Discontinuous interface depinning from a rough wall

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Depinning of an interface from a random self-affine substrate with roughness exponent ζ_s is studied in systems with short-range interactions. In two dimensions transfer matrix results show that for $\zeta_s < 1/2$ depinning falls in the universality class of the flat case. When ζ_s exceeds the roughness ($\zeta_0 = 1/2$) of the interface in the bulk, geometrical disorder becomes relevant and, moreover, depinning becomes *discontinuous*. The same unexpected scenario, and a precise location of the associated tricritical point, are obtained for a simplified hierarchical model. It is inferred that, in three dimensions, with $\zeta_0 = 0$, depinning turns first order already for $\zeta_s > 0$. Thus critical wetting may be impossible to observe on rough substrates.

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Wetting and depinning phenomena occur when the interface between two coexisting phases unbinds from an attractive substrate [1]. In two dimensions, where an Ising interface can be well represented by a directed path [2], critical wetting occurs as a rule, and first-order wetting is predicted only for special setups [1]. In three dimensions, on the other hand, numerical simulations have shown critical, first-order, and tricritical wetting for the Ising model. The same phenomena in random media have attracted a lot of attention recently. Many works [3-5] considered the effects of quenched disorder due to bulk impurities on interface depinning. Other studies addressed disorder restricted to a geometrically smooth *surface* (chemical surface disorder) [6]. Both bulk and chemical surface disorder may modify the universality class of the unbinding transition, but generally not its continuous, second-order character in two dimensions [1].

In the present paper we address the role of *geometrical* disorder due to wall roughness in determining the nature of the wetting transition. Disordered geometry is most amenable to theoretical treatment when characterized by simple scaling laws, like in the case of self-affine or fractal substrates. So far, the effects of such roughness were seldom discussed, mostly in connection with complete wetting [7–9]. In spite of this, real substrates with self-affine geometry are met in many situations and have been the object of recent experiments [8]. For these substrates the average transverse width of the wall scales with the longitudinal length X as X^{ζ_S} (0< ζ_S <1).

We show that in the two-dimensional (2D) Ising model the nature of the depinning transition changes drastically upon increasing the self-affine roughness exponent ζ_S . For $\zeta_S \lesssim 1/2$ depinning remains continuous as in the flat case, and disorder is irrelevant. For $\zeta_S \gtrsim 1/2$ an unusual *discontinuous* depinning occurs. Since the intrinsic roughness of a 2D interface is $\zeta_0 = 1/2$, it is natural to expect $\zeta_S = 1/2$ as precise threshold. The emerging scenario is that of geometrical disorder determining a tricritical phenomenon for depinning. We are able to locate the tricritical point by accurate renormalization group (RG) calculations on a hierarchical model, which further suggests $\zeta_S = 1/2$ as the tricritical threshold in 2D. Extrapolation of our results to the experimentally most relevant case of three dimensions (3D), where $\zeta_0 = 0$ in ordered bulk, suggests that a minute disorder in substrate geometry could suppress critical wetting in favor of a firstorder transition.

Let x and y be integer coordinates of points on a square lattice. A "wall" is given by a self-avoiding path directed according to the positive x axis (Fig. 1). To each wall step parallel to the x axis, a height S_x , equal to the ordinate of its left end, x, is associated. For simplicity we consider only wall configurations obeying the restriction $s_x = S_x - S_{x+1}$ $= \pm 1$. In order to generate wall geometries with a preassigned roughness exponent ζ_S , we used a randomized version of an algorithm due to Mandelbrot [10]. Given a wall profile, the interface can assume configurations obeying $h_x - h_{x+1} = 0, \pm 1$ and $h_x \ge S_x$, if h_x is the height of the horizontal step at x (Fig. 1). The interface is like a (partially) directed walk or polymer, and its Hamiltonian is

$$\mathscr{H} = \sum_{x} \left[\varepsilon (1 + |z_x - z_{x+1} + s_x|) - u \,\delta_{z_x,0} \right], \tag{1}$$

where $z_x \equiv h_x - S_x$, and $\varepsilon, u > 0$. According to (1), at temperature *T*, fugacities $\omega \equiv e^{-\varepsilon/T}$ and $k \equiv e^{u/T}$ are associated to each (horizontal or vertical) step of the walk, and to each horizontal step on the wall, respectively. With a wall profile covering a distance *X* the partition function is



FIG. 1. Example of rough substrate boundary (continuous) and interface (dotted) configuration.

