Facet formation in the negative quenched Kardar-Parisi-Zhang equation

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The quenched Kardar-Parisi-Zhang equation with negative nonlinear term shows a first order pinning-depinning (PD) transition as the driving force $F$ is varied. We study the substrate-tilt dependence of the dynamic transition properties in 1+1 dimensions. At the PD transition, the pinned surfaces form a facet with a characteristic slope $s_c$ as long as the substrate tilt $m$ is less than $s_c$. When $m<s_c$, the transition is discontinuous and the critical value of the driving force $F_c(m)$ is independent of $m$, while the transition is continuous and $F_c(m)$ increases with $m$ when $m>s_c$. We explain these features from a pinning mechanism involving a localized pinning center and the self-organized facet formation. [S1063-651X(99)12602-3]

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The pinning-depinning (PD) transition by an external driving force has been of much interest recently. Typical examples are interface growth in porous media under external pressure [1], dynamics of a domain wall under random fields [2,3], dynamics of a charge density wave under an external field [4], and vortex motion in superconductors under external current [5,6]. In the PD transition, there exists a critical value $F_c$ of the driving force $F$, such that when $F<F_c$, the interface (or charge, or vortex) is pinned by disorder, while for $F>F_c$, it moves with a constant velocity $v$. The velocity $v$ plays the role of order parameter in the PD transition, which typically behaves as

$$v \sim (F-F_c)^\theta.$$  

(1)

Recently, several stochastic models for the PD transition of interface growth in disordered media have been introduced [7,8]. It is believed that the models in 1+1 dimensions are described by the quenched Kardar-Parisi-Zhang (QKPZ) equation for the surface height $h$ [9],

$$\partial_t h = \nu \partial_x^2 h + \frac{\lambda}{2} (\partial_x h)^2 + F + \eta(x,h),$$  

(2)

where $\nu$ and $\lambda$ are constants and the noise $\eta$ depends on position $x$ and height $h$ with the properties of $\langle \eta(x,h) \rangle = 0$ and $\langle \eta(x,h) \eta(x',h') \rangle = 2D \delta(x-x') \delta(h-h')$. The QKPZ equation for $\lambda > 0$ exhibits a PD transition with $\theta \sim 0.64$ [8]. The surface at $F_c$ can be described by the directed percolation (DP) cluster spanned perpendicularly to the surface growth direction in 1+1 dimensions. The roughness exponent $\alpha$ of the interface is given as the ratio of the two correlation length exponents of the DP cluster, that is, $\alpha = \nu_1 \nu_2^{-1} \approx 0.63$ [7,8]. The coefficient $\lambda$ of the nonlinear term renormalizes to $\lambda_c$, which scales as $\lambda_c \sim (F-F_c)^{-\delta}$ ($\delta \sim 0.64$) [9]. This is obtained by measuring the substrate-tilt dependence of the velocity

$$v(F,m) \sim v(F,0) + \frac{\lambda_c}{2} m^2,$$  

(3)

where $m$ is the tilt of the initial substrate.

The origin of the nonlinear term in the QKPZ equation is different from that of the thermal KPZ equation with noise $\eta(x,t)$ [10]. For the quenched case, the nonlinear term is induced by the anisotropic nature of disordered media, while for the thermal case, it is induced by the lateral growth effect and is proportional to the velocity of the interface which vanishes at the threshold of the PD transition [11]. In particular, Tang et al. [10] showed in the context of vortex dynamics that the effective pinning strength takes the form $(\Delta_h + s^2 \Delta_x)^{2/3}(1 + s^2)^{2/3}$ where $s = \partial_x h$ is the local slope and $\Delta_h$ and $\Delta_x$ are the amplitudes of random forces in the $h$ and $x$ directions, respectively. When the medium is anisotropic, $\Delta_h \neq \Delta_x$ in general and the effective pinning strength depends on the local slope and generates the nonlinear term in Eq. (2) with $\lambda \propto (\Delta_h - \Delta_x)$. Therefore when $\Delta_h = \Delta_x$, i.e., when the surface is driven along the easy direction, $\alpha$ is negative.

