Near-equilibrium dynamics of crystalline interfaces with long-range interactions in (1+1)-dimensional systems

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The dynamics of a one-dimensional crystalline interface model with long-range interactions is investigated. In the absence of randomness, the linear response mobility decreases to zero when the temperature approaches the roughening transition from above, in contrast to a finite jump at the critical point in the Kosterlitz-Thouless transition. In the presence of substrate disorder, there exists a phase transition into a low-temperature pinning phase with a continuously varying dynamic exponent z>1. The expressions for the nonlinear response mobility of a crystalline interface in both cases are also derived.

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Various deposition growth models of interfaces have been investigated intensively in recent years [1,2]. The main interest of these studies stems from both practical applications and theoretical inquiries. The profile of a surface develops roughness gradually as the stochastically deposited particles accumulate. The primary features of interface growth are their nontrivial temporal and spatial scaling behavior. The scaling properties are manifested in the surface width [2]:

$$w(L,t) \sim L^{\alpha} f(t/L^{\alpha/\beta}),$$
 (1)

where L is the lateral size of the system, the scaling function $f(x) \sim x^{\beta}$ for $x \ll 1$, and $f(x) \to \text{const}$ for $x \gg 1$. The scaling behaviors are characterized by the roughness exponent α , and the exponent β . α features the long-time limit of the self-affine fractal structure as represented by the surface width $w(L,t) \sim L^{\alpha}$. At an early stage of growth, the surface width w(L,t) scales as t^{β} , where $\beta = \alpha/z$ and z is the dynamic exponent.

The discreteness of a lattice is an indispensable ingredient in either experiments or computer simulations. As is known, due to this effect the crystalline two-dimensional (2D) surface undergoes a roughening transition at a finite temperature. Such transitions of various systems have been observed experimentally in plastic and metal crystals. The theoretical understanding of this behavior is based on the discrete Gaussian solid-on-solid model (DGSOS) [1,3,4], in which the surface elastic energy is assumed to arise from the interactions between nearest neighbor atoms in a crystal. In addition, the periodic potential is introduced to account for the lattice discreteness.

One-dimensional systems with only short-range interactions should not have a phase transition. As a result, the DGSOS model in (1+1) dimensions does not exhibit a roughening transition [5]. However, in nature there exist various kinds of long-range interactions between atoms, such as the van der Waals force or the effective force due to bulk strain [6]. The general form of interactions is found to scale as some power law with the distance between atoms.

In view of this possibility, we consider a particular type of surface energy due to the long-range interactions between atoms in a crystal [6,7]. This model could be realized in vicinal surfaces whose steps are flat along one fixed direc-

tion. Here, we shall investigate the static and dynamic properties of a crystalline interface which undergoes the roughening transition in one dimension. Although qualitatively similar to the Kosterlitz-Thouless transition of the (2+1)-dimensional surface, the (1+1)-dimensional case exhibits different critical behaviors.

The 2D DGSOS model with bulk or substrate disorder has been investigated recently [8–10]. The disorder was found to have nontrivial effects on both the dynamical and static properties of the crystalline surface. The renormalization group (RG) analysis predicts a so-called superroughening transition. The low-temperature phase is dominated by disorder, and displays glassy behavior, identical to the vortex glass phase found in two-dimensional dirty type-II superconductors [11–14]. Here we shall incorporate the same type of disorder into the 1D interface with the elastic energy due to long-range interactions.

The motivation of this study is twofold. First, we would like to investigate the behavior of an interface with the elastic energy arising from long-range interactions in two different environments—pure and disordered. Secondly, current computer simulations of a 2D interface subject to quenched disorder are limited to modest spatial and temporal scales, and the present model could be used to probe more effectively the hydrodynamic limit.

The elastic energy of the interface caused by the long-range interactions [6,7] considered here is

$$\mathcal{H}_{0} = \frac{\rho}{2T} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \left[\frac{h(x) - h(x')}{x - x'} \right]^{2}$$
$$= \frac{K}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} |p| h(p) h(-p), \tag{2}$$

where h(x) is the height of the interface at position x, and ρ is the strength characterizing the elastic energy due to long-range interactions between atoms. The temperature T has been absorbed into the Hamiltonian \mathcal{H}_0 , and $K = 2\pi\rho/T$. Power counting shows that surface energy due to short-range interactions $\int dx (dh/dx)^2$ is irrelevant. Therefore we will not take it into account here.

The periodic potential inherited from the discrete nature of the lattice is given by

$$\mathcal{H}_{p} = \frac{\alpha}{a} \int_{-\infty}^{\infty} dx \cos[\gamma h(x)], \tag{3}$$

where α/a is the coefficient of the leading term due to the discreteness, and $\gamma=2\,\pi/b$ with a and b being lattice constants along and perpendicular to the base line, respectively. With this potential, the height of a surface should be regarded as a continuous variable within the interval $(-\infty,\infty)$. As in the DGSOS model, the higher harmonics are irrelevant near the critical point and can therefore be neglected.