5035

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$$\mathcal{Z}_X = \sum_{all \ walks} \omega^L k^l \tag{2}$$

where the sum is restricted, e.g., to walks from the origin (0,0) to any point (*X*, *y*), with $y \ge S_X$. *L* and *l* indicate total length and number of horizontal steps on the wall, respectively. \mathcal{Z}_X is a functional of the wall profile. In order to calculate it we use transfer matrices:

$$(\mathbf{T}_{s_{x}})_{m,n} = \omega [\delta_{n,m-s_{x}} + (\delta_{n,m-s_{x}-1} + \delta_{n,m-s_{x}+1})\omega]k^{\delta_{n,0}},$$
(3)

where *m* and *n* range on the allowed z_x and z_{x+1} , respectively. The partition function thus becomes

$$\mathscr{Z}_{X} = \sum_{l,p} \left(\prod_{x=0}^{X-1} \mathbf{T}_{s_{x}} \right)_{l,p} \phi_{0}(p),$$
(4)

where, with the left end of the interface grafted at the origin, $\phi_0(p) = \delta_{p,0}$. A wall profile corresponds to a sequence of factors \mathbf{T}_1 , \mathbf{T}_{-1} in the product of Eq. (4). \mathcal{Z}_X is thus given asymptotically in terms of the largest Lyapunov eigenvalue [11]

$$\lambda_{max} = \lim_{X \to \infty} \left[\frac{||(\Pi_{x=0}^{X-1} \mathbf{T}_{s_x}) \vec{\phi}_0||}{||\vec{\phi}_0||} \right]^{1/X} = \lim_{X \to \infty} \left[\frac{||\vec{\phi}_X||}{||\vec{\phi}_0||} \right]^{1/X}.$$
(5)

We verified that different long **T** sequences, i.e., wall profiles, lead to the same eigenvalue within good accuracy. Thus, the quenched free energy is $\ln\lambda_{max}(\omega,k,\zeta_S) = \lim_{X\to\infty} \ln \mathcal{D}_X/X$, where the bar indicates quenched averaging over wall profiles. In the random context depinning is most efficiently detected by studying the behavior of quantities which can be directly related to the components of $\vec{\phi}_X$. Examples are the average probability, $\overline{P_0}(\omega,k,\zeta_S) = \lim_{X\to\infty} 1/X \sum_{x=0}^{X-1} \phi_x^2(0)/||\vec{\phi}_x||^2$, that the horizontal step lies on the wall, and the average distance of the interface from the substrate, $\overline{\langle z \rangle} = \lim_{X\to\infty} 1/X \sum_{x=0}^{X-1} \sum_z z \phi_x^2(z)/||\vec{\phi}_x||^2$ [1]. For our determinations we used up to 50 independent profiles with $x \le 2^{20}$ for which the components of $\vec{\phi}_x$ were computed up to a distance from the wall $z_{max} \approx 2 \times 10^4$.

Rather than considering variations of P_0 or $\langle z \rangle$ along curves parametrized by temperature, we choose to follow $\omega = \text{const lines.}$ In the case $\zeta_S \lesssim 1/2$, e.g., upon approaching $k = k_c$ from above with $0 < \omega < 1$, $\overline{\langle z \rangle}$ is well fitted by $\overline{\langle z \rangle} = A(k-k_c)^{-\psi} + B$, with ψ always compatible with the exactly known flat wall value of 1 [1]. k_c of course depends on ω and ζ_s . Some ψ and k_c determinations are reported in Table I for $\omega = 1/2$. For $\zeta_S \leq 1/2$ disorder in the wall geometry does not appear to lead to a new universality class for depinning. By treating a different model with continuum many-body techniques, Li and Kardar [7] found secondorder depinning with $\psi = 1$ for all $\zeta_s < 1$. At variance with this conclusion we find here that the situation drastically changes for $\zeta_S \gtrsim 1/2$. In this range $\langle z \rangle$ has a much steeper, abrupt rise at k_c , so that the previous fit becomes clearly inappropriate.

