Dynamic scaling and crossover analysis for the Kuramoto-Sivashinsky equation

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Extensive numerical simulations of the discretized one-dimensional Kuramoto-Sivashinsky interface equation, in conjunction with a detailed crossover analysis, indicate that the large-scale fluctuations of this deterministic chaotic system are described by the noisy Burgers equation. As a consequence of a large effective interfacial tension, the asymptotic behavior is observed only after a long intermediate scaling regime. The skewness of the interfacial fluctuations is found to be a useful probe of the crossover.

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A central concept in the study of spatially extended chaos is the use of effective stochastic models for the large-scale properties of a chaotic system. This approach is at the heart of Kolmogorov's theory of fully developed turbulence and its ramifications [1], including more recent work in which stochastic forces are explicitly added to the equations of fluid dynamics [2,3]. Given the complexity of three-dimensional fluid turbulence, there has been much interest in finding simpler model systems where the emergence of stochastic large-scale behavior can be studied in some detail. A particularly promising candidate is the Kuramoto-Sivashinsky (KS) phase equation, which arises in various physical contexts such as chemical turbulence [4], flame-front propagation [5], and the dynamics of liquid films subject to gravity [6]. The scalar field $h(\mathbf{x},t)$ describing, e.g., the local phase of a cyclic chemical reaction [4] or the position of a flame front [5], satisfies

$$\frac{\partial}{\partial t}h = -\nabla^2 h - \nabla^4 h + (\nabla h)^2 , \qquad (1)$$

where all dimensionful parameters have been eliminated by rescaling. The only remaining control parameter is then the system size L, which governs the effective number of degrees of freedom of the system, in analogy with the Reynolds number in fluid turbulence. Due to the sign of the Laplacian term in (1) the trivial solution $h=0$ is unstable, with perturbations of wave vector $\mathbf{q}$ growing at the linear growth rate $\omega(\mathbf{q}) = \mathbf{q}^2 - \mathbf{q}^4$. This leads to a cellular local structure with a wavelength $l \approx 2\pi\sqrt{2}$ close to the maximum $q_0 = 1/\sqrt{2}$ of $\omega(\mathbf{q})$. For large L a turbulent steady state characterized by a finite density of positive Lyapunov exponents [7] is established in which the fluctuations generated by the instability are transferred by the nonlinear term to smaller wavelengths, where they are dissipated by the (stabilizing) fourth-order derivative.

It was suggested by Yakhot [8] that the large-scale properties of the one-dimensional KS equation are described by the stochastic model

$$\frac{\partial}{\partial t}h = \nu\nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta , \qquad (2)$$

where $\nu > 0$ and $\eta(x,t)$ is Gaussian white noise with covariance

$$\langle \eta(x,t)\eta(x',t')\rangle = D\delta(x-x')\delta(t-t') . \qquad (3)$$

Equation (2) was subsequently investigated by Kardar, Parisi, and Zhang (KPZ) [9] in the context of stochastic growth [10]. In the following we will interpret $h(x,t)$ as the height of a moving interface above a substrate point x at time t. It should also be noted that ∇h satisfies, according to (2), a noisy Burgers equation, which is closely related to fluid dynamics [2]. Comparing (1) to (2), it is apparent that the equivalence of the two equations requires the instability of the KS equation to have two rather different consequences on large scales: It should give rise to *both* a stochastic force with short-range correlations, and a positive effective interface tension ν.

The KPZ equation predicts a dynamic scaling form for the long-time, large-scale behavior of the correlations of

h, which is well understood in the case of one spatial dimension. The steady-state correlations of the discrete Fourier components $h(q,t)$, $q=2\pi n/L$, $n=\pm 1,\ldots,\pm L/2$, are

$$\langle h(q,t)h(-q,s)\rangle = \frac{A}{Lq^2} g_{ss}(q^z|t-s|)\,, \tag{4}$$

where $g_{ss}(0)=1$ and $\lim_{x\to\infty} g_{ss}(x)=0$, while the transient scaling form for an interface which is flat at time $t=0$ reads

$$\langle |h(q,t)|^2\rangle = \frac{A}{Lq^2} g_{tr}(q^z t) \tag{5}$$

with $g_{tr}(0)=0$ and $\lim_{x\to\infty} g_{tr}(x)=1$. The $1/q^2$ scaling of the equal time, steady-state correlations corresponds to an equilibriumlike equipartition law for the "velocity" field ∇h, which has been verified in several numerical studies of the KS equation [11,12]. In fact, as a consequence of a fluctuation-dissipation theorem for the KPZ equation [2], the equal time correlations are given *exactly* by the linear theory obtained by setting $\lambda=0$ in (2), which implies in particular that $A=D/2\nu$ in (4) and (5).