The negative QKPZ equation, i.e., the QKPZ equation with negative $\lambda$, is studied in [12]. In marked contrast to the $\lambda > 0$ case, the negative QKPZ equation describes a first order transition in the sense that the velocity $v$ shows a discontinuous jump at the PD transition. This is shown in the inset of Fig. 1. At the PD transition, the pinned surface takes the shape of a mountain with a constant slope as shown in Fig. 1. To elucidate the transition mechanism of the negative QKPZ equation, we study in this work the substrate-tilt dependence of the dynamic properties. We performed the direct numerical integration of Eq. (2) in one dimension with the discretized version used in [13,14]:

$$h(x,t+\Delta t) = h(x,t) + \Delta t \left[ h(x-1,t) + h(x+1,t) - 2h(x,t) + \frac{\lambda}{8} \left( h(x+1,t) - h(x-1,t) \right)^2 ight.$$  

$$\left. + F + \xi(x,[h(x,t)]) \right],$$  

(4)

where $[\cdots]$ denotes the integer part, and $\xi$ is uniformly distributed in $[-a/2,a/2]$, where $a = (10)^{2/3}$ is selected. We choose $\Delta t = 0.01$ and use the initial condition $h(x,0) = mx$.
and the helicoidal boundary condition $h(L+i,t)=h(i,t)+Lm$. Numerical results are discussed below in detail.

First, we measure the critical driving force $F_0$ and the facet slope at $m=0$ (no tilt) for several values of $\lambda$. $F_0$ is numerically defined as the value of $F$ at which no surface in the sample of up to 200 configurations is pinned until a large fixed time $t_0=10^8\Delta t$. Just below $F_0$, at least a finite fraction of the ensemble is pinned at $t_0$, showing the facet morphology. The facet slope is determined by sample averages of 100 configurations. Measured values of $F_0$ and $s_c$ are shown in Table I for $\lambda=-0.5,-1,-1.5$, and $-2$. Also shown are $v_0$, the velocity at $F_0$, i.e., the velocity discontinuity at the first order PD transition.

Next, we examine the tilt dependence of the surface growth. In general, one expects that the critical driving force $F_c(m)$ is $m$ dependent with $F_c(0)=F_0$. For small tilts, the first order nature of the PD transition and the morphology of the pinned surfaces at the transition do not change. Moreover, within our numerical accuracies, both the critical driving force and the critical facet slope are independent of the tilt $m$. We find this is so as long as $m$ is less than a critical tilt $m_c$, which is essentially the same as the facet slope $s_c$. That is, $F_c(m<m_c)=F_0$. When $m$ becomes larger than $s_c$, the surfaces at the pinned state cannot form a facet with slope $s_c$ by the helicoidal boundary condition and instead align along the substrate. In this case, the critical driving force $F_c(m)$ has to increase with $m$ to compensate for the tilt force. The schematic phase diagram in the $F-m$ plane is shown in Fig. 2(a). The positively moving phase is bounded by a horizontal line at $F=F_0$ for $m<m_c$ and a smooth curve $F_c(m)$ for $m>m_c$. The transition to the $v<0$ phase [the lower curve in Fig. 2(a)] is the continuous PD transition of the directed percolation universality class [9,10]. This region is better understood by rewriting the QKPZ equation in terms of $h’=-h$ as

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$F_0$</th>
<th>$s_c$</th>
<th>$v_0$</th>
<th>$\lambda_c^*$</th>
<th>$m_c^*$</th>
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<tr>
<td>$-0.5$</td>
<td>1.91</td>
<td>2.08</td>
<td>1.20</td>
<td>$-0.62$</td>
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<td>2.06</td>
<td>1.40</td>
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<td>$-1.52$</td>
<td>1.39</td>
</tr>
<tr>
<td>$-2.0$</td>
<td>2.09</td>
<td>1.26</td>
<td>1.42</td>
<td>$-1.89$</td>
<td>1.24</td>
</tr>
</tbody>
</table>
\[ \partial_t h' = v \partial_x^2 h' - \frac{\lambda}{2} (\partial_x h')^2 - F + \eta(x, h'). \]  

