Model for Nonequilibrium Wetting Transitions in Two Dimensions

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A simple two-dimensional (2D) model of a phase growing on a substrate is introduced. The model is characterized by an adsorption rate q, and a desorption rate p. It exhibits a wetting transition which may be viewed as an unbinding transition of an interface from a wall. For $p = 1$, the model may be mapped onto an exactly soluble equilibrium model exhibiting complete wetting with critical exponents $\gamma = 1/3$ for the diverging interface width and $x_0 = 1$ for the zero-level occupation. For $0 < p \neq 1$ a crossover to different exponents is observed which is related to a Kardar-Parisi-Zhang-type nonlinearity. [S0031-9007(97)04214-2]

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The interaction of a bulk phase (α) of a system with a wall or a substrate may result in very interesting wetting phenomena. In particular a layer of a second phase (β), which is preferentially attracted to the wall may be formed in its vicinity. As some of the parameters controlling the system, say temperature or chemical potential, are varied, the thickness of the β layer may diverge, leading to a wetting transition. Such transitions have been theoretically studied and experimentally observed in a variety of systems and models in thermal equilibrium (for a review, see Ref. [1]). Wetting transitions may be viewed as the unbinding of an interface from a wall. Within this approach one considers the interface configuration $h(r)$ which gives the height of the interface above the wall at point r. One then introduces an effective Hamiltonian of the form [2]

$$\mathcal{H} = \int d^{d-1}r \left\{ \frac{\sigma}{2} (\nabla h)^2 + V[h(r)] \right\}, \qquad (1)$$

where σ is the surface tension of the α-β interface, $V[h(r)]$ yields the effective interaction between the wall and the interface, and $d - 1$ is the interface dimension. The potential V which contains an attractive component may bind the interface to the wall. However, as the temperature or other parameters describing the system are varied, the attractive component of the potential may become weaker and it is no longer able to bind the interface, leading to a wetting transition. In $d = 2$ dimensions one usually distinguishes between critical wetting and complete wetting. Critical wetting is marked by the divergence of the interface width when the temperature T is increased towards the transition temperature T_W moving along the coexistence curve of the α and β phases. On the other hand complete wetting is characterized by the divergence of the interface width when the chemical potential difference between the two phases is varied, moving towards the coexistence curve at $T > T_W$. These types of transitions are associated with two different sets of critical exponents.

A very interesting question which has not been studied in detail so far is that of wetting transitions under *nonequilibrium* conditions. Here the β phase is adsorbed to the wall via a growth process whose dynamics, unlike that of equilibrium processes, does not obey detailed balance. This problem may be studied by considering the behavior of a moving interface interacting with a wall. Such transitions have been reported in recent studies of the dynamics of certain models of coupled maps [3].

In this Letter we introduce a class of nonequilibrium growth models of a one-dimensional interface interacting with a substrate. The interface evolves by both adsorption and desorption processes which in general do not satisfy detailed balance. By varying the relative rates of these processes, a transition from a binding to a nonbinding phase is found. For a particular value of the desorption rate, for which the dynamics happens to have detailed balance, the model may be mapped onto an exactly soluble equilibrium model which exhibits a complete wetting unbinding transition. The associated critical exponents are $\gamma = 1/3$ for the interface width and $x_0 = 1$ for the base level occupation. For generic values of the desorption rate, however, detailed balance is violated and a crossover to different exponents is observed.

Definition of the model.—The model is defined in terms of growth of a 1D interface, in which both adsorption and desorption processes take place. We consider a *restricted* solid-on-solid (RSOS) growth process, where the height differences between neighboring sites are restricted to take values $0, \pm 1$. The model is defined on a 1D lattice of N sites with associated height variables $h_i = 0, 1, \ldots, \infty$ and periodic boundary conditions. We use random sequential dynamics which are defined through the following algorithm: at each update choose a site i at random and attempt to carry out one of the processes:

(i) Adsorption of an adatom with probability $q/(q + p + 1)$:

$$h_i \to h_i + 1 . \qquad (2)$$

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(ii) Desorption of an adatom from the edge of an island with probability $1/(q + p + 1)$:

$$h_i \to \min(h_{i-1}, h_i, h_{i+1}) . \tag{3}$$

(iii) Desorption of an adatom from the interior of an island with probability $p/(q + p + 1)$:

$$h_i \to h_i - 1 \quad \text{if } h_{i-1} = h_i = h_{i+1} . \tag{4}$$

If the selected process would result in a violation of the RSOS constraint $|h_i - h_{i+1}| \leq 1$, the attempted move is abandoned and a new site i is selected. In addition, a hard-core wall at zero height is introduced, i.e., a process is carried out only if the resulting interface heights are non-negative. One can prove that these processes in general do not satisfy detailed balance.

