}')=&\tfrac{1}{2}[K(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;|\delta-\delta'|)+K(\mathbf{r}_\parallel,\mathbf{r}'_\parallel;\delta+\delta')][h(\mathbf{r}_\parallel)\\&-h(\mathbf{r}'_\parallel)]^2+\int d^Dx\int d^Dy\,J(\mathbf{r}_\parallel,\mathbf{x};\delta)M_0(\mathbf{x},\mathbf{y})\\&\times[h(\mathbf{x})-h(\mathbf{y})]^2J(\mathbf{r}'_\parallel,\mathbf{y};\delta')\\&-2\left[\int d^Dx\,K(\mathbf{r}_\parallel,\mathbf{x};\delta)[h(\mathbf{r}_\parallel)-h(\mathbf{x})]^2J(\mathbf{r}'_\parallel,\mathbf{x};\delta')\right.\\&\left.+(\mathbf{r}\leftrightarrow\mathbf{r}')\right].\end{aligned} \tag{2.23}$$

The first line in Eq. (2.22) is valid for $\delta'<\delta$, and $M_0(\mathbf{x},\mathbf{y})$ in Eq. (2.23) is defined as in Eq. (2.5) but with $h(\mathbf{y})=0$. The kernels J and K are given by Eqs. (2.10) and (2.15), respectively. The contribution G_0 in Eq. (2.21) corresponds to the Gaussian propagator for a half-space bounded by a flat surface with Dirichlet boundary conditions, i.e.,

$$G_0(\underline{r};\underline{r}')=\int\frac{d^Dp}{(2\pi)^D}\exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)]g_0(p;\delta,\delta') \tag{2.24}$$

with g_0 from Eq. (2.8).

III. MODULATED SURFACES

We now apply the results of the preceding section to patterned surfaces. The simplest example is provided by an uniaxial sinusoidal modulation with wavelength λ along, say, the x direction, i.e.,

$$h(x,\mathbf{Y})=a\cos(2\pi x/\lambda). \tag{3.1}$$

The other $(D-1)$ directions along the surface, denoted by $\mathbf{Y}$, remain translationally invariant. The Fourier transform of this height profile is

$$\hat{h}(\mathbf{k})=\frac{a}{2}(2\pi)^D\delta^{D-1}(\mathbf{K})\left[\delta\left(k_x-\frac{2\pi}{\lambda}\right)+\delta\left(k_x+\frac{2\pi}{\lambda}\right)\right], \tag{3.2}$$

where $\mathbf{k}$ is decomposed according to $\mathbf{k}=(k_x,\mathbf{K})$.

The nontrivial orders of the expansion of $G(\underline{r};\underline{r}')$ in h for fixed z and z' are given by

$$\begin{aligned}&G_1(\mathbf{r}_\parallel,z;\mathbf{r}'_\parallel,z')\\&\quad=-\frac{a}{2}e^{2\pi i/\lambda\cdot x'}\int\frac{d^Dp}{(2\pi)^D}\exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)]e^{-pz}\\&\qquad\times\exp\left[-\left|\mathbf{p}-\left(\frac{2\pi}{\lambda},0\right)\right|z'\right]+(\mathbf{r}_\parallel\leftrightarrow\mathbf{r}'_\parallel),\end{aligned} \tag{3.3}$$

$$G_2(\mathbf{r}_\parallel,z;\mathbf{r}'_\parallel,z') = -\frac{a^2}{4}\int\frac{d^Dp}{(2\pi)^D}\exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)]\left|\mathbf{p}-\left(\frac{2\pi}{\lambda},0\right)\right| \times e^{-pz}e^{-pz'} - \frac{a^2}{4}e^{4\pi i/\lambda\cdot x'}\int\frac{d^Dp}{(2\pi)^D} \times\exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)]\left|\mathbf{p}-\left(\frac{2\pi}{\lambda},0\right)\right|e^{-pz} \times\exp\left[-\left|\mathbf{p}-\left(\frac{4\pi}{\lambda},0\right)\right|z'\right]+(\mathbf{r}_\parallel\leftrightarrow\mathbf{r}'_\parallel). \tag{3.4}$$

For $\rho=|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|\to\infty$, the leading power law in ρ is the same as for a flat surface, but the amplitude is modulated by the shape of the surface in the vicinity of $\mathbf{r}_\parallel$ and $\mathbf{r}'_\parallel$. In particular, the first order result in Eq. (3.3) is consistent with Eqs. (2.11) and (2.12). For z, $z'\ll a$, λ the correlations follow more or less the surface modulation. Interestingly, for z, $z'\gg\lambda$, the correlations that are sensitive to the modulation, i.e., depend on λ, decay *exponentially* in z/λ. For instance, for $z=z'$ and $z/\lambda\to\infty$, one has $G_1\sim e^{-(2\pi/\lambda)z}$ and $G_2\sim e^{-(4\pi/\lambda)z}$. This exponential decay is due to the fact that the surface profile (3.1) has a perfect periodic shape. In contrast, a *local* perturbation on the surface would result in a perturbation of the correlations that decays only as a power law with the distance from the surface.

The corresponding orders of the lateral structure factor are given by

$$S_1(\mathbf{p},z;\mathbf{p}',z') = -\frac{a}{2}e^{-pz}e^{-p'z'}(2\pi)^D\delta^{D-1}(\mathbf{P}+\mathbf{P}') \times\left[\delta\left(p_x+p'_x-\frac{2\pi}{\lambda}\right)+\delta\left(p_x+p'_x+\frac{2\pi}{\lambda}\right)\right], \tag{3.5}$$

$$S_2(\mathbf{p},z;\mathbf{p}',z') = -\frac{a^2}{4}e^{-pz}e^{-p'z'}(2\pi)^D\delta^{D-1}(\mathbf{P}+\mathbf{P}')\left\{\left|\mathbf{p}-\left(\frac{2\pi}{\lambda},0\right)\right| \times\left[\delta\left(p_x+p'_x-\frac{4\pi}{\lambda}\right)+\delta(p_x+p'_x)\right]+\left|\mathbf{p}+\left(\frac{2\pi}{\lambda},0\right)\right| \times\left[\delta\left(p_x+p'_x+\frac{4\pi}{\lambda}\right)+\delta(p_x+p'_x)\right]\right\}. \tag{3.6}$$

These results indirectly characterize the surface in scattering experiments. For instance, the form of S_1 implies that the incident wave vector component p_x is scattered to $p'_x=p_x\pm2\pi/\lambda$ while the other components of $\mathbf{p}$ remain unchanged. The form of S_2 implies that p_x is scattered by $4\pi/\lambda$, 0, $-4\pi/\lambda$. In a scattering experiment with grazing incidence, the length scale perpendicular to the surface is set by the depth b that the evanescent wave penetrates the sample, giving rise to diffuse scattering and thereby probing the critical correlations close to the surface [3]. Since this diffuse scattering appears in addition to the contribution already present away from criticality [35], it can, in principle, be separated out by tuning the temperature deviation $T-T_c$. We assume that b is much larger than the height of the deformations. In this case, the above expansion in the deformations results in an expansion in powers of $h/b\ll1$ for the elastic scattering cross section, which allows one to distinguish the corresponding contributions via their intensities.

