Effect of long-range interactions in the conserved Kardar-Parisi-Zhang equation

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The conserved Kardar-Parisi-Zhang equation in the presence of long-range nonlinear interactions is studied by the dynamic renormalization-group method. The long-range effect produces new fixed points with continuously varying exponents and gives distinct phase transitions, depending on both the long-range interaction strength and the substrate dimension d. The long-range interaction makes the surface width less rough than that of the short-range interaction. In particular, the surface becomes a smooth one with a negative roughness exponent at the physical dimension $d=2$. [S1063-651X(98)02011-X]

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For the past decade the kinetic roughening of surfaces has attracted much interest [1]. The recent studies concentrate on measuring the scaling exponents that characterize the asymptotic behavior of the surface roughness on a large length scale and in a long time limit and finding the continuum equations. The problem of a rough surface not only is of practical importance in crystal growth, but also is related to the nonequilibrium statistical physics. Many computer simulations and theoretical approaches have been applied in the studies of the Kardar-Parisi-Zhang (KPZ) [2] equation and discrete molecular-beam-epitaxy growth models with various kinds of noise [3–7]. Among them, the Eden model [8], ballistic deposition [9], and the restricted solid-on-solid growth model [10] have been identified as a universality class corresponding to the KPZ equation for the coarse-grained height variable $h(\mathbf{r},t)$, which describes the surface as a function of coordinate $\mathbf{r}$ and time t. The KPZ equation has a nonlinear term of short range describing the lateral growth. However, there is poor agreement between the KPZ equation and the experimental data.

Recently, Mukherji and Bhattacharjee [11] proposed a phenomenological equation in the presence of long-range interactions to describe the kinetic roughening of the surface growth. The long-range effect of the nonlinear term in the KPZ equation is introduced by coupling the gradients at two different points. The roughness of the surface is found to depend on the long-range nature and several distinct phase transitions are observed. The long-range interactions decaying slower than $1/r^d$ (d is the substrate dimension) makes the KPZ fixed point with the short-range interaction be unstable. The surface then has the long-range roughness with different exponents depending on the power law of the long-range interactions. Other interactions decaying faster than $1/r^d$ are suppressed by the local interaction yielding the ordinary KPZ universality class.

In the kinetic roughening problems, the universality class of the dynamic systems depends on the symmetry of the order parameter, the dimensionality of space, and the conservation of the surface currents. Therefore, it would be interesting to examine how the long-range interaction in the conserved growth equation affects the roughness of the surface. Lauritsen [12] introduced a growth kernel equation (GKE) with a generalized conservation law described by an integral kernel. It describes the nonlocal interactions with the KPZ equation. Here we extend the phenomenological equation of Mukherji and Bhattacharjee to the conserved growth equation

$$\frac{\partial h(\mathbf{r},t)}{\partial t}=-K\nabla^4 h(\mathbf{r},t)+\eta_c(\mathbf{r},t)-\frac{1}{2}\nabla^2\int d\mathbf{r}'\,\vartheta(\mathbf{r}')\times\boldsymbol{\nabla}h(\mathbf{r}+\mathbf{r}',t)\cdot\boldsymbol{\nabla}h(\mathbf{r}-\mathbf{r}',t), \tag{1}$$

where $h(\mathbf{r},t)$, assumed to be a single-valued function of position $\mathbf{r}$, describes the height of the surface. The parameter K is a constant and η_c is a conserved random noise of zero mean with $\langle\eta_c(\mathbf{r},t)\eta_c(\mathbf{r}',t')\rangle=-2D_c\nabla^2\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$. Since the right-hand side of Eq. (1) can be written as the divergence of a current, the total volume under the surface is conserved. The kernel $\vartheta(\mathbf{r})$ includes long-range part that is connected to the underlying interactions. As in Ref. [11], we take $\vartheta(\mathbf{r})$ to have a short-range (SR) part $\lambda_0\delta(\mathbf{r})$ and a long-range (LR) part $\sim r^{\rho-d}$ or more precisely, in Fourier space, $\vartheta(\mathbf{k})=\lambda_0+\lambda_\rho k^{-\rho}$. Both Eq. (1) and the GKE have the conservation law and the long-range interaction in common. The GKE contains the KPZ equation with the generalized kernel. However, Eq. (1) has the nonlinear term with the long-range interaction as coupling the gradients at two different points. It takes into account with both the short-range part and the long-range part.