The action in Eq. (2) can also describe a variety of systems with quantum dissipations. A particular case is the electronic system involving a quantum wire with one impurity scattering center [15]. The Euclidean action of the electron at the impurity center is equivalent to the sum of Eq. (2) and Eq. (3).

The dynamics of interface growth considered here is governed by [3,4,16]

$$\frac{\partial h(x,t)}{\partial t} = \mu F - \mu \frac{\delta \mathcal{H}}{\delta h} + \eta(x,t), \tag{4}$$

where t is time, F is the driving force, μ is the mobility, and \mathcal{H} is the sum of \mathcal{H}_0 and \mathcal{H}_p . η is the thermal noise which obeys $\langle \eta(x_1,t_1)\eta(x_2,t_2)\rangle = 2\mu\delta(x_1-x_2)\delta(t_1-t_2)$, where the coefficient 2μ is chosen such that the system will reach the equilibrium states weighted by the Boltzmann factor $e^{-(\mathcal{H}_0+\mathcal{H}_p)}$. Consequently the fluctuation-dissipation theorem [17] will hold here in contrast to the case of far-from-equilibrium surface growth [18], which cannot be formalized by Eq. (4).

To facilitate the analysis of Eq. (4) we employ the formalism of Martin, Siggia, and Rose (MSR) [19,20]. In addition to h(x,t), the auxiliary field $\tilde{h}(x,t)$ is introduced as well as their conjugate source J(x,t) and $\tilde{J}(x,t)$. Upon averaging over the thermal noise the associated generating functional is obtained:

$$Z[J,\tilde{J}] = \int \mathcal{D}h \mathcal{D}\tilde{h} e^{\mathcal{S}_{\text{eff}}} = \int \mathcal{D}h \mathcal{D}\tilde{h} e^{\mathcal{S}_0 + \mathcal{S}_{\text{int}}}, \qquad (5)$$

where the effective MSR action \mathcal{S}_{eff} takes the form

$$\mathcal{S}_{0} = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} dt \left| Jh + \tilde{J}\tilde{h} + \mu \tilde{h}(p,t)\tilde{h}(-p,t) - \tilde{h}(-p,t) \right|$$

$$\times \left[\frac{\partial}{\partial t} h(p,t) - K\mu |p| h(p,t) \right] \right\}, \tag{6}$$

$$\mathcal{S}_{\text{int}} = -\frac{\mu \gamma \alpha}{a} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt \tilde{h}(x, t) \sin[\gamma h(x, t)]. \tag{7}$$

Here Eq. (5) will be treated by the RG technique. To perform the RG calculation, we follow the schemes of Amit *et al.* [21] and Neudecker [16]. Regularization of the Feynman integrals is established by introducing the infrared cutoff M and ultraviolet cutoff a into the free correlation function

$$C_0(x,t) = \langle h(x,t)h(0,0)\rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{1}{K|p|+M} e^{-\mu(K|p|+M)|t|} e^{-ipy}$$

with $y^2 = x^2 + a^2$.

In the absence of the periodic potential, the (1+1)-dimensional interface width scales as [22]

$$w^2(L,t) \sim \frac{\mu}{K} \ln \left[\frac{L}{a} f\left(K \frac{t}{L}\right) \right],$$
 (8)

where *L* is the linear size of the system, and the scaling function $\ln f(x) = -\ln 2 + \text{Ei}(4\pi x)$ with $\text{Ei}(-y) = -\int_{v}^{\infty} du (e^{-u}/u)$.

(i) Roughening transition in (1+1)-dimensional systems. To analyze Eq. (5) we calculate the perturbative correction to several vertex functions up to the lowest order in $\tau=1-(\gamma^2/2\pi K)$ and the second order in α , and use the minimal subtraction and the standard prescription to obtain the flow equations of various parameters [17,23] (details of the calculation will be published elsewhere).