TABLE I. Values of ψ and k_c at $\omega = 1/2$ from fits of $\langle z \rangle$.

ζs	ψ	k _c
0	1	4/3 ^a
1/3	1.01 ± 0.01	1.772 ± 0.001
2/5	1.01 ± 0.02	1.828 ± 0.001
1/2	$1.03~\pm~0.04$	1.908 ± 0.003

^aExact results for a flat substrate [1].

Further strong evidence of a change of the nature of the transition at $\zeta_S \approx 1/2$ comes from the behavior of $\overline{P_0}$ (Fig. 2). While for $\zeta_S \lesssim 1/2$, $\overline{P_0} \sim (k-k_c)^{\rho}$, for $k \rightarrow k_c^+$, with $\rho \approx 1$, as with flat substrate [1], for $\zeta_S \gtrsim 1/2$ a discontinuity in $\overline{P_0}$ shows up (Fig. 2), becoming sharper and sharper as finite-size effects are reduced. The amplitude of the discontinuous jump in $\overline{P_0}$ also increases with ζ_S .

Thus, for $\zeta_S \gtrsim 1/2$ substrate roughness is relevant and, moreover, drives the depinning transition first-order. $\zeta_S = 1/2$ is the natural candidate as border value between continuous and discontinuous regimes. Indeed, for $\zeta_S > 1/2$ the wall roughness exceeds the roughness $\zeta_0 = 1/2$ [5] of the interface.

Of course, we verified by numerical tests that different microscopic details of the wall construction, like alternative choices of step sizes, do not affect appreciably the estimates of exponents in the continuous regime, or the location of the threshold $\zeta_S \approx 1/2$.

In 2D, first-order depinning is quite unexpected in the context of interfacial phenomena. Only two special ways of obtaining it have been conceived so far, by introducing either an attractive defect line in the bulk [12], or longitudinally fully correlated disorder [13]. Here first order is caused by sufficiently strong geometrical surface disorder, which also reveals the opposite in its effects to its chemical counterpart. Indeed, while higher roughness induces first-order, in the defect line case chemical surface disorder drives the transition back continuous [14]. This latter effect is certainly what one would expect at first sight on the basis of experience with phase transitions [15]. Like in the special examples of Refs. [12,13], our first order depinning needs not be accompanied by off-coexistence prewetting phenomena.



FIG. 2. The probability P_0 as a function of k at $\omega = 1/2$ and for different ζ_S values.



FIG. 3. Construction rule of the DHL (level n=0 to level n=1) and schematic picture of the lattice at level n, with the four n-1 level units. A wall configuration (heavy) crossing the left units, and two polymer configurations (dotted) are reported. With such wall configuration Eq. (6) applies.

Extrapolation to 3D of our findings is natural and has remarkable and unexpected consequences. Systems with a dominance of short-range interactions are, e.g., metallic substrate adsorbates or, even more, type-I superconductors [16]. Since typically interfaces in pure systems are only logarithmically rough in 3D ($\zeta_0=0$), a minimum of substrate roughness should be sufficient to give first-order wetting. This offers a further possible explanation for the fact that critical wetting is so elusive from the experimental point of view [17]. A recent work predicts critical wetting for superconductor interfaces [16]. For such interfaces ζ_0 is not known, unfortunately, but could be rather small, if not zero. This means that special care in using smooth substrates should be exerted, in order to observe the predicted phenomenon.