The presence of a hard-core wall at $h = 0$ leads to a phase transition that takes place even in finite systems. This can be seen as follows: Without the wall the interface in a finite system has a finite width. For fixed $p > 0$ the parameter q controls the mean growth velocity of the interface, i.e., for large q the interface grows while for small q it moves downward. These two regimes are separated by a critical growth rate $q = q_c$ for which the mean velocity is zero. Therefore, on large time scales, a lower wall will affect only the interface dynamics if the interface does not move away from the wall, i.e., $q \leq q_c$, resulting in a smooth interface. In the growing phase $q > q_c$, however, the interface does not feel the wall. It is rough and propagates with a constant mean velocity. The phase transition line for an infinite system is shown in Fig. 1.

Throughout this paper we are particularly interested in the the mean growth velocity v in the growing phase, the occupation ρ_0 of the zero-height layer in the smooth phase, and the interface width in the smooth phase which

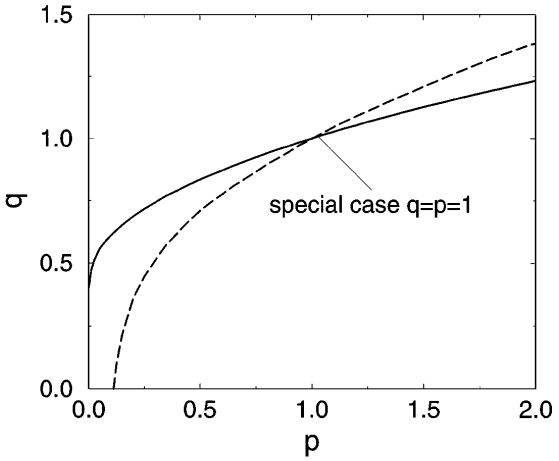

FIG. 1. Phase diagram for an infinite system. The wetting transition takes place along the solid line. Along the dashed line the growth velocity in the model without a wall does not depend on a global tilt of the interface, indicating that the effective Kardar-Parisi-Zhang (KPZ) nonlinearity vanishes. Both lines intersect in the point $q = p = 1$, where the microscopic processes obey detailed balance.

is defined by

$$w^2 = \frac{1}{N} \sum_{i=1}^{N} \left(h_i - \frac{1}{N} \sum_{j=1}^{N} h_j \right)^2 . \tag{5}$$

Consider now the thermodynamic limit $N \to \infty$. Near criticality in the growing phase $q > q_c$, we expect the interface velocity to scale like

$$v \sim (q - q_c)^y , \tag{6}$$

whereas in the smooth phase, $q < q_c$, the expected scaling for bottom layer occupation and width is

$$\rho_0 \sim (q_c - q)^{x_0} , \qquad w \sim (q_c - q)^{-\gamma} . \tag{7}$$

It would be interesting to find out how the critical exponents y, x_0, and γ depend on p. We note that the case $p = 0$ is special: In this case atoms cannot be desorbed from a completed layer, and the interface cannot move below its actual minimum height. This means that the hard-core wall becomes irrelevant. Therefore, the phase transition (which still exists for $p = 0$) relies on a completely different mechanism. The $p = 0$ transition is expected to belong to the universality class of a closely related model previously considered in Ref. [4]. It has been shown that in this case some of the critical exponents can be related to the universality class of directed percolation (DP). In particular one expects $x_0 = \beta$ and $y = \nu_\perp$, where $\beta = 0.276$ and $\nu_\perp = 1.73$ are the density and correlation length exponents, respectively, of DP. Here completed layers play the role of absorbing states from where the system cannot escape. For $p > 0$, however, the system is ergodic and one expects different critical exponents. Another special case is $p = 1$: here the system does satisfy detailed balance and can be solved exactly. In the following, we present our analysis of the wetting transition for $p = 1$. We then consider the general case for which the model does not have detailed balance.

