Critical Roughening of Interfaces: A New Class of Renormalizable Field Theories

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A renormalizable field theory is developed for (multi)critical roughening of interacting interfaces in systems of dimension $d < 3$. There is an infinite hierarchy of universality classes that mirrors the series of multicritical points in Ising systems. The relevant operator algebra of these theories is built up by local scaling fields that are singular distributions of the basic field variable. Critical indices, e.g., the exponent α_s of the specific heat, are obtained analytically in an ε expansion. The extension of our results to $d = 3$ is discussed.

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In recent years, much effort has been devoted to the study of low-dimensional manifolds such as domain boundaries, interfaces, polymers, or membranes. New experimental tools have been developed that make it possible to probe these objects in much detail. The structure of surfaces and interfaces can be studied on a microscopic scale using surface x-ray and neutron scattering, and even one-dimensional domain boundaries or surface steps can now be observed directly by atomic force microscopy.

The statistical mechanics of these systems is governed by the interplay between intermolecular forces and fluctuations due to thermal excitation or quenched disorder. If these fluctuations are strong enough, a single manifold is in a scale-invariant *rough* state. Ising domain walls in two dimensions or in three dimensions above the roughening temperature are an example.

In real systems, however, the position of a manifold may still be constrained by walls or defect planes, or by the presence of other manifolds, if they lead to an effective potential that is attractive over a microscopic range a and tends to zero at larger distances. For example, in the standard Ising model with a plane of weaker bonds, a domain wall is subject to an effective potential well; if the spin-spin interactions or the structure of the defect plane are more complex, the potential may have both attractive and repulsive parts within the range a. The discussion in the sequel includes such more general potentials.

At low temperature or weak quenched disorder, the manifold is then localized to the position of lowest energy up to fluctuations of order a and is hence smooth on larger scales, while at high temperature or strong disorder, it is in a delocalized state with shape fluctuations on all scales up to the size of the system. The *roughening, wetting,* or *unbinding transition* separating these two regimes [1] may be of first or second order. In the latter case, the size of typical fluctuations diverges as the critical point is approached from below. Close to criticality, as they become large compared to a, the fluctuations wipe out microscopic details of the interactions, i.e., they renormalize the binding potential. Universal scaling behavior emerges, at least for sufficiently short-ranged potentials.

So far, this type of transition has been studied by transfer matrix calculations for interfaces in two-dimensional systems and by functional renormalization group methods applied to the binding potential [2]. The latter methods reveal a rich pattern of fixed points in systems of dimension $d > 2$ [3]. However, the status of these results remained somewhat unclear since the functional renormalization involves various approximations and does not provide a systematic way of calculating measurable quantities, such as critical exponents [4].

In this Letter, we show that critical roughening transitions with short-ranged potentials define a new class of renormalized continuum field theories and, in a systematic ε expansion, we obtain the first analytic results on their critical indices for general dimensionality. We find an infinite hierarchy of multicritical universality classes that, in a remarkable way, mirrors the well-known series of bulk multicritical points in Ising systems. The latter series is represented by effective Hamiltonians with polynomial interactions ϕ^n in terms of the local order parameter $\phi(r)$, where $n = 4, 6, \ldots$. Nontrivial renormalization group fixed points bifurcate from the Gaussian fixed point at the borderline dimensions $d_n = 2+4/(n-2)$ and describe fluctuation-dominated critical ($n = 4$), tricritical ($n = 6$), or higher multicritical behavior *below* that dimension. For roughening transitions of $[d_\parallel = (d-1)]$-dimensional interfaces, there is again a series, labeled by $n = 0, 2, \ldots$, of fixed points bifurcating from the Gaussian fixed point at $d_{\parallel n} = 2 - 4/(n+3)$ and describing (multi)criticality *above* that dimension. More and more such fixed points appear as $d_\parallel$ approaches 2. The basic objects that build up these field theories, the local scaling fields, are very different from the Ising series: they are no longer polynomials in the basic field variable $\phi(r)$, but *singular distributions*, see Eq. (2) below.