IV. ROUGH SURFACES

The second order results are particularly useful when dealing with rough surfaces, where the quench averaged first order corrections vanish. Within the description using a height function $h(\mathbf{x})$, self-affine roughness is characterized by the behavior

$$\overline{[h(\mathbf{x})-h(\mathbf{y})]^2}\sim|\mathbf{x}-\mathbf{y}|^{2\zeta},\quad |\mathbf{x}-\mathbf{y}|\to\infty, \tag{4.1}$$

where the overbar denotes averaging over self-affine realizations of the surface profile, and ζ with $0<\zeta<1$ is the roughness exponent. Without restriction of the generality we choose the coordinate system so that $\overline{h(\mathbf{x})}=0$. In the limit of short distances $|\mathbf{x}-\mathbf{y}|$ it is reasonable to assume that the surface is smooth. This can be modeled by the Fourier transform,

$$\overline{[h(\mathbf{x})-h(\mathbf{y})]^2}=\omega^{2-2\zeta}|\mathbf{x}-\mathbf{y}|^2 \times\int\frac{d^Dp}{(2\pi)^D}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}p^{-D+2-2\zeta}e^{-p\lambda}. \tag{4.2}$$

While at large separations the above correlations grow as $|\mathbf{x}-\mathbf{y}|^{2\zeta}$, we have also introduced a cutoff length λ to regulate the behavior of the surface at short distances, and an overall amplitude length ω. The length λ characterizes the crossover from the analytic behavior for $|\mathbf{x}-\mathbf{y}|\ll\lambda$ to the behavior in Eq. (4.1) for $|\mathbf{x}-\mathbf{y}|\gg\lambda$. Apart from its physical significance, the appearance of the finite crossover length λ in Eq. (4.2) is also essential within the present theoretical approach (see Sec. V).

A characteristic feature of self-affine roughness is statistical translational invariance, since the right-hand side of Eq. (4.2) depends on the distance $|\mathbf{x}-\mathbf{y}|$ only. This implies that the averaged lateral structure factor $\overline{S}$ is proportional to $\delta^D(\mathbf{p}+\mathbf{p}')$, and depends on z, z', and $p=|\mathbf{p}|$ only. In order to maintain translational invariance, it is convenient to express the results for the correlation functions in terms of the local distance $\delta=z-h(\mathbf{r}_\parallel)$ from the surface rather than z (see Fig. 1). The two-point correlation function must now vanish as δ or δ' go to zero. On averaging $G(\underline{r};\underline{r}')$ over different surface profiles, the contribution G_{I} in Eq. (2.22) vanishes due to $\overline{h(\mathbf{x})}=0$, and the contribution G_{II} in Eq. (2.23) becomes translationally invariant with respect to the lateral components $\mathbf{r}_\parallel$ and $\mathbf{r}'_\parallel$. We thus introduce the lateral Fourier transform,

$$\overline{G_{\rm II}(\underline{r};\underline{r}')} = \int \frac{d^D p}{(2\pi)^D} \exp[i\mathbf{p}\cdot(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)] g_2(p;\delta,\delta'), \tag{4.3}$$

where $g_2(p;\delta,\delta')$ can be read off from the right-hand side of Eq. (2.23), i.e.,

$$\begin{aligned} g_2(p;\delta,\delta') = \tfrac{1}{2}[\mathcal{K}(p,|\delta-\delta'|) + \mathcal{K}(p,\delta+\delta')] \\ + \mathcal{K}(p,0)e^{-p(\delta+\delta')} - \mathcal{K}(p,\delta)e^{-p\delta'} \\ - \mathcal{K}(p,\delta')e^{-p\delta}. \end{aligned} \tag{4.4}$$

$\mathcal{K}(p,\delta)$ is the lateral Fourier transform of $K(\mathbf{x,y};\delta)\overline{|h(\mathbf{x})-h(\mathbf{y})|^2}$ and we have used the fact that the lateral Fourier transform of $M_0(\mathbf{x,y})\overline{[h(\mathbf{x})-h(\mathbf{y})]^2}$ appearing in the second line of Eq. (2.23) after averaging is given by $4\mathcal{K}(p,\delta=0)$. Using Eq. (4.2), $\mathcal{K}(p,\delta)$ can be expressed in terms of the convolution integral

$$\mathcal{K}(p,\delta) = \omega^{2-2\zeta} \int \frac{d^D k}{(2\pi)^D} U(|\mathbf{p}-\mathbf{k}|,\delta) k^{-D+2-2\zeta} e^{-k\lambda}, \tag{4.5}$$

where $U(p,\delta)$ is the lateral Fourier transform of $K(\mathbf{x,y};\delta)|\mathbf{x}-\mathbf{y}|^2$ given by

$$U(p,\delta) = \left[\delta - \frac{1}{2}p\delta^2 - \frac{D-1}{2}\left(\frac{1}{p} - \delta\right)\right] e^{-p\delta}. \tag{4.6}$$

In terms of the coordinates $\underline{r} = (\mathbf{r}_\parallel, \delta)$, the above results imply that the leading power law behavior of $\overline{G(\underline{r};\underline{r}')}$ for $\rho = |\mathbf{r}_\parallel - \mathbf{r}'_\parallel| \to \infty$ is the same as for a flat surface. The corresponding amplitude depends on the roughness, and is modified by a factor of $[1-\kappa(\omega/\lambda)^{2(1-\zeta)}]$ as compared to a flat surface, where $\kappa > 0$ is a number of order unity. The subleading correction of order $\overline{h^2}$ decays with the separation ρ with an additional factor of $\rho^{-2(1-\zeta)}$ compared to the leading term [see Eqs. (5.16) and (5.17) in Sec. V for $\varepsilon = 0$].

Note that $g_2(p;\delta,\delta')$ vanishes for $\delta=0$ or $\delta'=0$ as it should, according to the Dirichlet boundary condition at the surface. This would *not* be the case for $z=0$ or $z'=0$ if we carried out the expansion in $h(\mathbf{x})$ with fixed z and z'. However, the realization of the Dirichlet boundary condition for the Gaussian propagator is essential for the perturbation theory of the field theory described by Eq. (2.1). Moreover, $g_2(p;\delta,\delta')$ is an analytic function for small δ or δ' due to the finite crossover length λ in Eq. (4.5), which would otherwise be ill defined for $\lambda = 0$ if $\delta = 0$ and $\zeta < 1/2$.

V. INTERACTING THEORY

In this section we consider the asymptotic scaling behavior of the two-point correlation function near a self-affine rough surface for the n-vector model at the bulk critical point. By combining our previous results with the field-theoretic RG, we estimate the values of the corresponding critical exponents, using a double expansion in the surface deformations and in the deviation $\varepsilon = 4-d$ of the space dimension d from the upper critical dimension.

For the interacting field theory, governed by Eq. (2.1) with $u_0 \neq 0$, standard perturbation theory can be applied to get the correlation function near a surface of arbitrary but fixed shape,

$$\langle \Phi_i(\underline{r})\Phi_j(\underline{r}')\rangle = \delta_{ij}\mathcal{G}(\underline{r},\underline{r}';u_0), \tag{5.1}$$

with

$$\mathcal{G}(\underline{r},\underline{r}';u_0) = G(\underline{r},\underline{r}') - \frac{n+2}{3}\frac{u_0}{2} \times \int_V d^d R\, G(\underline{r};\underline{R})G(\underline{R};\underline{R})G(\underline{R};\underline{r}') + \mathcal{O}(u_0^2), \tag{5.2}$$

where the Gaussian propagator $G(\underline{r};\underline{r}')$ is given by Eq. (2.3). We are interested in the behavior of $\langle \Phi_i(\underline{r})\Phi_j(\underline{r}')\rangle$ in the limit for which the distance between $\underline{r}$ and $\underline{r}'$ is much larger than one or both of the vertical distances δ and δ' (see Fig. 1). If δ' is small, say, it is helpful to consider the so-called *surface operator* [1,2]

$$\Phi^\perp(\mathbf{r}'_\parallel) \equiv \partial_n \Phi(\underline{r}'), \tag{5.3}$$

where $\partial_n = [g(\mathbf{r}'_\parallel)]^{-1/2}[\partial_{\delta'} - \nabla h(\mathbf{r}'_\parallel)\cdot\nabla]$ denotes the normal derivative at $\mathbf{r}'_\parallel$ on the surface, with the determinant $g(\mathbf{y}) = 1 + [\nabla h(\mathbf{y})]^2$ of its induced metric [see Eq. (A10)]. In this way one avoids to deal with the irrelevant length δ' from the outset. For correlations vertically away from the surface, i.e., $\mathbf{r}_\parallel = \mathbf{r}'_\parallel$, we are thus led to consider

$$\langle \Phi_i(\underline{r})\Phi_j^\perp(\mathbf{r}_\parallel)\rangle = \delta_{ij}\mathcal{G}_\perp(\mathbf{r}_\parallel,\delta;u_0). \tag{5.4}$$

The loop expansion of $\mathcal{G}_\perp(\mathbf{r}_\parallel,\delta;u_0)$ is obtained by taking the normal derivative at $\mathbf{r}_\parallel$ of the right-hand side of Eq. (5.2).