Exactly soluble case, $p = 1$.—We first show that in this case the steady state satisfies detailed balance and that for $q < 1$ the probability of finding the interface in a particular configuration $\sigma_H = \{h_1, \ldots, h_N\}$ is given by the distribution

$$P(h_1, \ldots, h_N) = P(\sigma_H) = Z_N^{-1} \, q^{H(h_1, \ldots, h_N)} , \tag{8}$$

where

$$H = H(h_1, \ldots, h_N) = \sum_{i=1}^{N} h_i \tag{9}$$

is the sum of all heights. Here, the partition sum $Z_N = \sum_{h_1, \ldots, h_N} q^H$ runs over all interface configurations which respect the RSOS and the hard-core wall constraints.

In order to prove Eq. (8), notice that the processes (2)–(4) subjected to the RSOS constraint correspond to a change of H by one unit. Therefore, if the distribution of Eq. (8) is to hold in the steady state, the probabilities of finding the interface in states with total height H and $H + 1$ have to satisfy

$$P(\sigma_{H+1})/P(\sigma_H) = q . \tag{10}$$

As one can read off from the processes (2)–(4), any allowed transition $\sigma_H \to \sigma_{H+1}$ occurs with rate $w(\sigma_H \to \sigma_{H+1}) = q$. Moreover, for each such process $\sigma_H \to \sigma_{H+1}$, there is a reverse process $\sigma_{H+1} \to \sigma_H$ which takes place with a nonzero rate. For $p = 1$, this rate is given by $w(\sigma_{H+1} \to \sigma_H) = 1$ so that

$$w(\sigma_H \to \sigma_{H+1})/w(\sigma_{H+1} \to \sigma_H) = q \qquad (p = 1)\,. \tag{11}$$

Together with Eq. (10) this implies that the processes (2)–(4) satisfy detailed balance. Notice that the above consideration is consistent with the hard wall constraint $h_i \geq 0$. Equation (8) yields the steady state distribution only for $q < 1$. The unbinding transition takes place at $q = 1$ and the height distribution becomes time dependent for $q > 1$. For $p \neq 1$, detailed balance is violated. This can be proven by construction of explicit cycles of configurations in small systems for which the rates of moving clockwise and counterclockwise are unequal.

We now apply the transfer matrix formalism [5,6] to study the distribution (8). Let us define a transfer matrix T acting in spatial direction by

$$T_{h,h'} = \begin{cases} q^h & \text{if } |h - h'| \leq 1\,, \\ 0 & \text{otherwise,} \end{cases} \tag{12}$$

where $h, h' \geq 0$. Steady state properties can be derived from the eigenvector ϕ that corresponds to the largest eigenvalue μ of the transfer matrix $\sum_{h'=0}^{\infty} T_{h,h'}\phi_{h'} = \mu\,\phi_h$. From the squares of the eigenvector components one can derive various steady state quantities. For example, the probability ρ_h of finding the interface at height h is given by $\rho_h = \phi_h^2/\sum_{h'}\phi_{h'}^2$. Here we are particularly interested in the scaling behavior of bottom layer occupation ρ_0 and the width $w^2 = \sum_h (h - \overline{h})^2\rho_h$, where $\overline{h} = \sum_h h\rho_h$ denotes the mean height.

Close to criticality, where $\epsilon = 1 - q$ is small, one can carry out the continuum limit $\phi_h \to \phi(\tilde{h})$, replacing the discrete heights h by real-valued heights $\tilde{h}$. Then, the above eigenvalue problem turns into a differential equation [5] which, to leading order in ϵ, is given by

$$\left(\frac{\partial^2}{\partial\tilde{h}^2} + (3 - \mu) - 3\epsilon\tilde{h}\right)\phi(\tilde{h}) = 0\,. \tag{13}$$