Consider the effective Hamiltonian

$$\mathcal{H} = \int d^{d_\parallel} r \{[\nabla\phi(r)]^2 + V_a(\phi(r))\} \tag{1}$$

in terms of the interface displacement field $\phi(r)$ of canonical dimension $-\zeta = (d_\parallel - 2)/2 < 0$. For $d \leq 3$, the kinetic part describes a thermally rough interface on length scales larger than the bulk correlation length of the system, where overhangs can be neglected. The interface is subject to a translationally invariant effective potential $V_a(\phi)$ of microscopic range a [i.e., $V_a(\phi) = a^{-d}v(a^{-\zeta}\phi)$, the dimensionless shape function $v(z)$ varying with amplitudes of order 1 for $|z|\lesssim 1$ and decaying rapidly to zero for $|z|\gtrsim 1$], which is treated as a perturbation of the Gaussian theory ($V_a = 0$). In the continuum limit $a \to 0$, $V_a(\phi(r))$ becomes a distribution in the field variable $\phi(r)$ and can hence be expanded in the basis of distribution-valued scaling fields

$$\Phi_k^B(r) \equiv \sqrt{4\pi}\left(\frac{\partial}{\partial\phi(r)}\right)^k \delta(\phi(r)) \qquad (k = 0,1,2,\ldots)\,. \tag{2}$$

These "bare" Gaussian fields have canonical scaling dimensions

$$x_k = (k+1)\zeta\,. \tag{3}$$

In any dimension $d < 3$, only finitely many of them are relevant; they span the space of bona fide renormalizable binding potentials. The fields $\Phi_0^B, \Phi_2^B, \ldots$ are even, the fields $\Phi_1^B, \Phi_3^B, \ldots$ are odd under the $\mathbb{Z}_2$ symmetry $\phi \to -\phi$ of the Gaussian theory.

The Gaussian correlation functions of the fields $\Phi_k^B(r)$ are independent of the short-distance cutoff a, just like those of normal-ordered composite vertices $:\phi^k(r):$. However, in order to define these correlation functions, the functional integral has to be regularized in the infrared, e.g., by adding a "mass" term to the Hamiltonian: $\mathcal{H}_\mu = \int d^{d_\parallel}r[(\nabla\phi)^2 + \mu^2\phi^2]$. This is equivalent to studying the roughening in a finite layer, since the mass term $\mu^2\phi^2$ effectively restricts the transverse shape fluctuations to a finite width of order $\mu^{-\zeta}$. The universal quantities to be calculated below, which depend only on the short-distance structure of these correlation functions, are independent of μ in the "thermodynamic limit" $\mu \to 0$.

Using the regularized Hamiltonian $\mathcal{H}_\mu$, we obtain

$$\langle \Phi_{k_1}^B(r_1)\cdots\Phi_{k_N}^B(r_N)\rangle_\mu = \left(\frac{\partial}{\partial\phi_1}\right)^{k_1}\cdots\left(\frac{\partial}{\partial\phi_N}\right)^{k_N} \langle\sqrt{4\pi}\delta(\phi(r_1)+\phi_1)\cdots\sqrt{4\pi}\delta(\phi(r_N)+\phi_N\Phi)\rangle_\mu\Big|_{\phi_1=\cdots=\phi_N=0} \tag{4}$$

with

$$\langle\sqrt{4\pi}\delta(\phi(r_1)+\phi_1)\cdots\sqrt{4\pi}\delta(\phi(r_N)+\phi_N)\rangle_\mu = \int_{-\infty}^{\infty}\prod_{n=1}^{N}\frac{dq_n}{\sqrt{\pi}}\exp\left(-\frac{1}{2}\sum_{n,n'=1}^{N}G_\mu(r_n-r_{n'})q_nq_{n'} + i\sum_{n=1}^{N}\phi_nq_n\right)\;; \tag{5}$$

the free massive propagator

$$G_\mu(r) = \langle\phi(0)\phi(r)\rangle_\mu \propto \int d^{d_\parallel}p\,\frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{p^2+\mu^2} \tag{6}$$

is the sum of its scaling part

$$-\Delta_\mu(r) \equiv G_\mu(r) - G_\mu(0) = -|r|^{2\zeta}[1 + O(\mu^2r^2)] \tag{7}$$

(normalized for convenience) and the contact term

$$G_\mu(0) = A(d_\parallel)\mu^{-2\zeta} \tag{8}$$

[with $A(d_\parallel) = 2^{2\zeta}\Gamma(1+\zeta)/\Gamma(1-\zeta)$], which diverges as $\mu \to 0$.