By reinterpreting ω and k as monomer fugacity and Boltzmann factor for contacts, respectively, our model describes polymer adsorption [18]. Apart from a change in the ensemble ($\mathscr{Z} = \Sigma_X \mathscr{Z}_X$), the transfer matrices are the same. Criticality (Z dominated by infinite length polymer configurations) implies $\lambda_{max} = 1$. We find that $\lambda_{max}(1/2, k, \zeta_s) = 1$ for all $k \le k_c (1/2, \zeta_s)$, where k_c was defined above. For $k \ge k_c$ criticality occurs at $\omega < 1/2$, indicating that the polymer is adsorbed [18]. Indeed $\omega = 1/2$ marks criticality for the polymer in the bulk. The dependence of k_c on ζ_s shows that adsorption becomes more difficult with increasing roughness. One can also show that the fraction of monomers adsorbed on the wall should have the same singular behavior as P_0 , when moving at $\omega = 1/2$. Thus, like interface depinning, polymer adsorption undergoes a change from second to first order upon increasing ζ_s .

To gain more insight into this change, we stick to polymer language and consider a simplified model of adsorption defined on diamond hierarchical lattice (DHL) (Fig. 3). Selfavoiding paths on DHL have often been used to mimic directed polymers in 2D [19]. A wall joining the two ends is obtained as follows: at level n=0 of DHL construction the wall always coincides with the unique existing bond. For $n=n_{max}>0$, the wall is determined by backward iteration. Starting from n_{max} , at each level, n, we choose whether the wall passes through the left or right DHL units of level n-1, with probabilities $1-\Delta$ and Δ , respectively, and so on. If, e.g., we put $\Delta=0$, the process is deterministic and we create a single wall coinciding with the left border of the lattice. For $\Delta = 1/2$ we generate with equal probability all possible walls through the lattice. Given a wall, we consider



FIG. 4. P_0 on the DHL at $\omega = 1/2$ and for various Δ values. The dashed lines mark the discontinuities for $\Delta > 1/2$.

a polymer, with partition \mathcal{Z}_n , joining the ends of the lattice and laying, e.g., to the right of the wall. As in Eq. (2), ω and k are step and wall contact fugacities, respectively. For $\Delta = 0$ we deal with a polymer attracted (k > 1) by the left DHL border, which plays the role of a "flat," deterministic substrate. When Δ rises, the "roughness" of the now random wall increases. Transverse hills and valleys are felt more and more by the polymer. For a given wall, one can compute the polymer partition function iteratively, using $\mathcal{Z}_{b,n+1}$ $= 2\mathcal{Z}_{b,n}^2$ and

$$\mathcal{Z}_{n+1} = \mathcal{Z}_{n,1} \mathcal{Z}_{n,2} + \mathcal{Z}_{b,n}^2 \tag{6}$$

or

$$\mathcal{Z}_{n+1} = \mathcal{Z}_{n,1} \mathcal{Z}_{n,2}.$$
 (7)

Equation (6) or (7) is chosen, according to whether, at level n+1, the *n*th level diamonds, 1 and 2, crossed by the wall, are the left or the right ones, respectively. $\mathcal{Z}_{b,n}$ is clearly the "bulk" partition function on DHL at the *n*th level, in absence of wall. Initial conditions are $\mathcal{Z}_0 = k\omega$ and $\mathcal{Z}_{h,0} = \omega$. Considering first $\Delta = 0$, Eq. (6) induces a two-parameter RG mapping by putting $\mathscr{Z}_{b,1} = \omega'$ and $\mathscr{Z}_1 = \omega' k'$. Clearly the transformation of $\mathcal{Z}_{b,n}$ implies that the bulk criticality condition is $\omega = 1/2$ as in the Euclidean case. The value k = 1 is marginally unstable for $k \ge 1$ and separates adsorbed (k>1) from desorbed (k<1) regimes. Thus, for $\Delta=0$ a positive attraction is always sufficient to adsorb the polymer. Equation (6) applies for all n and the problem has a nontrivial fixed point with $\mathcal{Z}_{h}^{*}=1/2$ and $\mathcal{Z}^{*}=1/2$. $P_0(\omega = 1/2, k, \Delta = 0)$ can be extrapolated by iteration. Due to marginality, P₀ starts rising with zero slope, but continuously, for k=1 (Fig. 4). For $\Delta > 0$ the \mathcal{Z}_n 's become random variables and we must iterate their probability distribution, \mathcal{P}_n . This cannot be done exactly. However, starting from $\mathcal{P}_0 = \delta(\mathcal{Z} - k\omega)$, we follow the distribution at level *n* by iteratively sampling it. From a large number ($\simeq 10^6$) of \mathscr{Z} values distributed according to \mathcal{P}_{n-1} , we generate a sample distributed according to \mathscr{P}_n by choosing many pairs of \mathscr{Z} values and obtaining from each pair a new value of \mathscr{Z} according to Eq. (6) or (7), with probabilities $1 - \Delta$ and Δ ,