Up to now in this section we have considered a surface with arbitrary but fixed shape. In particular, for a *flat* surface, the one-loop addition in u_0 can be regularized and renormalized by minimal substraction of poles in $\varepsilon = 4-d$, leading to logarithmic contributions in the separation $r = |\underline{r} - \underline{r}'|$. This perturbative result can then be improved by RG, resulting in power laws in r with corresponding surface critical exponents [1,2]. For a self-affinely rough surface, the function $\mathcal{G}_\perp$ depends, of course, on the shape of this surface, i.e., on the height function $h(\mathbf{x})$. However, by averaging over different surface profiles, we expect that the average $\overline{\mathcal{G}_\perp}$ depends only on gross features characterizing the surface configurations, and, in particular, becomes independent of $\mathbf{r}_\parallel$ due to translational invariance. In the following we restrict ourselves to surfaces that are rough on large distances, and to contributions to $\mathcal{G}_\perp$ up to second order in $h(\mathbf{x})$. According to Eq. (4.2) we conclude that in this case the amplitude ω and the crossover length λ are the only remaining relevant length scales characterizing the different surface configurations.

In the next step, the resulting average $\overline{\mathcal{G}_\perp}(\delta;\omega,\lambda;u_0)$ has to be renormalized. For our perturbative calculations we use dimensional regularization and renormalization by minimal subtraction of poles in $\varepsilon = 4-d$ [38]. The reparametrizations

$$u_0 = 16\pi^2 \mu^\varepsilon Z_u u \tag{5.5}$$

and

$$\Phi = Z_\Phi^{1/2} \Phi_{\rm ren} \tag{5.6}$$

of the bulk parameter u_0 and the bulk field Φ in terms of their renormalized counterparts u and $\Phi_{\rm ren}$ are not affected by the presence of the surface. Here $Z_u = 1 + \mathcal{O}(u)$ and $Z_\Phi = 1 + \mathcal{O}(u^2)$ are the corresponding renormalization factors, and μ is the inverse length scale which determines the renormalization-group flow. Since all surfaces we average over are smooth on short distances, i.e., distances much smaller than the crossover length λ, we expect that the surface operator $\Phi^\perp$ is renormalized by the same renormalization factor Z_1 that would occur for a *flat* surface with Dirichlet boundary conditions. Thus,

$$\Phi^\perp = (Z_\Phi Z_1)^{1/2} \Phi_{\rm ren}^\perp , \tag{5.7}$$

with [2]

$$Z_1 = 1 + \frac{n+2}{3}\frac{u}{\varepsilon} + \mathcal{O}(u^2). \tag{5.8}$$

Using the above reparametrizations the renormalized, i.e., pole-free, counterpart of $\overline{\mathcal{G}_\perp}$ is given by

$$\overline{\mathcal{G}_{\perp,\rm ren}}(\delta;\omega,\lambda;u,\mu) = Z_\Phi^{-1} Z_1^{-1/2} \overline{\mathcal{G}_\perp}(\delta;\omega,\lambda;u_0). \tag{5.9}$$

This perturbative result can be improved using standard renormalization-group methods, by noting that $\overline{\mathcal{G}_\perp}$ does not depend on μ. The asymptotic scaling behavior is governed by the infrared (long-distance) stable fixed point for which

$$u = u^* = \frac{3\varepsilon}{n+8} + \mathcal{O}(\varepsilon^2), \tag{5.10}$$

and $\overline{\mathcal{G}_{\perp,\rm ren}}$ assumes the scaling form

$$\overline{\mathcal{G}_{\perp,\rm ren}}(\delta;\omega,\lambda;u,\mu) \sim \delta^{-(d-2+\eta_\perp)} f_\perp(\delta/\lambda;\omega/\lambda) \tag{5.11}$$

with the critical exponent $\eta_\perp$ for a flat surface. The scaling function $f_\perp$ is universal, but depends on the particular way we have introduced the crossover length λ in Eq. (4.2). Since all surfaces we average over are smooth on short distances, $f_\perp(0;\omega/\lambda)$ should be a finite number (in the following we suppress the dependence of $f_\perp$ on ω/λ for brevity). In the other limit $\delta/\lambda \to \infty$, the scaling function $f_\perp(\delta/\lambda)$ is expected to exhibit a power law that reflects the self-affine structure of the surface.

We have confirmed Eq. (5.11) explicitly to one-loop order according to Eq. (5.2), using the expansion of $G(\underline{r},\underline{r}')$ up to second order in $h(\mathbf{x})$ in Eqs. (2.21)–(2.23), and averaging using Eq. (4.2). Figure 2 illustrates this double expansion in graphical form [39].

We indeed find that the $1/\varepsilon$ poles generated by the surface operator $\Phi^\perp$ in Eq. (5.4) are removed by the renormalization factor Z_1 in Eq. (5.8), which provides a test of our calculation, and for the reasoning leading to Eq. (5.11). This calculation gives also the explicit form of the scaling function $f_\perp$ to first order in ε. We confirm, in particular, that $f_\perp(0)$ is a finite number, and that the logarithmic contributions of $f_\perp(\delta/\lambda)$ for $\delta/\lambda \to \infty$ can be recast in the form of a power law, i.e.,

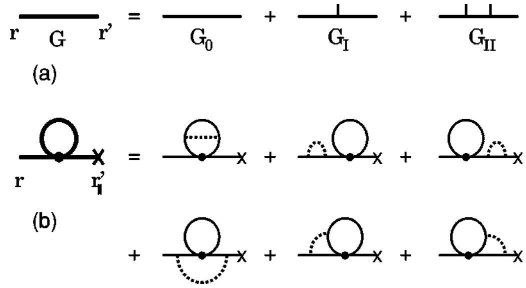

FIG. 2. (a) Representation of the full Gaussian propagator $G(\underline{r};\underline{r}')$ in Eq. (2.3) and its expansion up to second order in $h(\mathbf{x})$ according to Eqs. (2.21)–(2.23). The number of ticks corresponds to the order in $h(\mathbf{x})$. (b) The second order in $h(\mathbf{x})$ contribution to the one-loop integral in Eq. (5.2) decomposes into several parts. The dashed lines connecting the ticks indicate averaging over different surface profiles, using Eq. (4.2). The cross corresponds to the surface operator $\Phi^\perp$.

$$f_\tau(\delta/\lambda) \to \alpha + \beta(\delta/\lambda)^\psi. \tag{5.12}$$

Whereas both amplitudes α and β depend on ω/λ, the universal exponent ψ is independent of ω/λ and given by

$$\psi = \frac{3}{2}\frac{n+2}{n+8}\varepsilon - (2-2\zeta) + \mathcal{O}(\varepsilon^2). \tag{5.13}$$