Under rescaling factors $x \rightarrow e^{l}x$ and $t \rightarrow te^{lz}$ ($l = \ln y$ where y is the rescaling factor), the RG recursion relations of various parameters are given by

$$\frac{dK}{dl} = 0, (9)$$

$$\frac{dF}{dI} = F,\tag{10}$$

$$\frac{d\alpha}{dl} = \left(1 - \frac{\gamma^2}{2\pi K}\right)\alpha + O(\alpha^3),\tag{11}$$

$$\frac{d\mu}{dl} = \left[z - 1 - (\pi\alpha)^2\right]\mu. \tag{12}$$

We first discuss static properties. Equation (9) holds true for all orders of α , since there are no counterterms proportional to |p| in any order. Note that under the RG transformation only the terms proportional to powers of p, i.e., local in space, can be generated. Nonrenormalization of K is also justified by using the real space RG calculation [15]. On the other hand, in the case of a 2D crystalline interface the surface tension does suffer renormalization. As shown in Eq. (11) the sign of $\tau = 1 - (\gamma^2/2\pi K) = 1 - (T/T_c)$ determines the fate of coupling constant α , where $T_c = b^2 \rho$. When $\tau < 0$ or $T > T_c$, the flow of α under the RG transformation was driven to zero, and thus the lattice effect can be neglected. In the long-wavelength limit, the surface width $w(L,t=\infty)$ scales as $(\ln L)^{1/2}$, as implied from Eq. (8). On the other side of the transition $(T < T_c)$, as argued in Ref. [7], under the RG iteration coupling constant α flows to infinity. On a sufficiently large length scale, a mass term generated by the cosine term will dominate over the surface energy strength K. The interface is pinned at the minima of the periodic potential, and is led to a flat phase as also occurs in (2+1)-dimensional systems. Although there is no fixed point of α for $\tau > 0$, $\alpha(l) = \alpha(0)e^{\tau l}$ should hold as long as $l \ll 1/\tau = l_D$.

Next we turn to the dynamical properties of the interface in both phases. To facilitate the discussion, we give the expression of μ on the length scale l by integrating Eq. (11) and Eq. (12):

$$\mu(l) = \mu(0)e^{-[\pi^2\alpha(0)^2/2\tau](e^{2\tau l} - 1)}.$$
 (13)

The linear response mobility (as $F \rightarrow 0$) can be obtained by letting $l = \infty$ in Eq. (13). We find

$$\mu_M = \mu(0) e^{\pi^2 \alpha(0)^2 / 2\tau} \tag{14}$$

for τ <0 and μ_M =0 for τ >0. Here the parameters followed by (0) represent the corresponding bare values. In contrast to the roughening transition in the (2+1)-dimensional case, the linear response mobility decreases to zero as the temperature approaches the transition point from above. The higher order correction will not change this behavior qualitatively. In the case that the applied force F is finite, the movement of an interface is characterized by the nonlinear response mobility. Since F is a relevant field, on some sufficiently large length scale $l^* \sim -\ln F$, it will grow significantly. The pinning effect will be wiped out by the motion of an interface. Beyond this scale, the effect of the strength α , on the average, can be neglected. The mobility μ will scale normally, and its canonical dimension is zero. Consequently, the nonlinear response mobility is yielded by stopping the RG iteration up to this scale:

$$\mu(l^* \sim -\ln F) \sim \mu(0) \exp\left[-\frac{C}{\tau F^{2\tau}}\right], \quad \tau > 0 \quad (15)$$

where C is a constant depending on bare values of other parameters. Meanwhile l^* should be less than l_D , i.e., $-\ln F < 1/\tau$. Such a form of nonlinear response has been of interest in statics of the vortex glass phase of type-II superconductors. Here we see it can arise even in pure systems.

In the region far below the transition point the results presented here in general will not hold. However, one can resort to the activated-dynamics mechanism.

(ii) Depinning transition in (1+1) dimensions. Crystalline surface growth with bulk disorder or two-dimensional substrate disorder has been addressed recently. Here we shall study the dynamics of a (1+1)-dimensional interface with elastic energy in Eq. (2) subjected to substrate disorder.

In the presence of substrate disorder, the periodic potential [9] changes to

$$\mathcal{H}_{dis} = \frac{\alpha}{a} \int dx \cos\{\gamma [h(x) + d(x)]\}, \tag{16}$$

where d(x) is the quenched fluctuation of the substrate height uniformly distributed within the lattice spacing b. The correlation of d(x) under question is presumed to be of short range within lattice spacing a. In terms of the phaselike variable $\theta(x) = \gamma d(x)$, we assume

$$\langle e^{i\theta(x)}\rangle = 0,$$
 (17)

$$\langle e^{i\theta(x)}e^{-i\theta(x')}\rangle = a\,\delta(x-x').$$
 (18)

As can be seen in Eq. (17), substrate disorder acts to destroy the structure of a regular lattice, thereby eliminating

the roughening transition. However, as we show below, the correlation of disorder will lead to a new term which is relevant at lower temperatures.

After averaging over disorder θ , the corresponding MSR action becomes

$$S_{\text{int}} = \frac{\mu^2 g \gamma^2}{2a} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \tilde{h}(x,t) \tilde{h}(x,t')$$

$$\times \cos[\gamma h(x,t) - \gamma h(x,t')], \qquad (19)$$

where $g(0) = \alpha^2(0)/2$, and again higher harmonics are discarded.