The surface width $W(L,t)$ can be described by the dynamical scaling form $W(L,t)=L^\chi F(t/L^z)$, where L, χ, z, and F are the system size, the roughness exponent, the dynamic exponent, and the scaling function, respectively. For $\lambda_0=\lambda_\rho=0$, it becomes a linear equation evolving with the conservative surface diffusion, where the roughness exponent χ is $(2-d)/2$ and the dynamic exponent $z=4$. For the physical dimension $d=2$, $\chi=0$; thus the surface width is logarithmically rough as a function of system size L. Above

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two dimensions the linear equation with the conservative noise produces a negative roughness exponent, implying a smooth surface [13]. For $\lambda_\rho=0$ and $\lambda_0\neq0$, Eq. (1) becomes the conserved KPZ equation with a conservative noise [called the Sun-Guo-Grant (SGG) equation [7,14]], where the average height remains constant. For this local conserved growth equation, the dynamic renormalization-group (RG) calculation shows $\chi=(2-d)/3$ and $z=(10+d)/3$ [7]. For $d\geqslant2$, the nonlinear term is irrelevant and then the exponents are given by the linear theory with both λ_0 and λ_ρ being zero in Eq. (1). Here we show that a long-range part ($\lambda_\rho\neq0$) gives a new fixed point with continuously varying exponents and thus yields distinct phase transitions depending on both the parameter ρ of the long-range interactions and the substrate dimension d. This nonlocal λ_ρ term with positive ρ makes the surface less rough than in the case of $\lambda_\rho=0$. In particular, at the physical dimension $d=2$, the surface becomes a smooth phase with a negative roughness exponent rather than a logarithmically rough phase as in the SGG case.

Under the change of scale, the parameters in Eq. (1) make the changes $K\to b^{z-4}K$, $D_c\to b^{z-2\chi-d-2}D_c$, $\lambda_0\to b^{z+\chi-4}\lambda_0$, and $\lambda_\rho\to b^{z+\chi+\rho-4}\lambda_\rho$. In the absence of nonlinearity ($\lambda_0=\lambda_\rho=0$), K and D_c are scale invariant to yield $z_0=4$ and $\chi_0=(2-d)/2$. Using these values we find that the nonlinearities rescales as $\lambda_0\to b^{(2-d)/2}\lambda_0$ and $\lambda_\rho\to b^{(2+2\rho-d)}\lambda_\rho$. Thus the critical dimensions are given by $d_c=2+2\rho$ $(\rho>0)$ and $d_c=2$ $(\rho<0)$ for any nonzero λ_ρ. When $\rho>0$, if $d<d_c=2+2\rho$, the fixed point of the local interaction ($\lambda_\rho=0$, $\lambda_0\neq0$, and $z+\chi-4=0$) is unstable and thus a new fixed point is expected. If $2+2\rho\leqslant d$, the nonlinearities become irrelevant and the surface is controlled by the linear equation. For $\rho<0$, if $d<2$, the SGG fixed point is stable so that λ_0 is relevant rather than λ_ρ; otherwise the linear term is relevant. As a result, various phase diagrams depending on d and ρ appear.