In contrast, the nonlinearity has a crucial effect on the dynamic exponent z in (4) and (5), which takes the anomalous value $z=\frac{3}{2}$ for $\lambda\neq 0$. This prediction, which arises both from dynamic renormalization-group treatments of the KPZ equation [2,9] and a mode-coupling study of the KS equation [13], has, despite some suggestive early results [14,15], so far eluded direct verification in numerical simulations [12,16] of the KS equation. The discrepancy between the predictions of the stochastic model and the simulations has generally been attributed [12,16] to the existence of an intermediate-scaling regime where the linear term in (2) dominates the nonlinearity, but a quantitative study of the crossover behavior has not been carried out.

It is the purpose of this paper to provide such a study. We present numerical simulations of the KS equation which exceed previous work by several orders of magnitude in time and length scale, and combine them with precise estimates of the crossover scales predicted by the KPZ theory. This necessitates the numerical determination of the effective parameters entering the KPZ equation. Our central result is the observation of the onset of crossover to asymptotic KPZ scaling ($z=\frac{3}{2}$) on time scales which are consistent with the theoretical predictions, thus providing strong evidence that the dynamic correlations of the one-dimensional KS equation are indeed represented by the stochastic KPZ model.

We focus here on the *transient* behavior described by (5). The dynamic scaling exponent is measured through the interface width [9,10] which, in the large system limit $L\to\infty$, behaves as

$$\xi(t)^2 = \langle (h-\langle h\rangle)^2\rangle \sim t^{2\beta}\,, \tag{6}$$

where $\beta=1/2z$. In the intermediate scaling regime, where the nonlinearity in (2) can be neglected, $z=2$ and $\beta=\frac{1}{4}$. To estimate the time scale for the onset of the asymptotic regime with $\beta=\frac{1}{3}$, we first compute the width from the linearized ($\lambda=0$) KPZ equation. The result

$$\xi_{\lambda=0}(t)^2 = \frac{D}{\sqrt{2\pi\nu}} t^{1/2} \tag{7}$$

is then compared to the asymptotic behavior of the nonlinear equation, which, from dimensional considerations, takes the form [17]

$$\xi_{KPZ}(t)^2 = c_2 (A^2 \lambda t)^{2/3}\,, \tag{8}$$

where c_2 is a universal number with a numerical value close to 0.40 [17]. The crossover time estimate obtained by equating (7) and (8) is

$$t_c = \frac{2^5}{\pi^3 c_2^6} \frac{\nu^5}{D^2 \lambda^4} \approx \frac{252}{\nu g^2}\,. \tag{9}$$

Here we have introduced the KPZ coupling constant [9]

$$g = \frac{\lambda^2 D}{\nu^3} \tag{10}$$

which, in one dimension, has the units of an inverse length. While the fact that $\nu t_c \sim 1/g^2$ follows from purely dimensional arguments, the estimate of the prefactor which, somewhat surprisingly, is *not* of order unity, requires knowledge of the nontrivial amplitude c_2.

In practice, the crossover to the asymptotic KPZ regime will be observable only if t_c is small compared to the saturation time induced by the finite system size L. The saturation time can be estimated by equating (7) or (8) to the saturated width

$$\xi_\infty^2(L) = \frac{AL}{12} \tag{11}$$

obtained by summing over the $t\to\infty$ limit of the Fourier modes (5). The resulting criterion for the accessibility of the asymptotic regime is $L \gg L_c \approx 152/g$.

For completeness we note that analogous estimates can be obtained for the steady-state dynamic correlations governed by (4). In the steady state the width (6) is replaced by the correlation function

$$C(t) = \lim_{s\to\infty} \langle [h(x,t+s)-h(x,s) - \langle h(x,t+s)-h(x,s)\rangle]^2\rangle\,. \tag{12}$$

Following the procedure outlined above and using results [17] for the asymptotic behavior of $C(t)$ we find that the crossover from $t^{1/2}$ to $t^{2/3}$ behavior occurs at the time scale $t_c^{ss} \approx 63/(\nu g^2)$ which is observable in systems large compared to $L_c^{ss} \approx 108/g$. In the following we only discuss the transient behavior [18].

Next we turn to the numerical simulations of the KS equation. We have used a simple real-space scheme obtained by replacing all spatial and temporal derivatives by finite differences. The nonlinearity was discretized as $[(h_{i+1}-h_{i-1})/2\delta x]^2$, where $h_i(t)=h(i\delta x,t)$. The results presented here were calculated using a spatial discretization step $\delta x=1$, corresponding to about eight lattice points per cell wavelength l, and a time step $\delta t=0.1$. These parameters were chosen for reasons of numerical efficiency. Runs with smaller values of δt and δx indicated some changes in the effective KPZ parameters estimated below, but the qualitative behavior remained the same. We consider only periodic boundary conditions on h. The initial values $h(x,0)$ were chosen at random from a uniform distribution on the unit interval.