Perpendicular correlations are obtained when $\underline{r}$ moves into the bulk, while $\underline{r}'$ remains close to the surface, i.e., $\delta \to \infty$ with δ' fixed (see Fig. 1). Equations (5.4) and (5.11)–(5.13) then imply that the correlations decay as

$$\overline{\langle \Phi_i(\underline{r})\Phi_i(\underline{r}')\rangle} \sim \frac{1}{\delta^{d-2+\eta_\perp}} + \frac{a}{\delta^{d-2+\tilde{\eta}_\perp}} \tag{5.14}$$

where the first term corresponds to a flat surface with $\eta_\perp = 1 - \frac{1}{2}[(n+2)/(n+8)]\varepsilon + \mathcal{O}(\varepsilon^2)$ [1,2]. The second term describes the effect of self-affine roughness, with an amplitude a depending on ω, λ, and ζ, and the new universal exponent

$$\tilde{\eta}_\perp = \eta_\perp - \psi = (2-2\zeta) + 1 - 2\frac{n+2}{n+8}\varepsilon + \mathcal{O}(\varepsilon^2). \tag{5.15}$$

Similarly, when both points remain close to the surface, i.e., $\rho = |\mathbf{r}_\parallel - \mathbf{r}_\parallel'| \to \infty$ with δ and δ' fixed, the correlations decay as

$$\overline{\langle \Phi_i(\underline{r})\Phi_i(\underline{r}')\rangle} \sim \frac{1}{\rho^{d-2+\eta_\parallel}} + \frac{a'}{\rho^{d-2+\tilde{\eta}_\parallel}}. \tag{5.16}$$

In this case the flat surface is governed by $\eta_\parallel = 2 - [(n+2)/(n+8)]\varepsilon + \mathcal{O}(\varepsilon^2)$, while self-affine roughness gives

$$\tilde{\eta}_\parallel = (2-2\zeta) + 2 - 4\,\frac{n+2}{n+8}\,\varepsilon + \mathcal{O}(\varepsilon^2). \tag{5.17}$$

The corrections due to roughness now decay with a slower power as compared to the Gaussian case. Indeed, for a sufficiently large roughness exponent ζ, these corrections can even dominate the result for the flat surface. The borderline roughness exponent is $\zeta_\perp^* = 1 - \frac{3}{4}[(n+2)/(n+8)]\varepsilon + \mathcal{O}(\varepsilon^2)$ for perpendicular, and a different value of $\zeta_\parallel^* = 1 - \frac{3}{2}[(n+2)/(n+8)]\varepsilon + \mathcal{O}(\varepsilon^2)$ for parallel correlations. This is a surprising result from a naive point of view since, due to $\zeta < 1$, on larger and larger length scales a self-affine rough surface looks more and more like a flat surface. Note that this effect becomes only visible beyond the Gaussian approximation, which corresponds to $\varepsilon = 0$. By setting $\varepsilon = 1$ in the above expressions, one obtains the corresponding estimates for $d = 3$.

VI. TWO-DIMENSIONAL *XY* MODEL

To compare the results of the preceding section with a different interacting theory, we examine the correlations for a two-dimensional *XY* model below the Kosterlitz-Thouless temperature [40]. The order parameter in this system is the spin variable $s(\underline{r}) = e^{i\theta(\underline{r})}$, where $\theta(\underline{r})$ is the angle (phase) the spin makes with some reference axis. Even though the phase fluctuations are described by a Gaussian model, nontrivial spin-spin correlations are obtained. Below the Kosterlitz-Thouless temperature, the $d = 2$ dimensional *XY* model is well described by the spin-wave Hamiltonian (neglecting vortices) [41]

$$\beta\mathcal{H}\{\theta\} = \tfrac{1}{2}K \int d^2 r (\boldsymbol{\nabla}\theta)^2, \tag{6.1}$$

where $\underline{r} = (x,y)$. Correlation functions decay as power laws in this system. For instance, the two-point correlation function in the unbounded plane is given by [41,42]

$$\begin{aligned} G_b(\underline{r},\underline{r}') &= \langle e^{i\theta(\underline{r})} e^{-i\theta(\underline{r}')} \rangle \\ &= \exp[\mathcal{G}_b(\underline{r};\underline{r}') - \tfrac{1}{2}\mathcal{G}_b(\underline{r};\underline{r}) - \tfrac{1}{2}\mathcal{G}_b(\underline{r}';\underline{r}')] \end{aligned} \tag{6.2}$$

with

$$\mathcal{G}_b(\underline{r};\underline{r}') = \langle \theta(\underline{r})\,\theta(\underline{r}') \rangle = -\frac{1}{2\pi K}\ln(r/a), \tag{6.3}$$

where $r = |\underline{r} - \underline{r}'|$ and a is some lattice cutoff. This implies

$$G_b(\underline{r};\underline{r}') = \left(\frac{r}{a}\right)^{-\eta}, \tag{6.4}$$

where $\eta = 1/(2\pi K)$.

If the plane is bounded by a free surface (line) at $y = 0$, the correlation function $G(\underline{r},\underline{r}')$ in the half-space $y > 0$ is given by similar expressions as in Eq. (6.2), where now $\mathcal{G}(\underline{r},\underline{r}')$ satisfies the Neumann boundary condition at the surface [42]. The final result

$$G(x,y;x',y') \sim \left[\frac{[(x-x')^2 + (y-y')^2][(x-x')^2 + (y+y')^2]}{4yy'}\right]^{-\eta/2} \tag{6.5}$$

implies the surface critical exponents $\eta_\parallel = 2\eta$ and $\eta_\perp = \frac{3}{2}\eta$, which fulfill the scaling relation $2\eta_\perp - \eta_\parallel = \eta$ familiar from the surface critical behavior of *n*-vector models [1,2].

In order to study whether the nontrivial roughness dependence of correlations obtained in the preceding section is also present here, we now consider a deformed surface (line) with the same boundary conditions as above. Similar steps as outlined in Appendix A lead to the result for the two-point correlation function

$$G(\underline{r};\underline{r}') = \exp[\Gamma(\underline{r};\underline{r}') - \tfrac{1}{2}\Gamma(\underline{r};\underline{r}) - \tfrac{1}{2}\Gamma(\underline{r}';\underline{r}')] \tag{6.6}$$

with

$$\begin{aligned} \Gamma(\underline{r};\underline{r}') = \mathcal{G}_b(\underline{r};\underline{r}') - \int dx \int dx'\, \partial_n \mathcal{G}_b(\underline{r};X(x))\mathcal{M}(x,x') \\ \times \partial_{n'}\mathcal{G}_b(\underline{r}';X(x')), \end{aligned} \tag{6.7}$$

where ∂_n denotes the normal derivative acting on X, and $\mathcal{M}(x,x')$ is the functional inverse of $\partial_n\partial_{n'}\mathcal{G}_b(X(x),X(x'))$. As in Sec. II, we use the representation $X(x) = (x,h(x))$ in terms of the height profile $h(x)$, and expand $G(\underline{r};\underline{r}')$ up to second order in h. In particular, for a self-affinely rough surface, we find, using Eq. (4.1), that the surface correlations fall off with the simple relative factor of $r^{-2(1-\zeta)}$ as compared to a flat surface (line) (compare Sec. IV). We attribute this to the Gaussian nature of the fluctuations in the phase angle $\theta(\underline{r})$, which are retained in the asymptotics of correlations for $s(\underline{r})$.