The above equation implies that the negative QKPZ equation with negative \( F \) is equivalent to the positive QKPZ equation with positive \( F \) and vice versa. The negative velocity phase in the \( F > 0 \) region of Fig. 2(a) can be understood as a result of the positive QKPZ equation driven by a negative force which is not strong enough to overcome the effect of the positively driving nonlinear term. We confine our discussion to the upper curve of Fig. 2(a) below.

A typical data set for the velocity as a function of \( F \) and \( m \) in the positively moving phase is shown in Fig. 2(b), while Fig. 2(c) shows a three dimensional plot of \( v \) versus \( F \) and \( m \). At \( F = F_0 \) and for \( m < m_c \), \( v \) exhibits a discontinuous jump by \( \delta v(m) \). The lowest data in Fig. 2(b) shows this. Since \( \delta v(m) \) vanishes at \( m = m_c \), the point \( (F=F_0, m=m_c) \) may be regarded as a tricritical point in analogy with the equilibrium critical phenomena. Following [9], we measure \( \lambda_c \) by fitting the curves \( v(F, m) \) to Eq. (3) for small \( m \). Since it is insensitive to \( F \), we define \( \lambda_c \) as that obtained from \( F = F_0 \):

\[ \delta v(m) = v(F_0, m) = v_0 - \frac{|\lambda_c|}{2} m^2 + \ldots. \]  

The fifth column of Table I shows \( \lambda_c \). For \( F \) larger than but close to \( F_0, v(F, 0) \) is linear in \( F \). This together with Eq. (6) allows one to approximate \( v(F, m) \) as

\[ v(F, m) = v_0 + A(F - F_0) - \frac{|\lambda_c|}{2} m^2 + \ldots, \]  

where \( A \) is a constant. Setting \( v = 0 \) in Eq. (7), one obtains an approximate form for \( F_c(m) \) as

\[ F_c(m) = F_0 + \frac{|\lambda_c|}{2A} (m^2 - m_c^2), \]  

with \( m_c = (2v_0/|\lambda_c|)^{1/2} \). However, for larger \( m, v \) deviates from Eq. (7) and higher order terms in \( m \) become significant. To find \( F_c(m) \) and \( m_c \) more accurately, we fit the velocity curve for large \( m \) and estimate \( F_c(m) \) independently from the condition of \( v(F, m) = 0 \). This is justified since \( \theta = 1 \) generically for \( m \neq 0 \) [10]. In Fig. 3(a) we show the values of \( F_c(m) \) obtained in this way. The relation \( F_c(m_c) = F_0 \) then gives an independent estimate of \( m_c \), which is also shown in Table I. Note that \( m_c \) obtained in this way agrees well with the facet slope \( s_c \) as mentioned above. The value of \( m_c \) itself strongly depends on \( \lambda \) and could be fitted to a power law as \( m_c \sim |\lambda|^{-0.37} \) as shown in Fig. 3(b). Thus when \( \lambda = 0 \), \( m_c \) becomes infinite, which recovers the previous result that the critical force \( F_c(0) \) is independent of the substrate tilt in the quenched Edwards-Wilkinson universality class [9,10]. On the other hand, \( |\lambda_c| \) scales as \( |\lambda|^{0.8} \) in the inset of Fig. 3(b) and hence \( m_c \sim |\lambda|^{-0.37} |\lambda_c|^{0.46} \). This is to be compared with the zeroth order expression \( m_c \sim |\lambda|^{-0.5} \) in Eq. (8).