This equation, together with the boundary conditions $\phi(0) = \phi(\infty) = 0$, has a unique physical solution. Simple dimensional analysis indicates that the height variables scale as $h \sim \epsilon^{-1/3}$ and thus the width diverges as $w^2 \sim \epsilon^{-2/3}$. The occupation of the bottom layer in the continuum limit is given by $\rho_0 = \mathcal{N}^{-1}(\phi'(0))^2$, where $\mathcal{N} = \int d\tilde{h}\,\phi^2(\tilde{h})$ is a normalization factor. Since $\phi'(0) \sim \epsilon^{1/3}$ and $\mathcal{N} \sim \epsilon^{-1/3}$ one obtains a linear scaling law $\rho_0 \sim \epsilon$. The critical exponents for $p = 1$ are thus given by

$$x_0 = 1, \qquad \gamma = 1/3\,. \tag{14}$$

Numerical results.—In order to determine the critical exponents for other values of the growth rate p, we perform Monte Carlo simulations. The width w and the occupation of the bottom layer ρ_0 are measured in the smooth phase $q < q_c$. Depending on $\epsilon = q_c - q$, we first equilibrate a system of size 1500 over a time interval up to 4×10^6 time steps. Then the thermal averages of w and ρ_0 are measured over a time interval of the same size. Similarly, the interface velocity v is measured in the growing phase $q > q_c$.

The numerical data measured in the smooth phase are shown in Fig. 2. From the slopes in the double logarithmic plots we estimate the critical exponents (see Table I). For $p = 1$, the numerical results we obtain are consistent with the exact values derived above. In addition the velocity exponent is found to be $y = 1.01(3)$. For $0 < p < 1$ we observe a *crossover* to different critical exponents. Since the values differ from those in Eq. (14) by less than 30% and the crossover is extremely slow, it

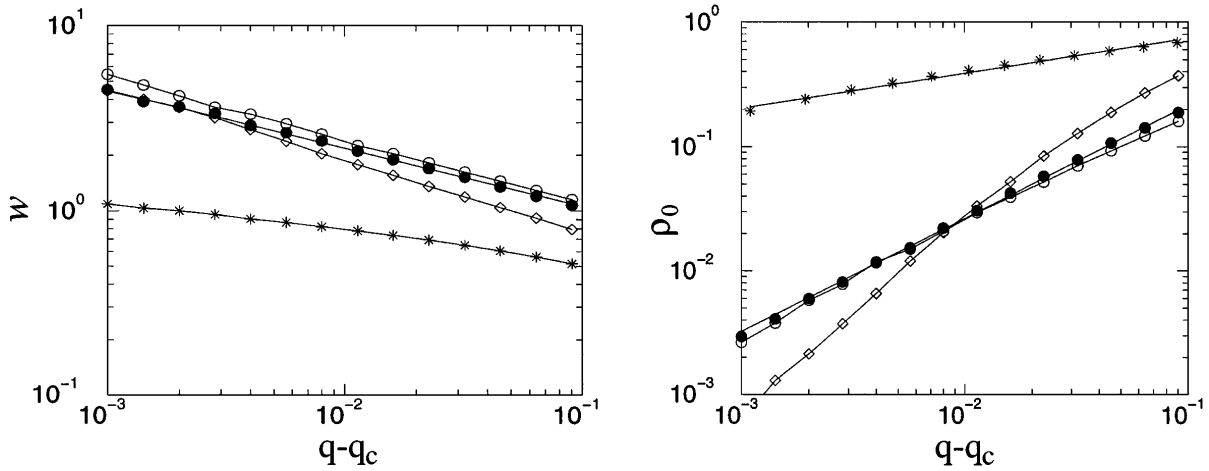

FIG. 2. Results obtained from Monte Carlo simulation of the growth model with 1500 sites. The width w and the bottom layer occupation ρ_0 are measured for ($\star$) $p = 0$, ($\diamond$) $p = 0.05$, ($\bullet$) $p = 1$, and ($\circ$) $p = 2.0$. For $p = 1$ we fitted straight lines. The curvature for $p \neq 1$ indicates a crossover to KPZ exponents.

TABLE I. Estimates for the critical exponents.

