Dynamic scaling of the width distribution in Edwards-Wilkinson type models of interface dynamics

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(Received 31 October 1995)

Edwards-Wilkinson type models are studied in $1+1$ dimensions and the time-dependent distribution $P_L(w^2,t)$ of the square of the width of an interface w^2 is calculated for systems of size L. We find that, using a flat interface as an initial condition, $P_L(w^2,t)$ can be calculated exactly and it obeys scaling in the form $\langle w^2 \rangle_\infty P_L(w^2,t) = \Phi(w^2/\langle w^2 \rangle_\infty, t/L^2)$, where $\langle w^2 \rangle_\infty$ is the stationary value of w^2. For more complicated initial states, scaling is observed only in the large-time limit and the scaling function depends on the initial amplitude of the longest wavelength mode. The short-time limit is also interesting since $P_L(w^2,t)$ is found to closely approximate the log-normal distribution. These results are confirmed by Monte Carlo simulations on a single-step, solid-on-solid type model (roof-top model) of surface evolution. [S1063-651X(96)07405-2]

PACS number(s): 05.40.+j, 05.70.Ln, 81.10.Aj

I. INTRODUCTION

Interfaces play an important role in a number of physical, chemical, and biological phenomena. Their fluctuations display universal features and, accordingly, models of interface motion have been analyzed and distinguished in terms of universality classes [1]. The classification usually proceeds by taking systems of various sizes L and measuring the time-evolution of the average of the square width, $\langle w^2 \rangle$, of the interface. Then the values of the static (ζ) and dynamic (z) exponents which determine the universality class are obtained [2] by observing the collapse of the data in accordance with the scaling form $\langle w^2 \rangle \sim L^{2\zeta} f(t/L^z)$.

In practice, this procedure is not so easy to realize since $\langle w^2 \rangle$ is an integral over all modes in the system and, consequently, large corrections to scaling are present. Recently, it was suggested [3] that an alternative and more detailed characterization of interfaces may be obtained through the probability distribution of the random variable w^2. The steady-state distribution function $P_L^{(s)}(w^2)$ has been calculated exactly for various growth models [3–5] and it has been found that $P_L^{(s)}(w^2)$ defines a scaling function $\Phi^{(s)}$,

$$\langle w^2 \rangle_\infty P_L^{(s)}(w^2) = \Phi^{(s)}(w^2/\langle w^2 \rangle_\infty), \tag{1}$$

which is a universal characteristic of the interface fluctuations.

The above scaling function, however, distinguishes only among static universality classes. For example, $\Phi^{(s)}(x)$ is the same for both the one-dimensional ($d=1$) Edwards-Wilkinson (EW) [6] and Kardar-Parisi-Zhang (KPZ) [7] equations since these models describe processes which have the same steady-state distributions and differ only in the scaling of their dynamics. Thus in order to distinguish among dynamical universality classes one should extend the static results to the time-dependent width distributions $P_L(w^2,t)$. This is what we shall do here for the simplest model of surface growth, the $d=1$ EW equation [6].

Since the EW equation is linear, much of the calculation can be done analytically (Sec. II) and, in particular, we can

derive $P_L(w^2,t)$ and the associated dynamical scaling function $\langle w^2 \rangle_\infty P_L(w^2,t)$ in closed form for the case of a flat initial surface. An interesting feature of the result is that the short-time limit is closely approximated by the log-normal distribution (Sec. III). Arbitrary initial conditions are harder to treat and we obtain general results only for the long-time limit where the dependence on the initial state disappears except for the initial amplitude of the longest wavelength mode (Sec. III).

In order to carry out a limited check of the universality of our results we used Monte Carlo (MC) simulations to study a single-step, solid-on-solid type model (''roof-top'' model) of surface evolution [8,9]. This model belongs to the EW universality class when the overall velocity of the surface is zero. Otherwise, it is in one universality class with the KPZ equation. Excellent agreement is found (Sec. IV) between the analytic and simulation results for the dynamical scaling function in the EW limit and, furthermore, we also find that this scaling function is easily distinguishable from the corresponding function obtained for the KPZ case.