Now we apply the RG analysis to the MSR action combining Eq. (6) and Eq. (19) in the same spirit as we did in the previous case. For the present theory the expansion parameters are $\tau' = 1 - (\gamma^2/K\pi)$ and g. We derive the recursion relations for $x \rightarrow xe^l$ and $t \rightarrow te^{lz}$ as follows:

$$\frac{dK}{dl} = 0, (20)$$

$$\frac{dF}{dl} = F,\tag{21}$$

$$\frac{dg}{dl} = \left(1 - \frac{\gamma^2}{K\pi}\right)g - 2g^2,\tag{22}$$

$$\frac{d\mu}{dl} = (z - 1 - \pi g)\mu. \tag{23}$$

As inferred from Eq. (22) above, the transition point is $T_{pc} = b^2 \rho/2$, i.e., $\tau' = 1 - (T/T_{pc}) < 0$. The coupling constant g pertaining to disorder flows to zero under the RG transformation. Below T_{pc} , g flows to a non-Gaussian fixed point $g^* = \tau'/2$.

As with the previous case, we first discuss the static properties. In the high-temperature phase, disorder is irrelevant and the surface width (or static height-height correlation function) is $w(L,t=\infty) \sim (\ln L)^{1/2}$. In contrast to the random DGSOS model, the marginal time-persistent parts [24–26] such as $\int \int \int dp dt dt' |p| \tilde{h}(p,t) \tilde{h}(-p,t')$ are not generated, since the term proportional to |p| is spatially nonlocal. The form of the static correlation function will rely on the existence of such a term, as in the 2D case. Near the transition point the height-height correlation functions of two phases will not be of any difference in contrast to the 2D random DGSOS model.

Next we turn to the dynamical properties. Above T_{pc} , $z\!=\!1$, and the linear response mobility remains finite and decreases to zero as the temperature approaches the transition point. The integration of the RG recursion relations gives the expression of the mobility at the scale l:

$$\mu(l) = \mu(0) \left[1 + \frac{2g(0)}{\tau'} (e^{\tau' l} - 1) \right]^{-\pi/2}$$
 (24)

and yields the linear response mobility:

$$\mu_M = \mu_0 \frac{|\tau'|^{\pi/2}}{[2g(0)]^{\pi/2}} \quad \text{as} \quad \tau' \to 0^+.$$
 (25)

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Below T_{pc} , due to the existence of an infrared stable fixed point g^* , the dynamic exponent z assumes a nontrivial value $1 + (\pi/2)[1 - (T/T_{pc})]$. The linear response mobility vanishes below T_{pc} .

Along the same line that we used to derive Eq. (15), the nonlinear response mobility below T_{pc} is given by

$$\mu \sim \mu(0) F^{(\pi/2)|\tau'|}$$
 (26)

to leading order in τ' .

The physical implications of the RG analysis in the low-temperature phase are the following: Unlike the case of the 2D interface, the time-persistent term in the 1D case is not generated under the RG transformation. Physically the interface with long-range interactions cannot afford costly elastic energy to adjust itself to follow the short-range correlated substrate disorder. In the low-temperature phase of the (2+1) random DGSOS model, the surface does follow disorder. In the present case, disorder is also relevant in the low-temperature phase. In the presence of a force, the traveling interface on the average is attractive to the local minima of the random periodic potential. This implies a larger dynamic exponent and a smaller mobility in the low-temperature phase than in the other phase.

It is straightforward to extend the calculations for the long-range elastic energy with other powers in the denominator of Eq. (2). The behaviors found are generic to systems with long-range interactions. The qualitative difference between systems with short- and long-range interactions is attributed to whether or not the interactions are renormalized.

In conclusion, we have investigated the dynamics of a (1+1)-dimensional crystalline interface with long-range interactions. The governing equation is cast in terms of the MSR formalism and is analyzed by using the RG technique. In the presence of a regular lattice, above T_c , the interface width is $w(L,t) \sim \{\ln[Lf(t/L)]\}^{1/2}$, and the linear response mobility is $\mu_M = \mu(0)e^{\pi^2\alpha(0)^2/2\tau}$. Below T_c the interface is flat. The nonlinear mobility is $\mu \sim \mu(0) \exp[-C/\tau F^{2\tau}]$.

In the presence of substrate disorder, above T_{pc} the interface width is $w(L,t) \sim \{\ln[Lf(t/L)]\}^{1/2}$. Below T_{pc} , the surface width is $w(L,t) \sim \{\ln[Lf(t/L^z)]\}^{1/2}$ with $z=1+(\pi/2)[1-(T/T_{pc})]$. The expression of the nonlinear mobility is also obtained for the disordered case.

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