Physics Letters A 379 (2015) 199–205

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

One dimensional conservative surface dynamics with broken parity: Arrested collapse versus coarsening

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ARTICLE INFO

Article history:
Received 4 September 2014
Received in revised form 7 November 2014
Accepted 12 November 2014
Available online 18 November 2014
Communicated by R. Wu

Keywords:
Surface dynamics
Coarsening
Scaling
Nonlinear partial differential equations

ABSTRACT

The conserved Kuramoto–Sivashinsky (cKS) equation describes the coarsening of an unstable solid surface that conserves mass and that is parity symmetric. When parity is a broken symmetry, a nonlinear third-order spatial derivative term must in general be included in the equation of motion. We show that the effects of this term can be dramatic. Numerical integrations reveal that if its coefficient is sufficiently large, a nearly constant speed "train of kinks" develops and coarsening appears to cease. An individual kink exhibits scaling behavior as it grows deeper and narrower until the fourth-order cKS nonlinearity averts a finite-time singularity.

1. Introduction

Nearly flat solid surfaces can become unstable against the formation of ripples, mounds or other structures that have a characteristic length scale that is much larger than the inter-atomic spacing. In these circumstances, a continuum equation of motion governs the surface dynamics. Provided that it does not develop overhangs, the surface may be described by specifying its height $h(x, y, t)$ above all points (x, y) in the x–y plane at time t.

In many cases, the total mass is conserved because material is not added to or removed from the solid. Matter may move over the solid surface or within a near-surface region, however, and this can lead to very rich and complex dynamics. Examples of problems of this kind include diffusion on solid surfaces [1], electromigration-induced drift on the surface of a conductor [2,3] and the dynamics of aeolian sand dunes [4,5]. A less familiar example is the ripples that can form when a solid surface is bombarded with a broad ion beam at oblique incidence [6]. If the ion energy is high enough, electronic rather than nuclear stopping is predominant, and sputtering is negligible. In this regime, the mass of solid is conserved but ion-induced plastic flow occurs within a thin layer at the surface of the solid [7].

A generic continuum model that conserves mass and that displays an instability is the conserved Kuramoto–Sivashinsky (cKS) equation

$$\partial_t h = -\partial_x^2 h - \frac{1}{2}\partial_x^4 h - \partial_x^2(\partial_x h)^2. \quad (1)$$

Note that we may assume without loss of generality that the spatial average of h is zero and that it has been assumed that h is independent of y for the sake of simplicity. The cKS equation is usually written without the coefficient $\frac{1}{2}$ before the fourth-derivative term, but we prefer this form because the maximally unstable mode has wavelength 2π rather than $2\sqrt{2}\pi$. The cKS equation models the step meandering instability on a surface characterized by the alternation of terraces with different properties [8]. It also describes the growth of an amorphous thin film by physical vapor deposition [9,10]—in this case, conserved dynamics are obtained by transforming to a frame that translates upward with constant velocity.

The behavior of the solutions to the cKS equation is now well understood [8,11–13]. A family of periodic steady-state solutions exists; these consist of nearly parabolic convex segments ("humps") that join at "kinks". These kinks are not discontinuities in $\partial_x h$, but are instead relatively narrow regions where $\partial_x^2 h$ is positive. For generic nominally flat initial conditions, a nearly periodic pattern with wave number $k \sim 1$ emerges at early times, but at longer times coarsening occurs: kinks merge and the average size of the parabolic segments grows in time. The cKS equation is viewed as a simple, paradigmatic model of coarsening in spatially extended nonlinear systems as a consequence. Several theoretical analyses as well as numerical integrations indicate that the characteristic length of the humps grows as $t^{1/2}$ and that the root-mean-square surface height grows as t^1 [8,11–13]; since most of

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http://dx.doi.org/10.1016/j.physleta.2014.11.015
0375-9601/

the surface is composed of nearly parabolic segments, the latter result is a natural consequence of the former.

In this paper, we will study a generalization of the cKS equation in which parity is a broken symmetry. The $x \to -x$ symmetry is broken by the applied electric field in the case of electromigration, by the wind in the case of aeolian dunes, and by the obliquely-incident ion beam in the case of ion-induced ripple formation. The symmetry could be broken in the growth of amorphous thin films by employing an obliquely-incident flux of atoms rather than a normally-incident one. In each case, an external driving force eliminates the $x \to -x$ symmetry.

When there is no $x \to -x$ symmetry, terms proportional to $\partial_x^3 h$ and $\partial_x(\partial_x h)^2$ must in general be added to the right-hand side of Eq. (1). The reason for this is that the $\partial_x^3 h$ and $\partial_x(\partial_x h)^2$ are of lower order in ∂_x than $\partial_x^4 h$ and $\partial_x^2(\partial_x h)^2$. Thus, we write

$$\partial_t h = -\partial_x^2 h - \frac{1}{2}\partial_x^4 h - \partial_x^2(\partial_x h)^2 + \alpha\partial_x(\partial_x h)^2 + \gamma\partial_x^3 h; \qquad (2)$$

note that there is no need to add a term proportional to $\partial_x h$ because such a term can be removed by a Galilean transformation. Eq. (2), with an additional nonlinear term $\partial_x(\partial_x h)^3$, has been shown to model aeolian sand dunes [4,5]. If the hydrodynamic model of ion-induced pattern formation is simplified using the lubrication approximation and if the ion energy is high enough that sputtering can be neglected, Eq. (2) results [14].[1] In addition, for $\alpha = 0$, it describes deposition and electromigration on a vicinal surface [2]. In this case, where only the linear third-order term is added to the cKS equation, the dynamics of the surface are hardly affected: there is overall drift, with the direction depending on the sign of γ, but coarsening takes place with the same power laws as for $\gamma = 0$ [2,4].