II. CALCULATION OF THE WIDTH DISTRIBUTION

A simple model of surface evolution governed by surface tension and noise is the EW equation [6]:

$$\frac{\partial h(x,t)}{\partial t} = \nu \frac{\partial^2}{\partial x^2} h(x,t) + \eta(x,t). \tag{2}$$

Here $h(x,t)$ is the height of the surface at sites $0 \leq x \leq L$, ν is a constant related to the dynamical surface tension, and η is a Gaussian white noise of strength Γ:

$$\langle \eta(x,t) \eta(x',t') \rangle = 2\Gamma \delta(x-x') \delta(t-t'). \tag{3}$$

For simplicity, we shall assume periodic boundary conditions. It should be noted, however, that free boundary condi-

tions may be more realistic in higher dimensions where comparisons with experiments are possible.

Our aim is to calculate the time-dependent distribution $P_L(w^2,t)$ for an arbitrary initial condition $h(x,0)$. The derivation follows along the line that has been worked out for the static case [3] with extra complications arising from time dependence as well as from initial conditions.

The quantity $w^2(t)$ is defined for a configuration $h(x,t)$ as the mean square fluctuations of the height:

$$w^2(t) = \overline{h^2} - \overline{h}^2, \qquad (4)$$

where the time-dependent average $\overline{f}(t)$ of a function $f(x,t)$ is obtained as its spatial average

$$\overline{f}(t) = \frac{1}{L}\int_0^L dx f(x,t). \qquad (5)$$

The first step of the calculation of $P_L(w^2,t)$ is writing it in terms of a path integral

$$P_L(w^2,t) = \int \mathscr{D}[h]\delta[w^2 - (\overline{h^2} - \overline{h}^2)]p(\{h\},t), \qquad (6)$$

where $p(\{h\},t)$ is the path probability that the surface evolves from an initial state $h(x,0)$ to a configuration $h(x,t)$ in time t. The dependence on the initial condition is not written explicitly though it is understood that this dependence is important for any finite t.

The Laplace transform of Eq. (6) gives the generating function of the moments of $P_L(w^2,t)$

$$G_L(\lambda,t) = \int_0^\infty d\zeta P_L(\zeta,t)e^{-\lambda\zeta}, \qquad (7)$$

and one finds that $G(\lambda,t)$ is the following path integral:

$$G_L(\lambda,t) = \int \mathscr{D}[h]p(\{h\},t)\exp[-\lambda(\overline{h^2} - \overline{h}^2)]. \qquad (8)$$

The next step is to note that the above path integral can be written as an infinite product of ordinary integrals provided the system is described in terms of the Fourier amplitudes. Indeed, let us write

$$h(x,t) - \overline{h}(t) = \sum_{n=-\infty}^{\infty} c_n(t)e^{ik_n x}, \qquad (9)$$

where $k_n = 2\pi n/L$ and $c_{-n} = c_n^*$ (note that $c_0 \equiv 0$, thus the $n=0$ Fourier mode can be left out from further considerations). The EW equation is replaced now by an infinite set of ordinary differential equations

$$\dot{c}_n(t) + \nu k_n^2 c_n(t) = \eta_n(t), \qquad (10)$$

where $\eta_n(t)$, defined as the Fourier transform of $\eta(x,t)$, is also an uncorrelated white noise. We can see that the Fourier modes with different n's are decoupled and evolve independently. Thus the probability of a path that an initial state characterized by a set of $\{c_n(0)\}$ evolve into $\{c_n(t)\}$ is just the product of probabilities $p_n[c_n(t)|c_n(0)]$ that $c_n(0)$ evolves into $c_n(t)$:

$$\hat{p}[\{c_n(t)\}|\{c_n(0)\}] = \prod_{n=-\infty}^{\infty} p_n[c_n(t)|c_n(0)]. \qquad (11)$$