VII. CONCLUSION AND OUTLOOK

We have developed a path-integral formulation for the study of correlation functions in a system that is confined by deformed or rough surfaces. Our results are generic for any system with long-ranged correlations. Examples include systems with a broken continuous symmetry, such as the *XY* model below the Kosterlitz-Thouless temperature, or a nematic liquid crystal, where the correlations are generated by the corresponding massless Goldstone modes; or critical fluids or magnets described by the *n*-vector model at the bulk critical point, which has been mostly considered in this work. The surface deformations can consist of specifically designed, regular patterns, or represent a self-affinely rough surface. Some conclusions and possible extensions of this paper are listed below.

(i) *Thermodynamic surface quantities*. Thermodynamic quantities can be obtained from derivatives of the free energy with respect to magnetic fields. To discuss surface behavior,

TABLE I. Scaling relations between critical exponents relevant to a rough surface, as derived from Eqs. (7.1) and (7.2), in terms of the bulk critical exponents η, ν, $y_b=\Delta/\nu$, and the roughness exponent ζ. For each exponent in the left column there is a corresponding exponent for a flat surface [1,2] that would be denoted without tilde (compare with Table III in Ref. [2]).

Critical exponent	Conditions	Scaling relation
$\tilde{\eta}_\perp$, $\tilde{\eta}_\parallel$ [Eqs. (5.14) and (5.16)]	$\tau=h_b=h_s=0$	$2\tilde{\eta}_\perp-\tilde{\eta}_\parallel=\eta+2-2\zeta$
$\tilde{y}_s$ [Eq. (7.1)]	$\tau\neq 0,\quad h_s\neq 0$	$\tilde{y}_s=\frac{1}{2}(d-\tilde{\eta}_\parallel+2-2\zeta)$
$\tilde{\chi}_1\sim\lvert\tau\rvert^{-\tilde{\gamma}_1}$	$\tau\neq 0\quad h_b=h_s=0$	$\tilde{\gamma}_1=\nu(2-\tilde{\eta}_\perp)$
$\tilde{\chi}_{11}\sim\lvert\tau\rvert^{-\tilde{\gamma}_{11}}$	$\tau\neq 0\quad h_b=h_s=0$	$\tilde{\gamma}_{11}=\nu(1-\tilde{\eta}_\parallel)$
$\tilde{m}_1\sim(-\tau)^{\tilde{\beta}_1}$	$\tau<0\quad h_b=h_s=0$	$\tilde{\beta}_1=\frac{\nu}{2}(d-2+\tilde{\eta}_\parallel+2-2\zeta)$
$\tilde{m}_1\sim\lvert h_b\rvert^{1/\tilde{\delta}_1}$	$\tau=h_s=0,\quad h_b\neq 0$	$\tilde{\delta}_1=\nu y_b/\tilde{\beta}_1$
$\tilde{m}_1\sim\lvert h_s\rvert^{1/\tilde{\delta}_{11}}$	$\tau=h_b=0,\quad h_s\neq 0$	$\tilde{\delta}_{11}=\nu\overline{y_s}/\tilde{\beta}_1$

we introduce distinct fields h_b and h_s in the bulk and close to the surface, respectively. Assuming that our underlying assumption of the validity of an expansion in $h(\mathbf{x})$ holds, the results for the two-point correlation function are consistent with the following form for the scaling of the leading singular part of the surface free energy per projected area:

$$f_s^{(\mathrm{sing})}=\xi^{-d+1}[g_s(h_b\xi^{y_b},h_s\xi^{y_s})+\xi^{-2(1-\zeta)}g_r(h_b\xi^{y_b},h_s\xi^{\tilde{y}_s})], \tag{7.1}$$

where $\xi\sim\lvert T-T_c\rvert^{-\nu}$ is the correlation length that diverges at the critical point. The first term in square brackets corresponds to a flat surface, with y_b and y_s describing the relevance of bulk and surface fields, respectively [1,2]. The second term gives the effect of surface roughness, with $\xi^{-2(1-\zeta)}$ reflecting the average increase in area.

By taking derivatives of Eq. (7.1), one can derive scaling relations between various surface critical exponents, in complete analogy to the case of a flat surface [1,2]. In the following we focus on the contributions generated by the surface roughness, which according to Eq. (7.1) appear *in addition* to the corresponding contributions for a flat surface. For example, the singular part of the *surface magnetization*, $-\partial f_s^{(\mathrm{sing})}/\partial h_s$, can be written as $m_1+\overline{m_1}$ so that $\tilde{\chi}_1=\partial\tilde{m}_1/\partial h_b$ and $\tilde{\chi}_{11}=\partial\tilde{m}_1/\partial h_s$ represent the contributions to the *local susceptibility* and the *layer susceptibility* generated by the surface roughness, respectively. Similarly, we suppose that the singular part of the two-point correlation function near the surface can be written as $G(\underline{r};\underline{r}')+\tilde{G}(\underline{r};\underline{r}')$, and $\tilde{G}(\underline{r};\underline{r}')$ behaves for $h_b=h_s=0$ as

$$\tilde{G}(\underline{r};\underline{r}')\sim\begin{cases}\lvert\underline{r}-\underline{r}'\rvert^{-(d-2+\tilde{\eta}_\parallel)}\Gamma_\parallel(\lvert\underline{r}-\underline{r}'\rvert/\xi), & \vartheta=0,\\ \lvert\underline{r}-\underline{r}'\rvert^{-(d-2+\tilde{\eta}_\perp)}\Gamma_\perp(\lvert\underline{r}-\underline{r}'\rvert/\zeta,\vartheta), & \vartheta>0,\end{cases} \tag{7.2}$$

where ϑ is the angle $\underline{r}-\underline{r}'$ makes with the surface, and $\Gamma_\perp$ vanishes for $\vartheta\to 0$. Equations (7.1) and (7.2) then imply the scaling relations between various critical exponents related to a rough surface shown in Table I.

Equations (5.15) and (5.17) for the *n*-vector model are consistent with the scaling relation for $\tilde{\eta}_\parallel$ and $\tilde{\eta}_\perp$ shown in Table I. However, to regain the results in Eqs. (5.14)–(5.17), we have to use a value of $\tilde{y}_s=1+[3n/2(n+8)]\varepsilon+O(\varepsilon^2)$ in Eq. (7.1), which is different from $y_s=1-[3/(n+8)]\varepsilon+O(\varepsilon^2)$. To motivate and justify this difference, we resort to an analogy in which the rough surface is replaced with a collection of edges with a (possibly scale-dependent) distribution of opening angles. Already for a single edge, describing correlations requires a distinct and angle-dependent value of y_e for the magnetic field close to the edge [43,44]. Similarly, results obtained recently for correlations in the vicinity of a fractal surface with fractal dimension d_f [22,23] cannot be obtained using the value of y_s for a flat surface [with ξ^{-d_f} replacing ξ^{-d+1} in Eq. (7.1) and omitting the second term in square brackets]. Thus $\tilde{y}_s$ can be regarded as inherently related to self-affine geometry. Interestingly, however, $\tilde{y}_s$ itself does not depend on the roughness exponent ζ, at least to order ε.

(ii) *Higher orders of the perturbation theory*. As the previous remark already indicates, higher order results in ε are necessary in order to check the generality of our results for the *n*-vector model. For the contributions up to second order in $h(\mathbf{x})$ (as considered here), we expect a systematic expansion in powers of ε, and one can calculate the $\mathcal{O}(\varepsilon^2)$ contributions of, e.g., $f_\perp$ and ψ in Eq. (5.12). All the information needed about the self-affinely rough surface is contained in Eq. (4.2). However, it is not clear how the perturbative calculation in $h(\mathbf{x})$, for a self-affinely rough surface, can be generalized to higher orders than the second. Such an attempt would require, in addition to Eq. (4.2), the knowledge of stochastic averages of three and more fields $h(\mathbf{x})$, which can also introduce new length scales. Regarding these obstacles, it would be desirable to complement our results with a nonperturbative approach, e.g., for the two-dimensional Ising model bounded by a self-affinely rough boundary.