The static amplitude $A=D/2\nu$ is estimated from the saturated width (11) as a function of system size. The local cellular structure of the KS interface leads to a large intrinsic width ξ_{intr}, which obscures the asymptotic scaling. To extract the large-scale contribution we fitted the numerical data to the form $\xi_\infty^2(L)=(A/12)L+\xi_{\mathrm{intr}}^2$ proposed by Kertész and Wolf [19] [Fig. 1(a)]. This yields the estimates $A\approx 0.154$ and $\xi_{\mathrm{intr}}\approx 1.15$, consistent with the value $A=0.158\pm 0.009$ obtained from the stationary Fourier spectrum shown in Fig. 1(b).

In Fig. 2 we show the time dependence of the width for two different system sizes. Here the intrinsic width has been eliminated by defining a smoothed interface, with the height at each grid point given by the mean of the $\Delta x=8$ nearest points, and measuring the width of the smoothed interface. In order to emphasize the intermediate scaling regime where $\beta=\frac{1}{4}$ we plot $\xi^2(t)/t^{1/2}$ as a function of t. This quantity is constant for times $20\leq t\leq 1000$, taking the value $D/\sqrt{2\pi\nu}=0.397\pm 0.001$ [cf. (7)]. Using the estimate for $A=D/2\nu$, we obtain the effective KPZ parameters $D=3.2\pm 0.1$ and $\nu=10.5\pm 0.6$. The surprisingly large number for ν which, as we shall see below, is really responsible for the slow crossover behavior, is consistent with estimates obtained by Zaleski [12] through a completely different method.

It remains to estimate λ, which is quite generally defined [20] through the expansion $v(\theta)\approx v_0+(\lambda/2)\theta^2+\cdots$ of the ensemble averaged growth rate $v=\langle\partial h/\partial t\rangle$ at a fixed macroscopic inclination $\theta=\langle\partial h/\partial x\rangle$. Comparing (1) and (2) and noting that the linear terms in (1) are invariant under an imposed tilt ($h\rightarrow h+\theta x$), one expects that $\lambda=2$ in the continuum limit. Measuring λ directly for the discretized KS equation with an average inclination imposed through helical boundary conditions $h(x+L)=h(x)+\theta L$ [20] (Fig. 3), we found a much larger value $\lambda=4.65\pm 0.15$, indicating that λ is quite sensitive to the spatial discretization [21]. The combination $A\lambda$ can also be obtained [17] from the dependence of the stationary growth rate at zero tilt on the system size L, which the KPZ theory predicts to be of the form [22] $v\approx v_\infty - A\lambda/2L$. Measurements for system sizes between $L=128$ and 1024 yielded $v_\infty\approx 0.496$ and $A\lambda\approx 0.695$, in good agreement with the value $A\lambda\approx 0.716$ obtained from the previous estimates.

Taken together these numbers imply that the KPZ coupling constant (10) is $g=0.060\pm 0.016$. Thus system sizes exceeding $L_c\approx 2500$ are necessary to observe asymptotic KPZ behavior, which explains the failure of previous numerical work [12,16]. The crossover time is estimated to be $t_c\approx 7000$, which is rather close to the point where our data (Fig. 2) deviate significantly from the $\beta=\frac{1}{4}$ behavior. In Fig. 2 we also display the prediction (8) for the asymptotic KPZ behavior, obtained from the above parameter estimates. The numerical data ap-

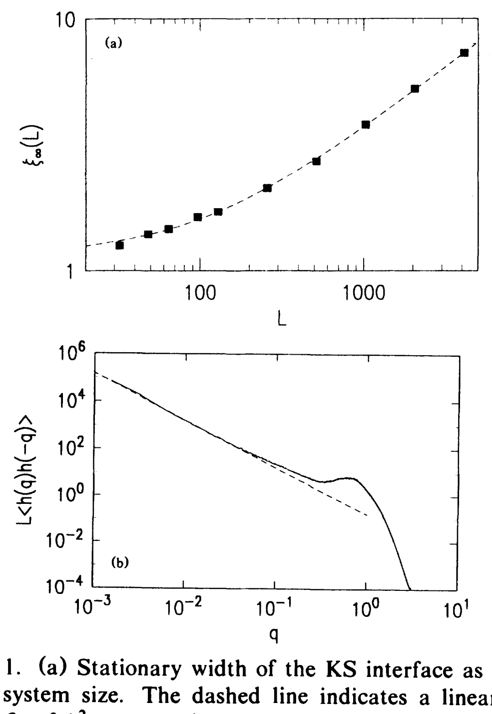

FIG. 1. (a) Stationary width of the KS interface as a function of system size. The dashed line indicates a linear least-squares fit of ξ_∞^2 vs L used to extract the asymptotic prefactor and the intrinsic width. (b) Fourier spectrum of the stationary height fluctuations for a system of size $L=4096$. The dashed line indicates the long-wavelength behavior A/q^2 with $A=0.158$. Note the peak at $q_0=1/\sqrt{2}$ corresponding to the cell wavelength l.