Equation (10) is well known as the Langevin equation of Brownian motion and thus $p_n[c_n(t)|c_n(0)]$ can be obtained from the Fokker-Planck description of the process [10]

$$p_n[c_n(t)|c_n(0)] = \frac{1}{2\pi\sigma_n^2(t)}\exp\left[-\frac{|c_n - \langle c_n(t)\rangle|^2}{2\sigma_n^2(t)}\right], \qquad (12)$$

where

$$\langle c_n(t)\rangle = c_n(0)e^{-\nu k_n^2 t}, \quad \sigma_n^2(t) = \frac{\Gamma(1 - e^{-2\nu k_n^2 t})}{L\nu k_n^2}. \qquad (13)$$

Now we can write the functional integral (8) as a product of integrals over the coefficients c_n

$$G_L(\lambda,t) = \mathcal{N}\prod_{n=1}^{\infty}\int dc_n dc_n^* p_n^2[c_n(t)|c_n(0)]e^{-2\lambda|c_n|^2}, \qquad (14)$$

where $\mathcal{N}$ is a normalization factor. Substituting $p[c_n(t)|c_n(0)]$ from (12), the Gaussian integrals can be calculated and the inverse Laplace transform of the result gives the time-dependent probability distribution in a scaled form which does not depend explicitly on L:

$$\langle w^2\rangle_\infty P_L(w^2,t)$$

$$\equiv \hat{\Phi}(x,\tau,\{s_{n0}\})$$

$$= \int_{-i\infty}^{i\infty}\frac{dy}{2\pi i}e^{xy}\prod_{n=1}^{\infty}\frac{\exp[-ys_{n0}^2 e^{-n^2\tau}/(1+ya_n)]}{(1+ya_n)}. \qquad (15)$$

Here $\langle w^2\rangle_\infty = L\Gamma/(12\nu)$ and

$$a_n = \frac{6}{(\pi n)^2}(1 - e^{-\tau n^2}), \qquad (16)$$

with the scaling variables given by

$$x = \frac{w^2}{\langle w^2\rangle_\infty}, \quad \tau = \frac{8\pi^2\nu t}{L^2}, \quad s_{n0}^2 = \frac{2|c_n(0)|^2}{\langle w^2\rangle_\infty}. \qquad (17)$$

In the case of a flat initial surface ($s_{n0}=0$), one can evaluate the integral (15) exactly by collecting contributions from simple poles at $-1/a_n$ and one finds a scaling function of two variables:

$$\Phi(x,\tau) \equiv \hat{\Phi}(x,\tau,\{0\}) = \sum_{m=1}^{\infty}\frac{1}{a_m}\exp\left\{\frac{-x}{a_m}\right\}\prod_{n=1,n\neq m}^{\infty}\frac{a_m}{a_m - a_n}. \qquad (18)$$

For any finite x, the above sum can be approximated by a finite number of terms and $\Phi(x,\tau)$ can be evaluated with a given accuracy. Difficulties arise only in the limit of $\tau\to 0$ where $\Phi(x,\tau)$ goes into a delta function. The evolution of $\Phi(x,\tau)$ obtained by numerical evaluation of (18) can be seen in Fig. 1.

We conclude this section by calculating the time dependence of $\langle w^2\rangle$ which will be needed for comparing the time
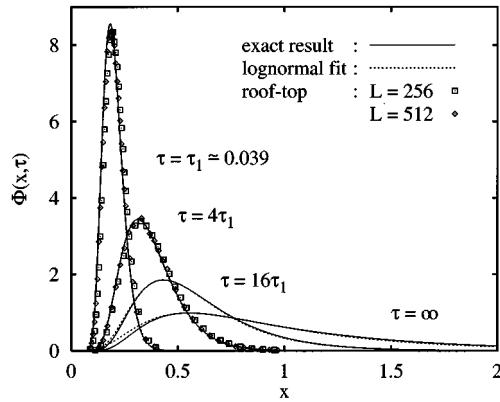
FIG. 1. Evolution of the scaling function of the width distribution in the case of a flat initial interface [Eq. (18)]. The scaling variables x and τ are given by Eq. (17). Exact results for the EW model are compared with log-normal fits and with Monte Carlo results on the ''roof-top'' model. The exact results and the log-normal fits are indistinguishable within linewidth for $\tau \lesssim 4\tau_1$.

