Steady states of the conserved Kuramoto-Sivashinsky equation

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Abstract

Recent work on the dynamics of a crystal surface [T. Frisch and A. Verga, Phys. Rev. Lett. 96, 166104 (2006)] has focused the attention on the conserved Kuramoto-Sivashinsky (CKS) equation: \( \partial_t u = -\partial_{xx}(u + u_{xx} + u_x^2) \), which displays coarsening. For a quantitative and qualitative understanding of the dynamics, the analysis of steady states is particularly relevant. In this paper we provide a detailed study of the stationary solutions and their explicit form is given. Periodic configurations form an increasing branch in the space wavelength–amplitude (\( \lambda–A \)), with \( d\lambda/dA > 0 \). For large wavelength, \( \lambda = 4\sqrt{A} \) and the orbits in phase space tend to a separatrix, which is a parabola. Steady states are found up to an additive constant \( a \), which is set by the dynamics through the conservation law \( \partial_t \langle u(x,t) \rangle = 0 \): \( a(\lambda(t)) = \lambda^2(t)/48 \).

Key words: Nonlinear dynamics, Coarsening, Instabilities, Crystal growth

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1 Introduction

The study of the growth processes of crystal surfaces [1,2,3] has turned out to be source of a variety of nonlinear dynamics. A first, general distinction should be made between a crystal growing along a high symmetry orientation (e.g., the face (100) of silicon) and one growing along a vicinal orientation (e.g., the face (119) of copper). In the former case, growth proceeds [4] via nucleation, aggregation of diffusing adatoms and coalescence of islands. The growth is intrinsically two-dimensional and the variable describing the growth dynamics is the local height \( z(x,y,t) \) of the surface, or alternatively, the local slope

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\( \vec{m}(x, y, t) = \nabla z(x, y, t) \). The ideal growth of a high-symmetry surface is called *layer-by-layer*. In the latter case (vicinal orientation), the surface is made up of a train of steps [5] which capture diffusing adatoms and advance. Since steps are neither created nor destroyed, a vicinal surface is usually described in terms of step positions \( \zeta_i(x, t) \), where \( i \) labels the steps. In this case the ideal growth is called *step-flow*.

The interest in the nonlinear dynamics of a crystal surface comes from the observation that growth is often unstable [6]. Layer-by-layer growth may be destabilized by mound formation, whose phenomenology has many similarities with thermal faceting [7], even if the driving force is kinetic rather than thermodynamic. The representative equation,

\[
\partial_t z = -\nabla \cdot \left[ \nabla^2 \vec{m} + \vec{J}(\vec{m}) \right],
\]

has strict resemblances with the Cahn-Hilliard equation [8], once we take the gradient of both sides.

The growth of a vicinal surface allows for more rigorous treatments and the original two-dimensional character of the growth can be often decomposed in the two spatial degrees of freedom, the coordinate \( x \) of the single step and the index \( i \) for different steps, according to the type of emerging instability. In fact, step flow may undergo two different types of instability: step bunching and step meandering. Step bunching means that the density of steps does not keep constant because steps prefer to gather in bunches separated by large terraces. Step meandering means that steps do not stay straight and start wandering.

The possibility that both instabilities appear at the same time is very rare [9]: typically, step bunching occurs while steps are straight and step meandering occurs while different steps wander in phase and their distance remains constant [10]. This means that the dynamics can be described by effective one-dimensional equations. For example, step bunching in the presence of large desorption can be described by the Benney equation [11],

\[
\partial_t u = -u_{xx} + \gamma u_{xxx} - u_{xxxx} + u_x^2,
\]

giving chaotical dynamics or a regular structure of stable bunches, depending on the strength of the propagative \( \gamma \)-term.

The dynamics of meandering depends on the asymmetry in the attachment kinetics to the steps: meandering occurs when adatoms preferentially attach to the ascending steps [12]. In the presence of strong evaporation, we get the well known Kuramoto-Sivashinsky equation [13], corresponding to the Benney equation when \( \gamma = 0 \) and producing spatio-temporal chaos. In the opposite
limit of vanishing evaporation and large asymmetry, a strongly nonlinear generalization of the Cahn-Hilliard equation was found [14]:

\[
\partial_t u = -A(u)\partial_{xx}[B(u) + C(u)u_{xx}] .
\] (3)

This equation may produce [15] a constant-wavelength pattern \((\lambda = \lambda_0)\) with diverging amplitude or a coarsening process, i.e., an increase in time of the wavelength \(\lambda\). This increase may be either perpetual, therefore defining the coarsening exponent \(n\), \(\lambda(t) \sim t^n\), or interrupted [16] at some length \(\lambda_{\text{max}}\).