Following a dynamic RG procedure [4,15], integrating out fast modes in the momentum shell $e^{-\ell}\Lambda\leqslant|\mathbf{k}|\leqslant\Lambda$ and performing the rescalings $r\to br$, $t\to b^z t$, and $h\to b^\chi h$, we derive the following flow equations for the coefficients, in a one-loop approximation:

$$\frac{dK}{d\ell}=K\left(z-4-\frac{D_cB_d}{K^3}\,\vartheta(1)\frac{d-4+3f(1)}{4d}\right), \tag{2}$$

$$\frac{dD_c}{d\ell}=D_c(z-2\chi-d-2), \tag{3}$$

$$\frac{d\lambda_0}{d\ell}=\lambda_0(z+\chi-4), \tag{4}$$

$$\frac{d\lambda_\rho}{d\ell}=\lambda_\rho(z+\chi-4+\rho), \tag{5}$$

where $f(a)=\partial\ln\vartheta(k)/\partial\ln k|_{k=a}$ and $B_d=S_d/(2\pi)^d$, S_d being the surface area of a d-dimensional unit sphere. Since the diagrams contributing to D_c have prefactors proportional to k^4, they correspond to higher derivatives in the original noise spectrum. Note that two scaling relations $z+\chi=4$ and $z+\chi=4-\rho$, which result from the nonrenormalization of λ_0 and λ_ρ in Eqs. (4) and (5), respectively, are the results of a one-loop approximation [16].

Defining the dimensionless parameters $U_0^2\equiv(D_c\lambda_0^2B_d)/K^3$, $U_\rho^2\equiv(D_c\lambda_\rho^2B_d)/K^3$, and $R=U_0/U_\rho$, we obtain the flow equations for U_0, U_ρ, and R:

$$\frac{dU_0}{d\ell}=U_0\left[\frac{2-d}{2}+\frac{3(d-4)}{8d}U_0^2+\frac{3U_\rho}{8d}(c_0U_0+c_1U_\rho)\right], \tag{6}$$

$$\frac{dU_\rho}{d\ell}=U_\rho\left[\frac{2-d+2\rho}{2}+\frac{3(d-4)}{8d}U_0^2+\frac{3U_\rho}{8d}(c_0U_0+c_1U_\rho)\right], \tag{7}$$

and $dR/d\ell=-\rho R$, where $c_0=(d-4)2^{-\rho}+d-4-3\rho$ and $c_1=(d-4-3\rho)2^{-\rho}$. The equation for R rules out the existence of any off-axis fixed point in the U_0 and U_ρ parameter space (except for $\rho=0$). From these equations we find that there are only two sets of axial fixed points in the two dimensional (U_0,U_ρ) space: for the short range, $(U_0^{*2}=4d(d-2)/3(d-4),U_\rho^{*2}=0)$, with $\chi+z=4$, and for the long range, $(U_0^{*2}=0,U_\rho^{*2}=4d(d-2-2\rho)/3(d-4-3\rho)2^{-\rho})$, with $\chi+z=4-\rho$. When $U_\rho=0$, the SR fixed point is stable for $d<2$, where $\chi=(2-d)/3$ and $z=(10+d)/3$, in agreement with the results of Sun, Guo, and Grant [7]. For $d\geqslant2$, U_0 is driven to zero as $\ell\to\infty$. The surface width is thus described by the linear equation yielding a smooth phase except for $d=2$ (logarithmically rough phase). Similarly, from Eq. (7) with $U_0=0$, the LR fixed point for $d<2+2\rho$ is stable. At this new LR fixed point, the exponents are given by

$$\chi=(2-d-\rho)/3,\quad z=(10+d-2\rho)/3. \tag{8}$$

These exponents are determined by Eqs. (3) and (5) in which D_c and λ_ρ are not renormalized in a one-loop approximation ($z-2\chi-d-2=0$ and $z+\chi=4-\rho$, respectively).

From these recursion relations, we can discuss the surface morphologies and the phase transitions for all d's and ρ's (see Fig. 1). Note that Eq. (1) is invariant under the $h\to-h$ and $\lambda\to-\lambda$ transforms. Therefore, we consider both positive and negative values of U_ρ and take $U_0\geqslant0$ without any loss in generality. As shown in Fig. 1, there are various (U_ρ,U_0) phase diagrams depending on the dimensionality d and the long-range interaction parameter ρ. We explain the phase diagrams in detail.