scale of MC simulations with the time scale of the EW equation. We find $\langle w^2 \rangle_t$ from the generating function as $-\partial_\lambda G(\lambda)|_{\lambda=0}$

$$\frac{\langle w^2 \rangle_t}{\langle w^2 \rangle_\infty} = 1 + \sum_{n=1}^{\infty} \left(s_{n0}^2 - \frac{6}{\pi^2 n^2} \right) e^{-\tau n^2}. \quad (19)$$

In the long-time limit ($e^{-\tau} \ll 1$) this expression reduces to

$$\frac{\langle w^2 \rangle_t}{\langle w^2 \rangle_\infty} = 1 + \left(s_{10}^2 - \frac{6}{\pi^2} \right) e^{-\tau} + O(e^{-4\tau}), \quad (20)$$

and one can see that $\langle w^2 \rangle_t$ approaches its steady-state value much faster if we start with an initial surface where s_{10}^2 is set to its steady-state value $s_{10}^2 = s_{1\infty}^2 = 6/\pi^2$. The above equation also suggest a method for finding out in simulations if the system has settled to its steady state. One can choose small ($s_{10}^2 \ll s_{1\infty}^2$) and large ($s_{10}^2 \gg s_{1\infty}^2$) initial values for s_{10}^2 and then $\langle w^2 \rangle_t$ approaches its steady-state value from below and above, correspondingly. If the two values converged, one may assume that the steady state has been reached. This type of checking for steady state is widely used in simulations of equilibrium systems such as the Ising model where completely ordered and disordered initial states are employed. Similar procedures, however, do not seem to have been followed in the simulations of surface evolution models.

For short times, one can change the sum (19) into an integral and $\langle w^2 \rangle_t - \langle w^2 \rangle_{t=0}$ can also be calculated

$$\langle w^2 \rangle_t = \langle w^2 \rangle_0 + \sqrt{2/\pi\nu}\,\Gamma t^{1/2} + O(t). \quad (21)$$

The above result is valid for a flat initial state as well as for an initial surface containing a finite number of nonzero Fourier terms ($s_{n0} \neq 0$ for $n \leq n_{max}$).

III. LONG- AND SHORT-TIME ASYMPTOTICS

The case of arbitrary initial conditions with nonzero s_{n0}'s is complicated by the presence of essential singularities in the function which is integrated in (15). As a consequence,

we are not able to evaluate the probability distribution in general. The representation (15) is useful however for finding the long- and short-time asymptotics of $\Phi(x,\tau)$.

For $\tau \to \infty$, one has to keep contributions which are proportional to $e^{-\tau} \ll 1$. It follows then that Φ depends on the initial state only through the initial amplitude s_{10} of the longest wavelength mode. The calculation of the terms which are proportional to $e^{-\tau}$ involves collecting contributions from both simple poles and quadratic singularities in (15) with the result that the s_{10} dependence appears in a prefactor in front of a new scaling function $\Psi(x)$:

$$\hat{\Phi}(x,\tau,\{s_{n0}\}) = \Phi_s(x) + \left(1 - \frac{s_{10}^2 \pi^2}{6} \right) \Psi(x) e^{-\tau} + O(e^{-2\tau}), \quad (22)$$

where

$$\Psi(x) = \frac{\pi^2}{3} \left(\frac{7}{4} - \frac{\pi^2}{6} x \right) \exp\left\{ -\frac{\pi^2}{6} x \right\}$$
$$- \frac{\pi^2}{3} \sum_{m=2}^{\infty} (-1)^{m-1} \frac{m^4}{1-m^2} \exp\left\{ -\frac{\pi^2}{6} m^2 x \right\}. \quad (23)$$

This scaling function $\Psi(x)$ is shown in Fig. 3 and discussed in Sec. IV.