(iii) *Multiscaling*. For a random fractal boundary, it has been shown [23] that correlation functions exhibit multiscaling, which means that the average (over fractal realizations of the boundary with given fractal dimension d_f) of their nth power does not scale in the same way as the nth power of their average. It would be interesting to see if similar behavior also applies to self-affine rough boundaries.

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APPENDIX A: PATH INTEGRAL FORMULATION FOR CORRELATION FUNCTIONS

In this appendix we introduce a method to evaluate correlation functions of a fluctuating field subject to boundary conditions at surfaces of arbitrary shape. We consider a scalar field Φ described by the Gaussian action

$$S\{\Phi\} = \int d^d r \left[\frac{1}{2}(\boldsymbol{\nabla}\Phi)^2 + \frac{\tau_0}{2}\Phi^2 \right], \tag{A1}$$

corresponding to Eq. (2.1) with $u_0 = 0$. In order to study the behavior of correlation functions for cases where more than one boundary surface is present, we consider N manifolds (objects) Ω_α with $\alpha = 1,...,N$. Each point on the manifold Ω_α is represented by a vector $X_\alpha(\mathbf{y}) = [X_\alpha^\mu(\mathbf{y}); \mu = 1,...,d]$. Assuming the Dirichlet boundary condition $\Phi = 0$ on the manifolds, a general correlation function with respect to the action (A1) can be written as

$$\langle \cdots \rangle = \frac{1}{Z_0} \int \mathcal{D}\Phi(\underline{r}) \prod_{\alpha=1}^{N} \prod_{X_\alpha} \delta(\Phi(X_\alpha)) \cdots e^{-S\{\Phi\}}, \tag{A2}$$

where

$$Z_0 = \int \mathcal{D}\Phi(\underline{r}) \prod_{\alpha=1}^{N} \prod_{X_\alpha} \delta(\Phi(X_\alpha)) e^{-S\{\Phi\}}. \tag{A3}$$

Correlation functions of Φ can then be deduced from the generating functional

$$Z\{J\} = \left\langle \exp\left[\int d^d r J(\underline{r}) \Phi(\underline{r}) \right] \right\rangle, \tag{A4}$$

which is normalized such that $Z\{0\} = 1$.

Following Refs. [32,33], we now express for each manifold Ω_α the boundary condition enforcing functional $\Pi_{X_\alpha} \delta(\Phi(X_\alpha))$ in terms of an auxiliary field $\Psi_\alpha(X_\alpha)$ as

$$\prod_{X_\alpha} \delta(\Phi(X_\alpha)) \equiv \int \mathcal{D}\Psi_\alpha(X_\alpha) \exp\left[i \int_{\Omega_\alpha} dX_\alpha \Psi_\alpha(X_\alpha) \Phi(X_\alpha) \right]. \tag{A5}$$

The Gaussian integration over Φ in Eqs. (A2) and (A3) can be performed, resulting in

$$Z\{J\} = \text{const}\, Z_b\{J\} \int \prod_{\alpha=1}^{N} \mathcal{D}\Psi_\alpha(X_\alpha) e^{-\tilde{S}_{\text{eff}}\{\Psi,J\}}, \tag{A6}$$

where

$$Z_b\{J\} = \exp\left[\tfrac{1}{2} \int d^d r \int d^d r' J(\underline{r}) G_b(\underline{r},\underline{r}') J(\underline{r}') \right] \tag{A7}$$

with the bulk two-point correlation function $G_b(\underline{r},\underline{r}')$ corresponding to the action (A1). The effective action $\tilde{S}_{\text{eff}}$ is given by

$$\begin{aligned} \tilde{S}_{\text{eff}}\{\Psi,J\} = \tfrac{1}{2} \sum_{\alpha\beta} \int_{\Omega_\alpha} dX_\alpha \int_{\Omega_\beta} dX_\beta \Psi_\alpha(X_\alpha) G_b(X_\alpha, X_\beta) \\ \times \Psi_\beta(X_\beta) - i \sum_\alpha \int d^d r \int_{\Omega_\alpha} dX_\alpha J(\underline{r}) \\ \times G_b(\underline{r}, X_\alpha) \Psi_\alpha(X_\alpha). \end{aligned} \tag{A8}$$

Note that evaluation of Eq. (A6) requires functional integration over the curved manifolds Ω_α. This is facilitated by expressing the functional measure $\int \mathcal{D}\Psi_\alpha(X_\alpha)$ in terms of the local coordinates $\mathbf{y}$, which itself comprise a flat manifold (the local coordinate system). To this end we introduce the new fields $\psi_\alpha(\mathbf{y}) \equiv \Psi_\alpha[X_\alpha(\mathbf{y})]$. However, this transformation requires some care regarding the integration measure $\int_{\Omega_\alpha} dX_\alpha$ in Eq. (A8) as well as the functional measure $\int \mathcal{D}\Psi_\alpha(X_\alpha)$ in Eq. (A6). The result is [45]

$$\int \prod_\alpha \mathcal{D}\Psi_\alpha(X_\alpha) e^{-\tilde{S}_{\text{eff}}\{\Psi,J\}} = \int \prod_\alpha \mathcal{D}\phi_\alpha(\mathbf{y}) e^{-S_{\text{eff}}\{\phi,J\}}, \tag{A9}$$

where the field $\phi_\alpha(\mathbf{y}) \equiv [g_\alpha(\mathbf{y})]^{1/4} \psi_\alpha(\mathbf{y})$ is given for each manifold Ω_α in terms of the determinant $g_\alpha(\mathbf{y})$ of its induced metric,

$$g_{\alpha,ij}(\mathbf{y}) = \sum_{\mu,\nu=1}^{d} \frac{\partial X_\alpha^\mu}{\partial y_i} \frac{\partial X_\alpha^\nu}{\partial y_j}. \tag{A10}$$

The new effective action S_{eff} is given by

$$\begin{aligned} S_{\text{eff}}\{\phi,J\} = \tfrac{1}{2} \sum_{\alpha\beta} \int d^D y \int d^D y' \phi_\alpha(\mathbf{y}) A_{\alpha\beta}(\mathbf{y},\mathbf{y}') \phi_\beta(\mathbf{y}') \\ - i \sum_\alpha \int d^d r \int d^D y J(\underline{r}) \omega_\alpha(\underline{r},\mathbf{y}) \phi_\alpha(\mathbf{y}) \end{aligned} \tag{A11}$$

with the kernels

$$A_{\alpha\beta}(\mathbf{y},\mathbf{y}') = [g_\alpha(\mathbf{y})]^{1/4} G_b(X_\alpha(\mathbf{y}), X_\beta(\mathbf{y}')) [g_\beta(\mathbf{y}')]^{1/4}, \tag{A12a}$$

$$\omega_\alpha(\underline{r},\mathbf{y}) = G_b(\underline{r}, X_\alpha(\mathbf{y})) [g_\alpha(\mathbf{y})]^{1/4}. \tag{A12b}$$

The functional measure $\int \mathcal{D}\phi_\alpha(\mathbf{y})$ on the right hand side of Eq. (A9) is the one conventionally used on a flat manifold. The corresponding Gaussian integrations can thus be performed, resulting in

$$Z\{J\}=Z_b\{J\}\exp\left[-\tfrac{1}{2}\int d^d r\int d^d r'\,J(\underline{r})K(\underline{r},\underline{r}')J(\underline{r}')\right] \tag{A13}$$

with the kernel

$$K(\underline{r},\underline{r}')=\sum_{\alpha\beta}\int d^D y\int d^D y'\,\omega_\alpha(\underline{r},\mathbf{y})A^{-1}_{\alpha\beta}(\mathbf{y},\mathbf{y}')\,\omega_\beta(\underline{r}',\mathbf{y}'). \tag{A14}$$