Note the following crucial feature of the correlation functions (5), for example, the two-point function

$$\begin{aligned}\langle\Phi_0^B(0)\Phi_0^B(r)\rangle_\mu &= 2\Delta_\mu(r)^{-\frac{1}{2}}[2G_\mu(0) - \Delta_\mu(r)]^{-\frac{1}{2}}\\ &= \sqrt{2/A(d_\parallel)}\mu^{x_0}|r|^{-x_0}[1 + O(|\mu r|^{x_2-x_0})]\,.\end{aligned} \tag{9}$$

Unlike the correlation functions of two and more points at a bulk critical point, they do not tend to a finite limit as $\mu \to 0$: *the critical theory vanishes.* This property ensures that in the thermodynamic limit, bulk correlation functions decay on the scale of the bulk correlation length, which remains finite at the critical roughening transition.

However, if the interface is localized by the potential V_a and hence there is a finite interface correlation length $\xi_\parallel$, the correlation functions of the fields Φ_k^B do not vanish for $\mu = 0$: the one-point function

$$\langle\Phi_0^B(r)\rangle_{\mathrm{loc}} \sim \xi_\parallel^{-x_0} \tag{10}$$

measures the probability of finding the interface position $\phi(r)$ in a microscopic neighborhood of the origin; the two-point function

$$\langle\Phi_0^B(0)\Phi_0^B(r)\rangle_{\mathrm{loc}} \sim \xi_\parallel^{-x_0}|r|^{-x_0}[1 + O(|r/\xi_\parallel|^{x_2-x_0})] \tag{11}$$

gives the return probability to the origin, etc. As $\xi_\parallel$ diverges, universal thermodynamic singularities occur in the derivatives of the interface free energy $f_s \sim \xi_\parallel^{-d_\parallel}$. For instance, the specific heat has a singular term

$$c_s \sim \int d^{d_\parallel}r\langle\Phi_0^B(0)\Phi_0^B(r)\rangle_{\mathrm{loc}} \sim \xi_\parallel^{-x_0}\int_0^{\xi_\parallel}R^{d_\parallel-1}\,dR\,R^{-x_0} \sim \xi_\parallel^{d_\parallel-2x_0} \tag{12}$$

for $d \geq 2$ [5], since the reduced temperature couples to the most relevant $\mathbb{Z}_2$-even scaling field Φ_0^B. Hence as a function of the reduced temperature, $\xi_\parallel$ and c_s diverge with exponents $\nu_\parallel = 1/(d_\parallel - x_0)$ and $\alpha_s = (d_\parallel - 2x_0)/(d_\parallel - x_0)$, respectively.

In general, the short-distance structure of these correlation functions is encoded in the operator algebra

$$\Phi_k^B(r_1)\Phi_l^B(r_2) = \sum_m C_{kl}^m(\mu^2 r_-^2)\, |r_-|^{-x_k - x_l + x_m} \Phi_m^B(r_+) + \cdots , \tag{13}$$

with $r_+ \equiv (r_1 + r_2)/2$, $r_- \equiv r_1 - r_2$. Its coefficients can readily be extracted from the integral representation (6) in the limit $|r_-| \to 0$, at least if Φ_k^B, Φ_l^B, and Φ_m^B are all relevant. By changing the integration variables q_1 and q_2 to $q_\pm \equiv q_1 \pm q_2$, performing the Gaussian integral over q_-, and Taylor expanding all terms analytic in r_-, we obtain

$$\sqrt{4\pi}\delta(\phi(r_1) + \phi_1)\sqrt{4\pi}\delta(\phi(r_2) + \phi_2) = \Delta_\mu(r_-)^{-\frac{1}{2}} \exp\left(-\frac{\phi_-^2}{\Delta_\mu(r_-)} - \frac{\Delta_\mu(r_-)}{4}\frac{\partial^2}{\partial\phi_+^2}\right)\sqrt{4\pi}\delta(\phi(r_+) + \phi_+) \tag{14}$$

with $\phi_\pm \equiv (\phi_1 \pm \phi_2)/2$, up to terms involving gradient fields. Inserting this in (5) then shows that the coefficients $C_{kl}^m(\rho^2)$ are analytic in their argument and, as $\rho^2 \to 0$, tend to a finite limit

$$C_{kl}^m = \sum_{j_1=0}^{k}\sum_{j_2=0}^{l}(-1)^{k-j_2}(-2)^{-\frac{1}{2}(k+l+m)}\binom{k}{j_1}\binom{l}{j_2}\frac{c(k+l-j_1-j_2)}{(m-j_1-j_2)!!} \tag{15}$$

if $k + l + m$ is even; otherwise they vanish by symmetry. $c(j)$ is defined as $(j-1)!!$ if j is even and 0 otherwise, and only terms with $j_1 + j_2 \le m$ are included in the sum.