respectively. The resulting \mathscr{Z} 's constitute a sample of \mathscr{P}_n . This procedure could be iterated for $n \leq 40$ with extremely high accuracy.

 P_0 at $\omega = 1/2$ is plotted as a function of k in Fig. 4 for different Δ 's. For $0 \le \Delta \le 1/2$, P_0 rises continuously from zero as $c(k-k_c)$. Thus, $\rho=1$ for $0 < \Delta < 1/2$. The slope c and k_c are both increasing with Δ . Apart from c=0 at $\Delta = 0$, due to the accidental marginality, such behavior reproduces what is observed in 2D when $\zeta_S < 1/2$. For $\Delta < 1/2$ the polymer is more "rough" than the wall. Only when $\Delta = 1/2$ does the latter have the same freedom to develop through the DHL as a polymer has within the "bulk." On the other hand, $\Delta > 1/2$ corresponds qualitatively to $\zeta_S > 1/2$, because the polymer feels more and more the wall limiting its options when developing through the DHL. For $\Delta = 1/2$ we have evidence that $c = \infty$, with a still continuous transition. This infinite slope indeed anticipates a sharp discontinuity in P_0 for $\Delta > 1/2$. So, the hierarchical model contains ingredients reproducing, at least qualitatively, the scenario emerging for the Euclidean model, and gives a suggestive indication of the way in which continuous transitions switch to first order at the expected threshold $\zeta_s = 1/2$.

The dependence of k_c on Δ mimics that on ζ_s in 2D, and further motivates the correspondence between Δ and ζ_s in the two cases. We stress that, since all paths have the same length, and there is no natural recipe for defining a transversal distance on DHL, the notion of roughness must always be mediated in some way: here we can link roughness to Δ . Our hierarchical model provides a remarkable example of the tricritical transition we are dealing with in this paper, and allows an essentially exact determination of its location and properties. Moreover, the threshold we find at $\Delta = 1/2$ is strongly suggestive of the precise location of the tricritical point in the Euclidean case.

Summarizing, in 2D, interface depinning or directed polymer adsorption on rough substrate with $\zeta_S < 1/2$ are continuous and in the same universality as in the flat case. For $\zeta_S > 1/2$ roughness is relevant and, moreover, the transitions acquire an unusual, discontinuous nature. This result, not anticipated so far [7], warns that some continuum approaches may not be able to catch the correct physics of depinning from rough substrates. We expect similar properties, and the same threshold $\zeta_S = 1/2$, for directed polymer adsorption on a self-affine surface in 3D. Indeed, directed polymers have no upper critical dimension, and for them $\zeta_0 = 1/2$ in all *d*. Although the single polymer adsorption regime is not easily accessible experimentally, we believe that our results should be relevant for stretched polymers [20].

In 3D the interface of a pure system typically has $\zeta_0 = 0$ [5]. We thus conjecture that depinning occurs discontinuously as soon as $\zeta_S > 0$, in cases when the interactions are predominantly short range, like in metallic systems. Our results also bear on the observability of the recently predicted critical wetting in the case of type-I superconductors [16], which is perhaps the most strict physical example of short-range interface-substrate interactions.

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