	$p = 0$	$p = 0.05$	$p = 1.0$	$p = 2.0$
q_c	0.3991(5)	0.5564(2)	0.9999(2)	1.2329(5)
x_0	0.27(1)	1.51(6)	0.96(5)	1.02(5)
γ	0 (log.)	0.41(3)	0.32(3)	0.37(3)
y	1.69(5)	0.98(3)	1.01(3)	1.00(3)

is difficult to determine these exponents precisely. Our estimates are $y = 1.00(3)$, $x_0 = 1.5(1)$, and $\gamma = 0.41(3)$. Similar results are obtained for $p > 1$ except for x_0 which is close to one in this case. Finally, for $p \to 0$, we observe another crossover. This is consistent with the results of Ref. [4] which indicate that the interface width diverges logarithmically at the $p = 0$ transition.

General considerations.—Equilibrium wetting of a 2D Ising system has been studied in Refs. [5,7]. It was shown that a column of weak bonds (which acts as an attractive potential for the domain wall separating the up and down states) located at the boundary induces a wetting transition at some finite temperature T_W. At the critical wetting transition the interface width diverges with $\gamma = 1$.

The transition found for $p = 1$ is of a different nature. In this case, $(1 - q)$ acts as a chemical potential difference between the two coexisting phases. For $q < 1$ the chemical potential difference drives the interface towards the wall, resulting in a smooth interface. On the other hand, for $q > 1$ the interface is driven away from the wall, resulting in a KPZ-like rough moving interface [8]. The critical behavior associated with the transition is thus that of *complete* wetting.

For $p \neq 1$, the mapping to equilibrium is impossible since detailed balance is violated. Here a KPZ-type nonlinearity is expected to be responsible for the different exponents we observe. Within this approach, one describes the system by the Langevin equation

$$\frac{\partial h(r,t)}{\partial t} = v_0 + \sigma \nabla^2 h(r,t) - \frac{\partial V[h(r,t)]}{\partial h(r,t)} + \lambda [\nabla h(r,t)]^2 + \zeta(r,t), \tag{15}$$

where $\zeta(r,t)$ is a zero-average Gaussian noise field with variance $\langle \zeta(r,t)\zeta(r',t')\rangle = 2D\delta^{d-1}(r - r')\delta(t - t')$ and V is the effective interaction between the wall and the interface. This equation has been studied recently [9,10] in the context of nonlinear diffusion with multiplicative noise. A simple scaling argument suggests that the width exponent corresponding to the wetting transition described by this equation is given by

$$\gamma = (2 - z)/(2z - 2), \tag{16}$$

where z is the dynamic exponent. For a 1D interface $z = 3/2$, yielding $\gamma = 1/2$. Our numerical results indicate that the width exponent γ is larger for $p \neq 1$ as compared with its $1/3$ value at $p = 1$, although it seems to be smaller than $1/2$. However, in view of the very slow crossover expected in this problem (see below) it is possible that γ is indeed $1/2$, but more extensive simulations close to q_c would be needed to observe it.

The bottom layer occupation ρ_0 may be related to ξ^{-1}, where ξ is the correlation length. Thus, we expect x_0 to be equal to the correlation length exponent ν, which for the KPZ equation is given by $\nu = 1/(2z - 2)$, yielding $x_0 = 1$ in 1D. However, the numerical results suggest that this scaling argument is valid only for $p > 1$, whereas for $0 < p < 1$ much larger values for x_0 are obtained. This may be related to the existence of *different* universality classes in both cases, corresponding to the distinction between an "upper" and a "lower" wall in Ref. [10].

In order to verify this picture we made a numerical estimate of the effective nonlinear KPZ term corresponding to the RSOS model considered in this work. This is done by comparing the growth velocities of a flat and a tilted interface in absence of a wall. We find that the nonlinearity is indeed nonvanishing in the (p, q) plane, except on a particular line (the dashed line in Fig. 1). As expected, this line and the phase transition line are different and intersect in the point $q = p = 1$. At all other points on the transition line the nonlinear term is *not* vanishing, and the KPZ-like exponents are expected to be valid. Since λ is small in the vicinity of the $q = p = 1$ point, very slow crossover phenomena occur, making it difficult to observe the true exponents in this region. Moreover, the interaction between the wall and the interface strongly depends on the sign of λ. This may lead to different exponents x_0 for the bottom layer occupation on the two sides of the special point.

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