Specifically, consider now an interface subject to a $\mathbb{Z}_2$-symmetric potential:

$$\mathcal{H} = \mathcal{H}_\mu + g_B \int d^{d_\parallel} r\, \Phi_n^B(r) \tag{16}$$

with n even. The bare coupling constant g_B has canonical scaling dimension

$$\varepsilon = d_\parallel - x_n = \frac{n+3}{2}\left(d_\parallel - 2 + \frac{4}{n+3}\right) \tag{17}$$

and is hence relevant if $d_\parallel$ is *larger* than the borderline dimension $d_{\parallel n} = 2 - 4/(n+3)$. With the operator algebra (15) at hand, it is relatively straightforward to renormalize this theory in perturbation theory. Unlike in the case of polynomial interactions, however, we cannot rely on Feynman diagrammatics since none of the scaling fields Φ_k^B has trivial multipoint correlation functions that factorize according to Wick's theorem. Therefore it is appropriate to carry out the renormalization at the level of the operator algebra, treating all scaling fields Φ_k^B on an equal footing [6].

The interface free energy per area $\mu^{-d_\parallel}$ can be expanded in powers of the dimensionless bare coupling constant $u_B = \mu^{-\varepsilon} g_B$,

$$F(u_B) = F(0) + \sum_{N=1}^{\infty} F_N u_B^N , \tag{18}$$

where

$$F_N = \mu^{-d_\parallel + N\varepsilon}\frac{(-1)^N}{N!}\int d^{d_\parallel} r_2 \cdots d^{d_\parallel} r_N \langle \Phi_n^B(0)\Phi_n^B(r_2)\cdots\Phi_n^B(r_N)\rangle_\mu^c(0) \tag{19}$$

is an integral over connected correlation functions of the Gaussian theory. If these integrals are defined with a short-distance cutoff a, powerlike singularities appear that are to be read off from the operator algebra. For small positive ε, the terms $C_{nn}^k \langle\Phi_k^B\rangle_\mu(0)\int d^{d_\parallel} r_2 |r_2|^{-2x_n + x_k}$ with $k < n$ generate *ultraviolet* singularities proportional to $a^{(k-n)x_0+\varepsilon}$ in F_2; additional singularities appear at higher order. They only lead to a cutoff-dependent shift in the critical couplings $g_B^{(k)}$ of Φ_k^B and are automatically subtracted if the integrals are defined by analytic continuation to higher dimensions. But since the regularized Nth order integral is proportional to $\mu^{d_\parallel - N\varepsilon}$, the perturbation series is *infrared* divergent at order $N = d_\parallel/\varepsilon$ in the limit $\mu \to 0$. This is cured by the ε expansion, which consists in absorbing the poles in ε of (19) into a renormalized coupling constant $u = Z(u)u_B$. To order u_B^2, we obtain

$$F(u_B) = F(0) - \mu^{-x_n}\langle\Phi_n^B\rangle_\mu(0)\left[u_B - \frac{1}{2}\left(\frac{s_n C_{nn}^n}{\varepsilon} + O(\varepsilon^0)\right)u_B^2\right] + O(u_B^3) , \tag{20}$$

where s_n denotes the surface of the $d_{\parallel n}$-dimensional unit sphere, and hence $Z(u) = 1 - (s_n C_{nn}^n/2\varepsilon)\, u + O(u^2)$. The resulting beta function [7]

$$\beta(u) \equiv \mu\partial_\mu u = -\varepsilon u + \frac{s_n}{2} C_{nn}^n\, u^2 + O(u^3) \tag{21}$$

has the infrared fixed point $u^* = (2/s_n C_{nn}^n)\,\varepsilon + O(\varepsilon^2)$.

Additional singularities appear in the perturbation expansion of the bare correlation functions $\langle\Phi_{k_1}^B(r_1)\cdots \times\Phi_{k_N}^B(r_N)\rangle_\mu(u_B)$. By an analogous argument, we find that to leading order all poles can be absorbed into the definition of renormalized fields $\Phi_k(u) = \tilde{Z}_k(u)\Phi_k^B$ with $\tilde{Z}_k(u) = 1 + (s_n C_{kn}^k/\varepsilon)u + O(u^2)$ [8]. This determines the scale-dependent dimensions [7] $x_k(u) = x_k + s_n C_{kn}^k u + O(u^2)$, whose fixed point values

$$x_k^* = x_k(u^*) = x_k + \frac{2C_{kn}^k}{C_{nn}^n}\varepsilon + O(\varepsilon^2) \tag{22}$$

govern the infrared asymptotics of the solutions of the Callan-Symanzik equation.