The case of vanishing desorption and weak asymmetry has been recently considered by T. Frisch and A. Verga [17], who found the equation

\[
\partial_t u = -\partial_{xx}(u + u_{xx} + u_x^2) ,
\] (4)

which has been called the conserved Kuramoto-Sivashinsky (CKS) equation. The equation has been solved numerically and appears to give rise to a coarsening pattern, whose exponent, according to similarity arguments [17], is \(n = \frac{1}{2}\). A similar equation, with an extra propagative term \(\gamma u_{xxx}\), arises in step bunching dynamics with vanishing desorption [18] and in a completely different domain, sand-ripple dynamics [19]. The propagative term breaks the \(x \to -x\) symmetry, but does not seem to change the long-time behavior: perpetual coarsening with \(n = \frac{1}{2}\) is preserved. Additional discussion about this equation can be found in the last Section.

Most times, coarsening occurs because the Partial Differential Equation (PDE) describing the dynamics has a branch of steady states whose wavelength is an increasing function of their amplitude. These steady states are unstable with respect to phase fluctuations [20] and the profile evolves in time keeping close to the stationary branch.

In Ref. [17] the authors remark that the profile emerging from the CKS equation can be thought of as a superposition of parabolas and that a stationary parabola is a particular solution of the equation. In this paper we aim at a detailed characterization of the steady states of the CKS equation. This will be mainly done analytically, giving the general exact relation between \(u\) and \(u_x\), i.e., determining the trajectories in phase space.
2 Steady states

The steady states of the CKS equation (4), satisfy the second-order nonlinear differential equation

\[ u + u_{xx} + u_x^2 = a + bx . \] (5)

Since the constant \( b \) must vanish in order to get limited solutions, while the constant \( a \) can be trivially absorbed into a uniform shift of \( u(x) \) and be set to zero, the problem reduces to solving the differential equation

\[ u_{xx} = -u - u_x^2 . \] (6)

Interpreting \( x \) as a time, this equation describes the dynamics of a harmonic oscillator subject to an additional force proportional to the square velocity. It can be easily solved by evaluating the derivative of \( u_{xx} \equiv F \),

\[ F_x = -u_x - 2u_x u_{xx} = -u_x(1 + 2F) , \] (7)

so that

\[ \frac{du}{dF} = -\frac{1}{1 + 2F} , \] (8)

whose integration starting from a zero-velocity initial condition, \( u(0) = A \) and \( u_x(0) = 0 \), that implies \( F(0) = -A \), gives the first integral

\[ 2(A - u) = \ln \left| \frac{1 + 2F}{1 - 2A} \right| , \] (9)

or

\[ 1 + 2F = \pm (1 - 2A) e^{2(A-u)} ; \] (10)

a continuity argument allows us to drop the minus sign

\[ F = -u - u_x^2 = -\frac{1}{2} + (1 - 2A) e^{2(A-u)} , \] (11)

making it apparent that if \( A \geq \frac{1}{2} \) the force is strictly negative and the trajectory is not limited. On the other hand, if \( A = A_+ \), with \( 0 < A_+ < \frac{1}{2} \), the particle initially acquires a negative velocity, but the increasing positive contribution to the force \( F \) will eventually restore \( u_x = 0 \) at some position.
Fig. 1. Trajectories in the phase space \((u, u_x)\) of the limiting parabola \(u_x^2 = \frac{1}{2} - u\) (thick full line) and of the periodic steady states: \(A_- = 1\) (dotted), \(A_- = 2\) (short dashed), \(A_- = 4\) (dot dashed), and \(A_- = 8\) (long dashed). The thin full lines correspond to the approximation \(u_x^2 = 2A_- (u + A_-)\), valid close to \(u = -A_-\).

\(u = -A_- < 0\); the converse occurs starting from \(A = -A_- < 0\), so that a periodic orbit occurs for any \(A < \frac{1}{2}\). The pairs of turning points \((A_+, -A_-)\) are solution of

\[
(1 - 2A_+) e^{-(1 - 2A_+)} = (1 + 2A_-) e^{-(1 + 2A_-)},
\]

that maps the interval \([0, \frac{1}{2}]\) onto the interval \((-\infty, 0]\). Eventually, we can write the trajectories in the phase space \((u, u_x)\) as

\[
u_x^2 = \frac{1}{2} - u - (\frac{1}{2} - A) e^{2(A - u)};
\]

these are plotted in Fig. 1 for a choice of values of \(A_-\). If \(A_+ = \frac{1}{2}\), we obtain the separatrix \(u_x^2 = \frac{1}{2} - u\), which corresponds to the parabolic trajectory \(u(x) = \frac{1}{2} - (x - x_0)^2/4\).