Using $A^{-1}_{\alpha\beta}(\mathbf{y},\mathbf{y}')=[g_\alpha(\mathbf{y})]^{-1/4}M_{\alpha\beta}(\mathbf{y},\mathbf{y}')[g_\beta(\mathbf{y}')]^{-1/4}$, where $M_{\alpha\beta}(\mathbf{y},\mathbf{y}')$ is the functional inverse of $G_b(X_\alpha(\mathbf{y}),X_\beta(\mathbf{y}'))$ (with respect to both $\mathbf{y}$, $\mathbf{y}'$ and the indices α, β), one finds that the factors of $[g_\alpha(\mathbf{y})]^{1/4}$ in Eq. (A14) cancel. From Eqs. (A12)–(A14) one can thus read off the final result for the two-point correlation function,

$$G(\underline{r},\underline{r}')=G_b(\underline{r},\underline{r}')-\sum_{\alpha,\beta=1}^{N}\int d^D y\int d^D y'\,G_b(\underline{r},X_\alpha(\mathbf{y}))\times M_{\alpha\beta}(\mathbf{y},\mathbf{y}')G_b(\underline{r}',X_\beta(\mathbf{y}')). \tag{A15}$$

Choosing $N=1$, corresponding to only one manifold, gives Eq. (2.3).

APPENDIX B: SHORT DISTANCE EXPANSION OF THE STRESS TENSOR

In this appendix we consider the expansion of the two-point correlation function for a general massless field theory described by a Hamiltonian $\mathcal{H}\{\Phi\}$, to first order in the deformations of the height profile of a bounding surface. To this end, we introduce a new type of short-distance expansion of the stress tensor near a surface with the following scale-invariant boundary conditions: (a) the Dirichlet boundary condition $\Phi=0$ corresponding to the ordinary surface universality class, and (b) the boundary condition $\Phi=\infty$ describing critical adsorption, corresponding to the extraordinary universality class.

A deformed surface S given by the height profile $h(\mathbf{x})$ (see Fig. 1) can be obtained from the flat surface S_0 with $h(\mathbf{x})=0$ by means of a coordinate transformation, which maps the space $(\mathbf{x},z)$ on the space $(\hat{\mathbf{x}},\hat{z})$. We define this transformation by

$$\hat{\mathbf{x}}=\mathbf{x},\qquad \hat{z}=z+h(\mathbf{x})\Theta(z), \tag{B1}$$

where $\Theta(z)$ is an arbitrary differentiable function with $\Theta(z)=1$ for $z\leqslant z_0$ with some $z_0>0$, and which vanishes for $z\to\infty$. We denote the Hamiltonian with the flat surface S_0 by $\mathcal{H}$ and the Hamiltonian with a deformed surface S by $\hat{\mathcal{H}}$. According to the definition of the stress tensor T_{ik} [46–48] the change of $\mathcal{H}$ generated by the coordinate transformation (B1) can be written as

$$\hat{\mathcal{H}}-\mathcal{H}=-\int_{\mathrm{HS}}d^d r\sum_{k=1}^{d}\left[\frac{\partial}{\partial r_k}[h(\mathbf{x})\Theta(z)]\right]T_{zk}(\underline{r})+O(h^2), \tag{B2}$$

where HS denotes the half-space $\underline{r}=(\mathbf{x},z)$ with $z\geqslant 0$. Using the property $\Sigma_k\partial_k T_{ik}=0$ and the divergence theorem, one obtains

$$\hat{\mathcal{H}}=\mathcal{H}+\int_{\mathbb{R}^D}d^D x\,h(\mathbf{x})T_{zz}(\mathbf{x},z=0)+O(h^2). \tag{B3}$$

The contribution to first order in h is located *at* the (flat) surface and does not depend on the specific choice of $\Theta(z)$. The higher order contributions $O(h^2)$ cannot be transformed in this way, and will not be addressed in the following. $T_{zz}(\mathbf{x},0)=\lim_{\delta\to 0}T_{zz}(\mathbf{x},\delta)$ represents a surface operator, which does not, however, need to be renormalized at the surface, so that its scaling dimension equals its canonical inverse length dimension of d [49,50].

In the following we consider the cumulant $\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle^C$ of the two-point correlation function in the system described by $\mathcal{H}\{\Phi\}$ above the deformed surface S. Using Eq. (B3) one finds

$$\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle^C=\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C-\int d^D x\,h(\mathbf{x})\times\langle T_{zz}(\mathbf{x},0)\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C+O(h^2), \tag{B4}$$

where $\langle\,\rangle_0^C$ denotes the cumulant within the half-space HS bounded by the flat surface S_0. We now consider the limit $\rho=|r_\parallel-r_\parallel'|\to\infty$ (see Fig. 1), so that we can use the short-distance expansion (SDE) of the order parameter $\Phi(\underline{r})$ near the surface. For the first term $\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C$ in Eq. (B4), the SDE is well known: (a) for the Dirichlet boundary condition $\Phi=0$, the SDE is given by [1,2]

$$\Phi(\mathbf{r}_\parallel,z)=a z^{(\eta_\parallel-\eta)/2}\frac{\partial}{\partial z}\Phi(\mathbf{r}_\parallel,z)|_{z=0}+\cdots, \tag{B5a}$$

where $\partial_z\Phi(\mathbf{r}_\parallel,z=0)$ is a surface operator, $\eta_\parallel$ is a surface critical exponent, and a is a nonuniversal amplitude; (b) for the boundary condition $\Phi=\infty$, the SDE has the form [49,50]

$$\frac{\Phi(\mathbf{r}_\parallel,z)}{\langle\Phi(\mathbf{r}_\parallel,z)\rangle_0}=I+b_T z^d T_{zz}(\mathbf{r}_\parallel,z=0)+\cdots, \tag{B5b}$$

where $\langle\Phi(\mathbf{r}_\parallel,z)\rangle_0$ is taken at the critical point of the field theory, and I is the identity operator. The amplitude b_T is universal. Equation (B5) in conjunction with the scaling behavior $\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C\sim\rho^{-(d-2+\eta)}f(z/\rho,z'/\rho)$ [1,2] gives the result for a flat surface

$$\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C\sim(zz')^{(\eta_\parallel-\eta)/2}\rho^{-(d-2+\eta_\parallel)},\quad \rho\to\infty. \tag{B6}$$

For boundary condition (b), one has $\eta_\parallel=d+2$ [49,50], and the property $\langle T_{zz}\rangle=0$ has been used.