Comparing Eq. (22) with (20), one can see that the same prefactor, $s_{10}^2 - 6/\pi^2$, appears in front of $e^{-\tau}$ in both cases. Thus the relaxation of the scaling function is also accelerated if s_{10} is chosen to be the steady-state value $s_{1\infty}$. Furthermore, it also follows that the steady-state distribution can also be bracketed by choosing small and large initial values for s_{10}.

Now we turn to the description of the short-time limit of $\Phi(x,\tau)$ in case of a flat initial condition. The description is based on an earlier observation [11] that the fluctuations of chemical reaction fronts which are supposed to belong to the EW universality class produce a $\Phi(x,\tau)$ which is rather well approximated by log-normal distribution [12]

$$\Phi(x,\tau) \approx \mathcal{L}(x,x_0,\sigma) = \frac{1}{\sqrt{2\pi}\sigma x} \exp\left\{ -\frac{\ln^2(x/x_0)}{2\sigma^2} \right\}, \quad (24)$$

where $x_0(\tau)$ and $\sigma(\tau)$ are fitting parameters which can be determined from various considerations. We have determined $x_0(\tau)$ and $\sigma(\tau)$ by equating both the maxima and positions of the maxima x_m of the two functions $\Phi(x,\tau)$ and $\mathcal{L}(x,x_0,\sigma)$. The values of x_m and $\Phi(x_m,\tau) = \Phi_m(\tau)$ have been determined numerically from (18) and then σ was obtained by solving the following equation:

$$\sqrt{2\pi}\,x_m \Phi_m \sigma = e^{-\sigma^2/2}, \quad (25)$$

and finally, x_0 was expressed as $x_0 = x_m \exp(\sigma^2)$. For sufficiently short times, the width of the distribution goes to zero and $\sigma \to 0$. In this limit the expressions for x_0 and σ simplify to $x_0 \approx x_m$, and $\sigma \approx 1/(\sqrt{2\pi}\,x_m \Phi_m)$.

The results of this fitting procedure can be seen in Fig. 1. Qualitatively, the fit is quite good over the whole time inter-
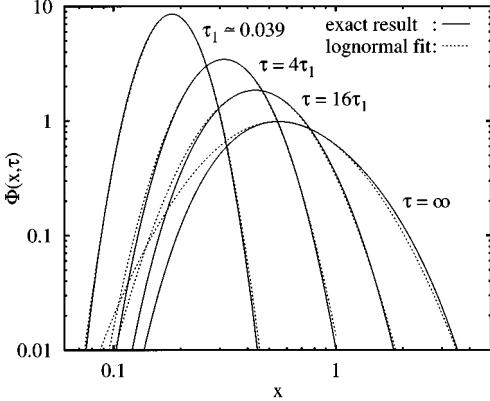
FIG. 2. The analytical results and the log-normal fits of Fig. 1 on a log-log plot.

FIG. 3. Scaling function $\Psi(x)$ describing the long-time relaxation of the width distribution [Eq. (22)]. The theoretical curve for the EW model is compared with the Monte Carlo results for both the EW and KPZ limits of the ''roof-top'' model. The initial states are either flat or contain a single sine perturbation with the longest available wavelength.

val and it clearly becomes excellent at short times. In order to make the quality of the short-time fit more apparent, we have redrawn the curves of Fig. 1 on a log-log plot with the results shown on Fig. 2. As one can see again, the log-normal fit becomes better at small times and, at $\tau = 0.039$, the fit becomes practically indistinguishable from $\Phi(x,\tau)$ in an interval where the function decreases from its maximum value by three orders of magnitude.