Thus for each $n = 0, 2, \ldots$, we obtain an interacting continuum field theory $\mathcal{T}_n$ that describes the universal long-distance behavior of the system (17) at the critical roughening point above the borderline dimension $d_{\parallel n}$; below that dimension, the fixed point $\mathcal{T}_n$ is unstable and, at least for a sufficiently weak potential strength, the long-distance behavior of the system (17) is Gaussian. The theory $\mathcal{T}_0$ governs the scaling of an unbound interface subject to a purely repulsive potential, while the higher theories $\mathcal{T}_2, \mathcal{T}_4, \ldots$ form a hierarchy of multicritical universality classes: the fixed point $\mathcal{T}_n$ has the n relevant scaling fields $\Phi_0, \Phi_1, \ldots, \Phi_{n-1}$ (the field Φ_{n+1} is redundant and the fields $\Phi_n, \Phi_{n+2}, \Phi_{n+3}, \ldots$ are irrelevant), and we expect a series of crossover phenomena $\mathcal{T}_n \to \mathcal{T}_{n-2} \to \cdots \to \mathcal{T}_0$.

As follows from (16) and (23), all scaling fields Φ_k have first-order contributions to their anomalous dimensions, which turn out to be *negative* for some relevant fields Φ_k. Hence, in contrast to the Ising series, these fields become more relevant under the renormalization group flow. In the case $n = 2$, for example, the two relevant fields Φ_0 and Φ_1 have dimensions $x_0^* = x_0 - 16\varepsilon + O(\varepsilon^2)$ and $x_1^* = x_1 + 8\varepsilon + O(\varepsilon^2)$, respectively, with $\varepsilon = (5/2)(d_\parallel - 6/5)$. This gives the exponents $\nu_\parallel = 1/(d - x_0^*) = 5/4 - (415/16)\varepsilon + O(\varepsilon^2)$ and $\alpha_s = (d_\parallel - 2x_0^*)/(d_\parallel - x_0^*) = 1/2 + (245/8)\varepsilon + O(\varepsilon^2)$.

Physically, the anomalous dimensions in (23) describe the fact that in the universality classes $\mathcal{T}_n$, typical interface shape configurations characterized by correlation functions of the fields Φ_k differ from the Gaussian ensemble because a nonzero critical potential well or bump is present at the origin.

In two dimensions, the only such universality class is the theory $\mathcal{T}_0$ with borderline dimension $d_{\parallel 0} = 2/3$ (all higher fixed points are unstable). At this fixed point, the decay of the one-point function $\langle \Phi_0(r) \rangle_\mu \sim \mu^{x_0^*}$ and the two-point function $\langle \Phi_0(0)\Phi_0(r) \rangle_\mu \sim \mu^{x_0^*}|r|^{-x_0^*}[1 + O(|\mu r|^{x_2^* - x_0^*})]$ is faster than for a free interface; this could be observed in finite-size studies of the two-dimensional Ising model with a line of stronger bonds. The results of the ε expansion are also in good agreement with exact transfer matrix calculations [9].

In three dimensions, there may be an infinite sequence of universality classes $\mathcal{T}_n$ according to the ε expansion. The fact that the fields Φ_k acquire anomalous dimensions indeed suggests that they are an interesting set of observables with power-law correlation functions even in $d = 3$, where an unbound interface is only logarithmically rough. But for the multicritical theories, low-order calculations are expected to fail quantitatively (as they do for the multicritical Ising models [10]), and the exponents should be determined numerically. This sequence of models is also relevant from a field-theoretic point of view: Does the local operator algebra, the analytic continuation of (16), have the structure imposed by ($d_\parallel = 2$)-dimensional conformal invariance? In analogy to the Ising series, it is then likely to be related to a minimal conformal theory [11].

Although we have limited ourselves to the study of temperature-driven roughening transitions, our approach should be useful more generally. Issues of interest include wetting transitions (where the $\mathbb{Z}_2$ symmetry is broken) and universality classes of interacting membranes below the persistence length (that are distinguished from interfaces by the form of the Gaussian propagator G_μ).

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