For the second term $\int d^D x h(\mathbf{x})\langle T_{zz}(\mathbf{x},0)\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C$ on the right hand side (rhs) of Eq. (B4), the above procedure cannot be applied directly because the integration of $T_{zz}(\mathbf{x},0)$ separates the points $\underline{r}$ and $\underline{r}'$ from the surface. To proceed, it is illustrative to consider first the case of a *constant* height field $h(\mathbf{x})=h_0$. In this case, the integration of $T_{zz}(\mathbf{x},0)$ simply amounts to a surface shift in the form [51]

$$h_0\int d^D x\langle T_{zz}(\mathbf{x},0)\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C = h_0\left(\frac{\partial}{\partial z}+\frac{\partial}{\partial z'}\right)\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C . \tag{B7}$$

Consider for illustration the case for which only $\underline{r}=(\mathbf{r}_\parallel,z)$ is close to the surface, i.e., $z\ll z'$. Since $\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C$ for small z behaves like a power in z, the z derivative on the rhs of Eq. (B7) is larger than the z' derivative by an amount of order z'/z. Now we recall that for the boundary conditions (a) and (b), correlations near the surface are *suppressed*, so that one can expect that on the left hand side of Eq. (B7) actually only a small integration region around $\mathbf{r}_\parallel$ contributes to the z derivative on the rhs. This suggests the operator product expansion

$$T_{zz}(\mathbf{x},0)\Phi(\mathbf{r}_\parallel,z)=\Delta(\mathbf{x}-\mathbf{r}_\parallel,z)\frac{\partial}{\partial z}\Phi(\mathbf{r}_\parallel,z)+\cdots \tag{B8}$$

for ($\mathbf{x}$, 0) close to $\underline{r}=(\mathbf{r}_\parallel,z)$, where $\Delta(\mathbf{x},z)$ is a representation of the delta function $\delta^D(\mathbf{x})$ in D dimensions, i.e.,

$$\int d^D x\Delta(\mathbf{x},z)=1, \quad \lim_{z\to 0}\Delta(\mathbf{x},z)=\delta^D(\mathbf{x}). \tag{B9}$$

Note that $\partial_z\Phi(\mathbf{r}_\parallel,z)$ on the rhs of Eq. (B8) is *not* a surface operator, since the z derivative is taken at a distance $z>0$ from the surface. The validity of Eq. (B8) can be verified for various cases. For two-dimensional systems at criticality bounded by a line with the boundary condition (a) or (b), it follows from the local form of the conformal Ward Identity [42]. For the Gaussian model with the boundary condition (a), it can easily be verified for any dimension d. For a Φ^4 model at criticality with boundary condition (b), Eq. (B8) is consistent with the form of $\langle T_{zz}(\mathbf{x},0)\Phi(\mathbf{r}_\parallel,z)\rangle_0$ known from conformal invariance arguments for any d with $2\leqslant d\leqslant 4$ [49,50]. For this system we have checked Eq. (B8) also for the correlation function $\langle\varphi(\underline{r})\varphi(\underline{r}')\rangle_0$ with $\varphi(\underline{r})=\Phi(\underline{r})-\langle\Phi(\underline{r})\rangle$ [50] to first (one loop) order in the Φ^4 interaction.

Let us go back to $\int d^D x h(\mathbf{x})\langle T_{zz}(\mathbf{x},0)\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C$ on the rhs of Eq. (B4) with z and z' fixed. In order to obtain its leading behavior for $\rho\to\infty$, the $\mathbf{x}$ integration can be divided in two regions. Within one region, $\mathbf{x}$ is far away from both $\mathbf{r}_\parallel$ and $\mathbf{r}_\parallel'$. Hence Eq. (B5) can be applied to both points $\mathbf{r}_\parallel$ and $\mathbf{r}_\parallel'$. Within the complement region, $\mathbf{x}$ is either close to $\mathbf{r}_\parallel$ or to $\mathbf{r}_\parallel'$ so that Eq. (B8) can be used. Due to the z derivative in Eq. (B8) in conjunction with the scaling behavior quoted below Eq. (B5), the contribution arising from the second integration region is by a factor ρ/z or ρ/z' larger than the contribution from the first integration region. Using Eq. (B6), we conclude that the leading contribution for $\rho\to\infty$ of the second term on the rhs of Eq. (B4) is given by $[A(\underline{r})+A(\underline{r}')]\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle_0^C$ with the amplitude $A(\underline{r})$ in Eq. (2.12). Thus we obtain the leading scaling behavior of $\langle\Phi(\underline{r})\Phi(\underline{r}')\rangle^C$ for $\rho\to\infty$ quoted in Eq. (2.11).

APPENDIX C: STRUCTURE OF THE LOOP EXPANSION

We consider the diagrams on the right hand side of Fig. 2(b). According to Eq. (5.2), in the $(\mathbf{p},\delta)$ representation, the distances δ_0 of the Φ^4 vertices [dots in Fig. 2(b)] from the surface have to be integrated using $\int_0^\infty d\delta_0$. To one loop order, only the three diagrams in the first line of Fig. 2(b) exhibit short-distance singularities at $\delta_0=0$. These diagrams consist of the following components:

 $= g_0(p;\delta,\delta_0)$ [see Eq. (2.8)] ; (C1)

 $= e^{-p\delta_0}$; (C2)

 $= g_2(p;\delta,\delta_0)$ [see Eq. (4.4)] ; (C3)

 $= -p\mathcal{K}(p,0)\,e^{-p\delta_0} + p\mathcal{K}(p,\delta_0) - \Omega\, e^{-p\delta_0}$ (C4)

with the constant $\Omega=\partial\mathcal{K}(p,\delta)/\partial\delta|_{\delta=0}$.

 $= \mathcal{A}\,\delta_0^{1-D}$ (C5)

with the constant

$$\mathcal{A}=-\int\frac{d^D\alpha}{(2\pi)^D}\frac{1}{2\alpha}e^{-2\alpha}, \tag{C6}$$

 $= \int\frac{d^D p}{(2\pi)^D}\left[\mathcal{K}(p,0)\,e^{-2p\delta_0} - 2\,\mathcal{K}(p,\delta_0)\,e^{-p\delta_0}\right] = \Omega\,\mathcal{B}\,\delta_0^{1-D} + F_1(\delta_0)$, (C7)

where the function $F_1(\delta_0)$ is regular for $\delta_0\to 0$. The constant $\mathcal{B}$ is given by

$$\mathcal{B}=D^{-1}\int\frac{d^D\alpha}{(2\pi)^D}[\tilde{U}_0(\alpha)e^{-2\alpha}-2\tilde{U}(\alpha)e^{-\alpha}], \tag{C8}$$

where $\tilde{U}_0(p\delta)=U(p,0)/\delta$ and $\tilde{U}(p\delta)=\tilde{U}(p,\delta)/\delta$, with $U(p,\delta)$ from Eq. (4.6). Note that in Eq. (C7) the terms in square brackets in Eq. (4.4), which correspond to the first line in Eq. (2.23), do not contribute.

Writing $\mathcal{A}=\mathcal{A}_0+\varepsilon\mathcal{A}_1+O(\varepsilon^2)$ and $\mathcal{B}=\mathcal{B}_0+\varepsilon\mathcal{B}_1+O(\varepsilon^2)$ with $\varepsilon=4-d$, one finds that $\mathcal{A}_0=\mathcal{B}_0$. This nontrivial fact is the reason why the $1/\varepsilon$ poles due to the short-distance singularities of the first and the third diagram in the first line of Fig. 2(b) cancel each other. The second diagram can be written as $\mathcal{A}[1/\varepsilon-C_E-\ln(p)]$  $+F_2(p,\delta)$, with Euler's constant C_E and a pole-free function $F_2(p,\delta)$. The $1/\varepsilon$ pole in this expression is then removed by the factor $Z_1^{-1/2}$, with

Z_1 from Eq. (5.8), that multiplies the zero-loop contribution  of the correlation function. The remaining, regular contributions, including those from the diagrams in the second line of Fig. 2(b), contain additional logarithmic terms in δ which are not present if the surface was flat. One can then identify these logarithmic contributions, and show that they can be recast in the power law according to Eqs. (5.11)–(5.13). It should be noted, however, that here this exponentiation is not entirely based on an RG argument, but relies on the plausible assumption that the self-affine structure of the surface should result in pure power laws (without logarithmic corrections) for the decay of correlation functions.

An analogous calculation leads to the quoted results for lateral correlations. Since in this case both points are located near the surface, only four of the six diagrams in Fig. 2(b) are different from each other.

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