(i) $\rho>0$. The effective nonlinearity U_ρ is dominant over U_0; thus the phase in all space (U_ρ,U_0) except for $U_\rho=0$ is determined by the long-range λ_ρ term in Eq. (1). For $d<2-\rho$, the LR fixed point is stable and the surface is the LR rough phase with the positive roughness exponent (we call it the LR rough phase) given by Eq. (8). If $U_\rho=0$, the SR rough phase with the positive roughness exponent [$\chi=(2-d)/3$, we call it the SR rough phase] exists such that a phase transition takes place between two LR rough phases when the sign of U_ρ is changed. The critical behavior ($U_\rho=0$) follows the SGG nonlinear equation with the SR rough phase. For $d=2-\rho$, the surface is the logarithmically rough phase with a zero roughness exponent (we call it the log rough phase). For $2-\rho<d<2+2\rho$, the phase is controlled by the LR fixed point and the surface is the LR smooth phase

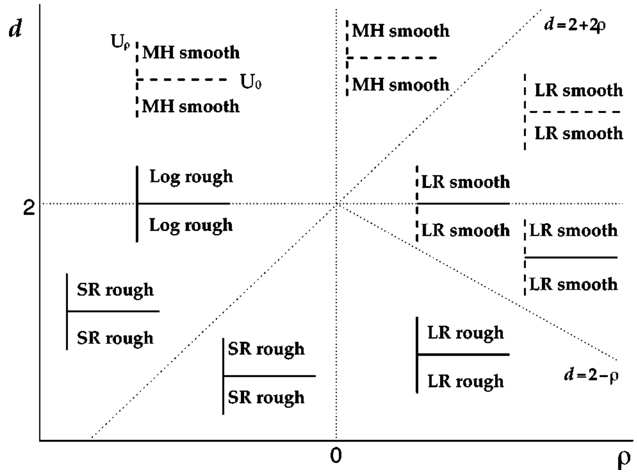

FIG. 1. U_ρ (y axis) vs U_0 (x axis) phase diagram in (ρ,d) space. On the x axis and y axis of the phase diagrams, the solid lines denote the rough phase and the dotted lines a smooth phase. The detailed meanings of the corresponding rough or smooth phase are explained in Table I. For $\rho>0$, the long-range effect makes the surface less rough than for the case of $\rho=0$ (see the region $2-\rho \leqslant d \leqslant 2$ for $\rho>0$).

due to the negative value of the roughness exponent [$\chi=(2-d-\rho)/3$, we call it the LR smooth phase]. In addition, the various critical behaviors depending on both value of ρ and dimension d are shown in Fig. 1. Phases at the critical line ($U_\rho=0$) are SR rough for $2-\rho \leqslant d<2$, log rough for $d=2$, and MH smooth for $2<d<2+2\rho$. Here the MH smooth phase is defined by the linear equation with a negative roughness exponent [$\chi=(2-d)/2$, we call it the Mullins-Herring (MH) smooth phase]. For $d \geqslant 2+2\rho$, both the LR and SR fixed points are irrelevant, so only the MH smooth phase of the linear equation exists. Therefore, various phase transitions take place when the sign of U_ρ is changed, except for the region $d \geqslant 2+2\rho$ where no phase transition occurs for all values of U_ρ and U_0. At physical dimension $d=2$, it is well known that for the short-range interaction ($U_\rho=0$ and $U_0 \neq 0$), the SR fixed point (the SGG equation) is irrelevant, so the surface is logarithmically rough. However, if $U_\rho \neq 0$ and $\rho>0$ (that is, for the long-range interaction), the LR fixed point is relevant and the surface becomes LR smooth with the negative exponents given by Eq. (8). We thus find that the nonzero U_ρ term with $\rho>0$ can make the surface less rough than the logarithmically rough phase of the case $\rho=0$ (see Table I).