In order to understand the origin of the discontinuous PD transition for \( \lambda < 0 \), we examine the noise distribution on the perimeter sites of critically pinned surfaces. It is found that the noise strengths around the site at the valley in Fig. 1 are relatively small, corresponding to large pinning strengths. Meanwhile, when \( \lambda \ll 0 \), surfaces tend to form a flat facet to make the term \( (\lambda/2)(\partial_x h')^2 \) negatively large, leading to a large pinning strength. However, the curvature force \( \nabla^2 h \) is almost zero on the hillside, but is positive at the valley. Thus the sites around the valley are pinned by balancing the driving forces due to the curvature and the external force \( F \) with the pinning forces due to the noise and the nonlinear term. Once the sites around the valley are pinned, the stable slope \( s_c \) of the facet is selected in a self-organized way: Suppose that a surface is formed with a facet of slope \( s < s_c \). Then the velocity of the sites on the hillside would be positive according to Fig. 2(b). The pinning strength due to \( \lambda/2s^2 \) is not strong enough to resist the external force, and the sites on the hillside move upward, and tend to make the slope of the facet larger. When the slope becomes larger than \( s_c \), however, the nonlinear term is too strong, and the sites on the hillside move downward, reducing the slope. Thus the slope \( s_c \) becomes stable, and surfaces form a facet with the slope \( s_c \) as shown in Fig. 1. Since the surface pinning is initiated at the sites around the valley, once the pinning site is broken by an external force which is slightly bigger than \( F_0 \), the surface grows with a finite velocity, leading to the first order transition. On the other hand, when \( \lambda > 0 \), the nonlinear term is positive, and enhances the external driving force. Thus surfaces do not form a facet. The surface pinning is mainly due to local noise strengths as can be pictured in the DP cluster. Thus the pinned sites are not localized but scattered all over the system, so that the PD transition is continuous.

It would be interesting to observe the tilt dependence of the negative quenched KPZ equation from a stochastic.

![FIG. 3. (a) The depinning critical \( F_c(m) \) versus the substrate tilt \( m \) for several values of \( \lambda \). (b) Estimated numerical data for the critical tilt \( m_c \) versus \( \lambda \). The broken line \( m_c \sim |\lambda|^{-0.37} \) is a least squares fit. Inset: The \( \lambda \) dependence of \( \lambda_c \) showing \( |\lambda| \sim |\lambda_c|^{0.8} \).](Image 336x469 to 540x733)
model. The Sneppen A model [12,15] is known to belong to the negative QKPZ universality class. In the Sneppen A model, the restricted solid-on-solid (RSOS) condition is imposed on the height difference of neighboring columns. Because of this restriction, the surface tilt cannot be larger than a maximum value. If the maximum tilt is less than the critical slope \( s_c(\lambda) \) of the stochastic model, the tricritical behavior would not be observed in simulations because the coefficient \( \lambda \) is not controllable. Recently a PD transition similar to the negative QKPZ equation is found in a seemingly different system, the driven Frenkel-Kontorova model [16], where the PD transition is also discontinuous and the displacement at the pinned state looks like Fig. 1. However, the tricritical behavior has not been studied yet in this system.

In summary, we have investigated the tilt-dependent behavior of the negative quenched QKPZ equation. We observed and explained that there exists a characteristic substrate tilt \( m_c \) such that the PD transition is discontinuous when the substrate tilt \( m \) is less (greater) than \( m_c \). The characteristic tilt \( m_c \) is found to be the same as the facet slope \( s_2 \) of the critically pinned surfaces which are formed in a self-organized way and depends on the nonlinear term coefficient \( \lambda \) as \( m_c \sim |\lambda|^{-0.37} \). Moreover, the threshold force \( F_c(m) \) for the PD transition is independent of \( m \) for \( m \leq m_c \) and increases with increasing \( m > m_c \). The effective nonlinear term coefficient \( \lambda \) remains finite as \( F \) approaches \( F_0 \).

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