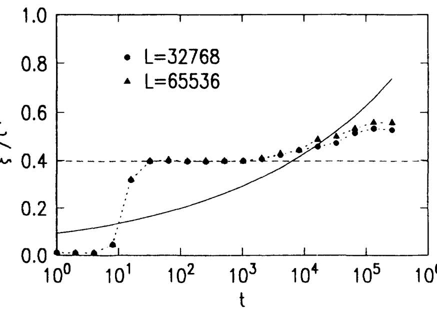

FIG. 2. Time dependence of the interface width. The data for system size $L=32768$ (65536) constitute an average over 152 (70) independent runs. The dashed line indicates the estimate $D/\sqrt{2\pi\nu}=0.397$ and the solid line shows the asymptotic behavior $\xi^2(t)=0.092t^{2/3}$ predicted by the KPZ theory.

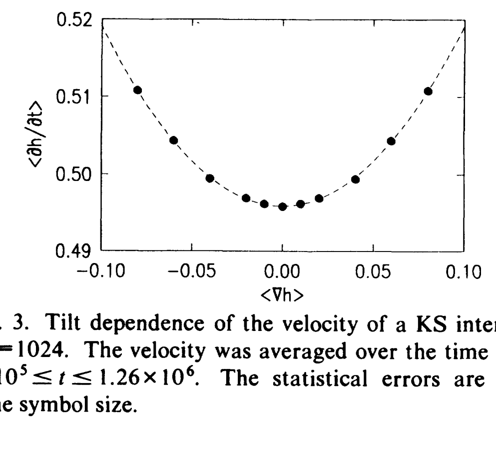

FIG. 3. Tilt dependence of the velocity of a KS interface of size $L=1024$. The velocity was averaged over the time interval $4.19\times 10^5\leq t\leq 1.26\times 10^6$. The statistical errors are smaller than the symbol size.

pear to approach the KPZ behavior up to $t \approx 10^4$, where the size dependence of the width becomes observable, indicating the onset of saturation effects.

This picture is confirmed by measuring the skewness $s = \langle (h - \langle h \rangle)^3 \rangle / (\xi)^{3/2}$ of the interface fluctuations. The asymptotic KPZ regime is characterized by a universal skewness of magnitude $|s| \approx 0.29$ and a sign equal to the sign of λ [17], while the surface fluctuations in the intermediate ($\lambda = 0$) scaling regime are Gaussian with $s = 0$. In Fig. 4 we show simulation results for the skewness in the KS equation. The skewness is nonzero and positive, consistent with the fact that $\lambda > 0$. After a peak associated with the initial exponential instability, it increases roughly logarithmically in time and reaches a maximum value of 0.26, close to the KPZ prediction. The sharp decrease of the skewness at the latest times is, again, indicative of saturation effects, which are known to set in early and abruptly for this quantity [17].

In summary, we have presented extensive numerical simulations which strongly support Yakhot's conjecture [8] that the one-dimensional deterministic KS equation belongs to the universality class of noisy interface models described by KPZ [9]. The existence of an extended intermediate scaling regime, which has hampered previous numerical work, could be traced back to the large value of the effective interfacial tension ν [23]. We expect a study similar to the present one to be very illuminating (though much harder to carry out) in the two-dimensional case, where the equivalence between the KS equation and the noisy KPZ model was recently conjectured [24] to break down.

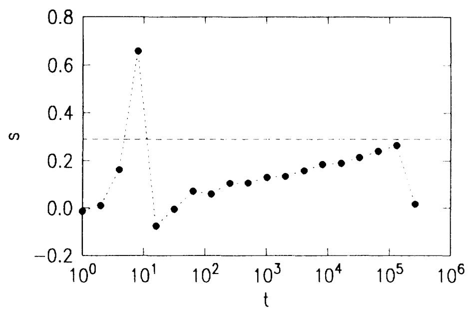

FIG. 4. Skewness of the KS interface as a function of time. The system size is $L = 32\,768$ and the data constitute an average over 40 independent runs. The skewness $s = 0.29$ characterizing a KPZ interface is indicated by the dashed line.

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