Eq. (13) can be rewritten in a more familiar form,

\[
\frac{u_x^2}{2} + V(u) = E = \frac{1}{4},
\]
Fig. 2. Effective potentials $V(u)$ for bound states, $A < \frac{1}{2}$ (dotted lines), for the separatrix, $A = \frac{1}{2}$ (dash-dotted line), and for unbounded states, $A > \frac{1}{2}$ (dashed line). The “energy” of the particle is $E = \frac{1}{4}$ (full line) in all cases. The condition $V(u) = E$ identifies the turning points. Inset: the potential $V^*(h) = \frac{1}{2}(h + e^{-2h})$ (full line) and the energy $E^* = \frac{1}{2}(1 - A) - \frac{1}{4} \ln(1 - A)$ (dotted line), valid for $A < \frac{1}{2}$.

showing that the system satisfies the conservation of a pseudo-energy $E = \frac{1}{4}$, with a potential

$$V(u) = \frac{u^2}{2} + \frac{1}{2} \left( \frac{1}{2} - A \right) e^{2(A-u)}$$

(15)

that depends on the boundary (initial) conditions. The above discussion about closed and open orbits becomes a straightforward analysis of the potential shape, as reported in Fig. 2.

It appears from the figure that the potential keeps its shape: this can be checked analytically by considering a shift in the $u$ variable, $u(x) = h(x) + q_0$; for $q_0 = A + \frac{1}{2} \ln \left| \frac{1}{2} - A \right|$ the first integral (14) can be rewritten as

$$\frac{h_x^2}{2} + V^*(h) = E^*(A),$$

(16)

with $E^*(A) = \frac{1}{2}(1 - A) - \frac{1}{4} \ln \left| \frac{1}{2} - A \right|$, and the $A$-independent potential

$$V^*(h) = \frac{1}{2}(h \pm e^{-2h})$$

(17)
Fig. 3. Periodic steady states configurations, corresponding to $A_- = 1$ (dotted), $A_- = 2$ (short dashed), $A_- = 4$ (dot dashed), and $A_- = 8$ (long dashed). The thick full lines corresponds to the limiting parabola $u = \frac{1}{2} - x^2/4$. Small inset: the minima of the configurations and the approximations $u = -A_- + A_- x^2/2$ (thin full lines). Large inset: wavelength $\lambda$ as a function of the amplitude $A_-$. The full line is the asymptotic relation $\lambda = 4\sqrt{A_-}$.

where the sign $+$ ($-$) is valid for $A < \frac{1}{2}$ ($A > \frac{1}{2}$). For bounded states, the energy minimum is $E^*(0) = \frac{1}{4}(1 + \ln 2)$ and coincides with the minimum of the potential $V^*(h=\ln 2/2)$ (trivial orbit). The potential $V^*(h)$ and a representative value of the energy $E^*$ are plotted in the inset of Fig. 2.

The numerical results for the periodic configurations $u(x)$ in real space are shown in Fig. 3. It is useful to determine the amplitude $A_-$ in the negative $x$ direction, as a function of $A_+$, through the condition (12). For $A_+ \to 0$, it is easily found that $A_-/A_+ \to 1$, while in the important limit $A_+ \to \frac{1}{2}$, $A_-$ diverges logarithmically according to

$$A_- e^{-2A_-} \approx \frac{1}{2} - A_+$$

i.e.,

$$A_- \approx -\frac{1}{2} \ln(1 - 2A_+)$$

In proximity of $u = -A_-$, bounded trajectories have a minimum with a curvature that diverges as $A_- \to \infty$, as shown by the expansion $u = -A_- + \varepsilon$ in
Eq. (13), which gives
\[ u \approx -A_+ + \frac{A_-}{2} (\delta x)^2 + O[A_-^2 (\delta x)^4] . \] (20)

This approximation is shown as thin full lines, both in Fig. 1 and in Fig. 3. The quadratic and quartic terms are of the same order when |\( \delta x \)| \( \approx 1/\sqrt{A_-} \), which sets the size of the high-curvature region. In fact, the slope \( u_x(\delta x = 1/\sqrt{A_-}) \approx \sqrt{A_-} \) joins to the same slope of the limiting parabola \( u = \frac{1}{2} - x^2/4 \), when \( u \approx -A_- \).