In this paper, we will study the solutions of Eq. (2), which we will refer to as the parity broken conserved Kuramoto–Sivashinsky (pb–cKS) equation. We find through direct numerical integrations (Section 2) that the nonlinear third order term can have a dramatic effect on the character of the solutions. In particular, it seems to drive a transition between qualitatively different long-time behaviors. There is a large region in the α–γ parameter space in which the solutions do not appear to exhibit coarsening, but instead become aperiodic traveling waves as t grows large. These traveling waves exhibit kinks, just like the solutions to the cKS solutions; but, unlike the latter, the depth and curvature of the kinks saturate almost as soon as the nonlinear effects become significant. Section 3 presents a scaling analysis of the development of kinks which is in good agreement with the numerical integrations when α is large. In Section 4 we conclude with a summary of our findings.

2. Numerical method and results

A Galerkin method is employed in the numerical calculations. We apply periodic boundary conditions on the interval $0 \le x \le 2\pi\nu$ and write $h(x,t)$ as a finite trigonometric series, that is,

$$h(x,t) = \sum_{n=1}^{N}\left[a_n(t)\cos(nx/\nu) + b_n(t)\sin(nx/\nu)\right]. \qquad (3)$$

This leads to a set of nonlinear first order differential equations for the coefficients. The $n = 0$ term is omitted because conservative dynamics implies $da_0/dt = 0$, and vertical translation invariance implies that a_0 does not appear in any of the equations for the other coefficients; thus a_0 can be taken to be identically zero. The choice of wave number cutoff N is described below. We may assume without loss of generality that $\alpha \ge 0$ because if it is not, we may make the replacement $x \to -x$; the parameter γ can take on any real value.

[1] The effect of the nonlinear term $\alpha\partial_x(\partial_x h)^2$ has also been studied for ion energies low enough that nuclear stopping is predominant [15]. In the low energy regime, sputtering is not negligible and the dynamics are not conservative.

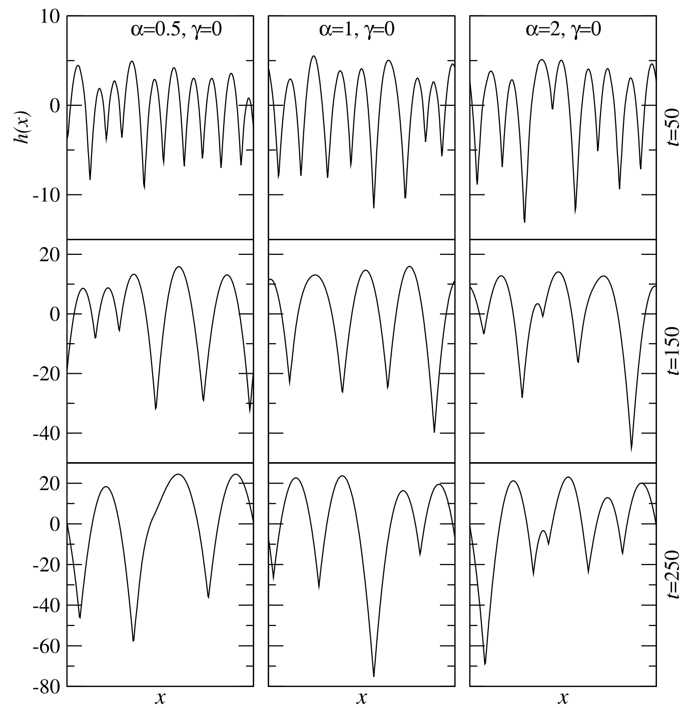

Fig. 1. Snapshots of $h(x,t)$ for $\alpha = 0.5$ (left column), 1.0 (middle column) and 2.0 (right column) at several times. The x values in the plots cover the entire domain $(0, 40\pi)$. The vertical scales are the same for all plots in a row.

Numerical integrations were carried out with the Livermore solver [16] using the analytic Hessian, wrapped by SciPy [17]. Initial conditions were drawn from random Gaussian distributions for the Fourier coefficients with standard deviations sufficiently small, typically $\langle a_n^2\rangle^{1/2} = \langle b_n^2\rangle^{1/2} = 0.1/N^{1/2}$, so that the system was in the linear regime. The N values we typically used were on the order of hundreds, and we spot checked for finite-N artifacts. Most of the numerical integrations we report were carried out with ν in the range of 20 to 40, and were thus comparable in effective size to direct numerical integrations of the cKS equation in the literature [13]. For all parameter values (α, γ, ν) we have explored, the finite-time singularity associated with the parity-breaking nonlinear term (discussed in Section 3 below) was suppressed by the cKS nonlinearity—but the number of function and Hessian evaluations per unit of time that the integration algorithm settled on varied by four orders of magnitude, depending on the parameter values. When singularities were encountered in numerical integrations, they were found to be artifacts which could be eliminated by increasing N and/or reducing the initial time step.

We begin the presentation of our numerical investigations by setting $\gamma = 0$, so that only the nonlinear parity-breaking term is present, and examining how the results evolve with increasing α. In Fig. 1 we show a sequence of snapshots of the surface at different times for several values of α. These results show that the surface coarsens in time for sufficiently small values of α, just as it does for $\alpha = 0$. There are several ways in which the dynamics for $\alpha > 0$ differs in detail from cKS dynamics, however. In the cKS equation, coarsening occurs through merging of kinks [18], as shown in Fig. 2. For $\alpha > 0$, a small hump will merge into the left side of a larger hump, and rather than the two kinks associated with the small hump merging, the right kink of the