(ii) $\rho<0$. The LR fixed point is irrelevant on the ground that U_0 is dominant over U_ρ. So the short-range term in Eq. (1) that describes the nonlinearity of the SGG equation determines the surface behavior in all space (U_ρ, U_0). If $U_0=0$, it is a LR rough phase for $d<2+2\rho$ and a MH rough phase for $2+2\rho \leqslant d<2$. Here the MH rough phase has the positive roughness exponent given by the linear equation $\chi=(2-d)/2$. If $U_0 \neq 0$, the SR fixed point is stable for $d<2$ and the surface is always short-range rough. When $d \geqslant 2$, both the SR and LR fixed points are no longer stable for any value of U_0, so the phase is governed by the linear equation. Therefore, the phases are logarithmically rough for $d=2$ and MH smooth for $d>2$. Unlike the case of $\rho>0$, no phase transitions take place for all spaces of U_ρ and U_0.

We have also studied Eq. (1) with a nonconservative noise η instead of a conservative noise η_c. The nonconservative noise η is a white noise of zero mean with $\langle \eta(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle = 2D\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$. There are two sets of axial fixed points. The phase diagrams in this growing surfaces are essentially the same as Fig. 1 if the dimensionality is replaced by $d \to d-2$. At the SR fixed point, $d_c=4$, $\chi=(4-d)/3$, and $z=(8+d)/3$, in agreement with the equation introduced by Lai and Das Sarma [3]. At the new LR fixed point with $d_c=4+2\rho$, the exponents are given by $\chi=(4-d-\rho)/3$ and $z=(8+d-2\rho)/3$, which are obtained from the nonrenormalization of D and λ_ρ in a one-loop ap-

TABLE I. Various phases depend on both ρ and d. These phases correspond to the diagrams in Fig. 1. There are six different phases: LR rough if $\chi=(2-d-\rho)/3$ is positive, LR smooth if $\chi=(2-d-\rho)/3$ is negative, SR rough if $\chi=(2-d)/3$ is positive, MH rough if $\chi=(2-d)/2$ is positive, MH smooth if $\chi=(2-d)/2$ is negative, and log rough if $\chi=0$.

ρ	d	Phase of U_0 (x axis)	Phase of U_ρ (y axis)
$\rho<0$	$d<2+2\rho$	SR rough	LR rough
	$2+2\rho \leqslant d<2$	SR rough	MH rough
	$d=2$	log rough	log rough
	$d>2$	MH smooth	MH smooth
$\rho>0$	$d<2-\rho$	SR rough	LR rough
	$d=2-\rho$	SR rough	log rough
	$2-\rho<d<2$	SR rough	
	$d=2$	log rough	LR smooth
	$2<d<2+2\rho$	MH smooth	
	$d \geqslant 2+2\rho$	MH smooth	MH smooth

proximation. Experimental results for the growth of Fe films on Fe(001) using a high-resolution low-energy electron diffraction technique [17] show $\chi=0.79\pm0.05$ and $\beta=\chi/z=0.22\pm0.02$ for $d=2$. This value belongs to the region $d<2+2\rho$ $(\rho<0)$ in Table I so the surface is LR rough with $U_0=0$. If $\chi<2/3$ and $\beta<2/5$ for $d=2$, the positive value of ρ can be adjusted to fit the experimental data. At this point, it is unclear whether the experimental system really possesses the long-range interaction such as that of Eq. (1). We thus strongly encourage the examination of other systems with long-range interactions.

In summary, we have studied the conserved KPZ equation in the presence of long-range interactions. For positive values of ρ, the long-range nonlinear term makes the surface less rough and produces different values of the exponents from those of the SGG equation. In particular, at physical dimension $d=2$, the surface is smooth for $\rho>0$, while the surface is logarithmically rough for $\rho=0$. However, the long-range nonlinear term becomes irrelevant for negative values of ρ and the surface is controlled by the SGG fixed points.

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