As for the unbounded states, \( A > \frac{1}{2} \), it is worth noting that they diverge at a finite value \( x_\infty \); in the mechanical analogy, this means that the particle escapes to infinity in a finite time. We can determine \( x_\infty \) integrating Eq. (13) once more:
\[ x_\infty = -\int_A^\infty \frac{du}{u_x} = \frac{1}{\sqrt{2}} \int_0^\infty \frac{ds}{\sqrt{s + (2A - 1)(e^s - 1)}} \] (21)
and, for large \( A \),
\[ x_\infty \approx \frac{1}{\sqrt{4A}} \int_0^\infty \frac{ds}{\sqrt{e^s - 1}} = \frac{\pi}{\sqrt{4A}} . \] (22)

Finally, in the large inset of Fig. 3 we plot the wavelength \( \lambda \) of the steady states as a function of their amplitude \( A_- \). The full line, \( \lambda = 4\sqrt{A_-} \), gives the analytical approximation valid for large \( A_- \). It can be determined from the asymptotic parabola \( u = \frac{1}{2} - x^2/4 \) imposing \( u(\lambda/2) = -A_- \), or equivalently, from the mechanical analogy for the potential \( V^* \) (see inset of Fig. 2).

3 Steady states and dynamics

In the Introduction we have argued that steady states are important because dynamics proceeds evolving along the family of steady states of increasing wavelength \( \lambda \). In the case of the CKS equation special attention should be paid to the constant \( a \) appearing in Eq. (5) and to the conserved character of Eq. (4). We are now going to show that the conservation law fixes the value of \( a \), as a function of \( \lambda \). Afterwards, we explain that for the dynamics \( a \) is the time dependent vertical shifting of the surface profile.

On the one hand, the conserved dynamics requires that the spatial average \( \langle u(x, t) \rangle \) is time independent; on the other hand, \( \langle u(x) \rangle \neq 0 \) and does depend
on $\lambda$. Therefore, the family of steady states which is relevant for the dynamics is

$$u_\lambda(x) = u(x) + a(\lambda),$$

(23)

where the constant $a$ satisfies the condition

$$a(\lambda) = -\langle u(x) \rangle.$$ (24)

In the above notation, $u(x)$ means the general steady state (of wavelength $\lambda$) found in the preceding Section. For large $\lambda$, the average value of $u(x)$ can be safely determined by approximating it with the arc of the (separatrix) parabola, so that

$$\langle u(x) \rangle = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} dx \left( \frac{1}{2} - \frac{x^2}{4} \right) + o(\lambda^2) = -\frac{\lambda^2}{48} + o(\lambda^2).$$ (25)

Therefore, we get

$$a(\lambda) = \frac{\lambda^2}{48}.$$ (26)

4 Conclusions and discussion

The starting and only assumption of this work is that steady states of increasing wavelength play a central role in the dynamics of the CKS equation and, in particular, in the coarsening process. This assumption is based on previous work [20] on a plethora of different PDE for which this connection has been well established. It is also supported by numerical work [17] on the CKS eq., showing that the system indeed coarsens with a profile made up of a sequence of arcs of parabola.

In Section 2 we have analytically found all the steady states and in Section 3 we have determined the relation between vertical shifting of the profile and coarsening process. The theory of the phase diffusion equation [20], which would allow a more rigorous derivation of the coarsening exponent $n = \frac{1}{2}$ [17], can not easily be applied to the CKS equation, because the linear operator coming from the Frechét derivative is not self-adjoint, a feature that the CKS equation shares with the Kuramoto-Sivashinsky equation.

The fact that the surface profile is made up of arcs of parabola joined by vanishing regions of diverging amplitude (angular points) suggests an alternative
dynamical description: the system is made up of a sequence of “particles” (the angular points) which tend to annihilate, and therefore the system tends to coarsen. Is it possible to study the effective dynamics of these particles?

Let us finally comment on a modified version of the CKS equation [18,19],

$$\partial_t u = -\partial_{xx}(u + u_{xx} + u_x^2 + \gamma u_x), \quad (27)$$

where a third-order dispersive drift term has been added to the right-hand-side. This equation has been mentioned in the Introduction as emerging in two different domains: growth of a vicinal surface subject to a step-bunching instability and sand ripple dynamics. According to numerics [18], Eq. (27) displays a surface profile which is not much different from the profiles shown by the CKS equation. Also, the system seems to coarsen with the same law, \(\lambda \sim \sqrt{t}\).

It may be tempting to treat Eq. (27) along the same lines followed for the CKS equation. The first remark is that periodic steady states should now be replaced by travelling periodic configurations. In fact, Eq. (27) does not have periodic stationary solutions because of the \(\gamma\)-term. Nonetheless, one might look for periodic solutions depending on \((x - vt)\). It would be interesting to understand if there is a branch of travelling periodic configurations in the space \(\lambda - A\) and if dynamics coarsens following this branch, as for the CKS equation.

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