A more quantitative description of the quality of the log-normal fit can be given by defining a relative distance between the two functions as

$$\ell(\tau) = \max_x \frac{|\Phi(x,\tau) - \mathscr{L}(x,x_0,\sigma)|}{\Phi_m(\tau)}. \qquad (26)$$

This distance increases with τ and reaches its maximum value $\ell_{\max} = \ell(\infty) \approx 0.14$ in the stationary state. For $\tau \to 0$, we find that $\ell \sim \tau^{1/2}$ and $\ell < 0.01$ for $\tau < 0.02$. Although the diminishing relative distance actually comes from the ratio of a strongly divergent $\Phi_m(\tau) \sim \tau^{-3/4}$ and a less divergent maximum distance $\max_x|\Phi - \mathscr{L}| \sim \tau^{-1/4}$, plots of the two functions which extend from zero to their maxima are indistinguishable (see Fig. 1) for $\tau < 0.1$.

IV. MONTE CARLO SIMULATIONS

In order to see if the dynamic scaling found for the width distribution had the expected universality, we carried out Monte Carlo simulations for a ''roof-top'' model of surface evolution [8,9]. In this model the height of the surface is characterized by a single-valued function h_i at sites $i = 1,2,\ldots,L$ and periodic boundary conditions $h_{i+L} = h_i$ are imposed. The height differences are restricted to $h_{i+1} - h_i = \pm 1$ and the evolution consists of particles being deposited at local minima or evaporating from local maxima of the surface with rates p_+ and $p_- = 1 - p_+$, respectively. If $p_+ = p_- = 1/2$, the model belongs to the universality class of EW model while for $p_+ \neq p_-$ the universality class is that of the KPZ equation [9].

For equal rates, one can obtain [9] an exact expression for $\langle w^2 \rangle_t$ and comparing the result with the solution of the EW Eq. (19), the time scale of the MC simulation can be related to that of the EW equation. In this way one finds that the parameters ν and Γ should be set to $\nu = \Gamma = 1/2$. Then the

x's and τ's in the MC data and in the EW equation are related in a unique way and there are no parameters to fit when the Φ's are compared. Figure 1 shows both the $\Phi(x,\tau)$'s obtained from simulation and the theoretical curves of the EW model. One finds good agreement although a small systematic shift of the MC curves towards larger values of x can be observed. This shift is due to the fact that, in the ''roof-top'' model, the initial surface is not entirely flat ($w_{t=0}^2 = 1/4$) in variance with the $w_{t=0}^2 = 0$ used in the theoretical calculation. This difference should disappear in the $L \to \infty$ limit and, indeed, one can see that the difference is smaller for the $L = 512$ sample as compared to the $L = 256$ system.

We have also examined the function $\Psi(x)$ which characterizes the scaling of the long-time relaxation of the distribution function in the EW model (23). Since one can find a large enough time window where $\langle w^2 \rangle_\tau - \langle w^2 \rangle_\infty \sim e^{-\tau}$ for all x, the function $\Psi(x)$ can be determined accurately and, as can be seen from Fig. 3, there is an excellent agreement with the theoretical curve. Thus we can conclude that the ''roof-top'' model which belongs to the EW universality class for $p_+ = p_- = 1/2$ indeed produces the same time-dependent distribution $\Phi(x,\tau)$ as the EW equation.

In order to investigate if the $\Phi(x,\tau)$'s characterizing the EW and the KPZ classes were distinguishable, we have also studied the long-time behavior of the ''roof-top'' model for unequal rates ($p_+ = 1$, $p_- = 0$). In this case, we find that $\langle w^2 \rangle_\infty P_L(x,t) - \Phi(x,\infty)$ decays with time exponentially $\exp(-\alpha_L t)$, with a relaxational rate, α_L independent of x and, as can be seen in Fig. 3, the coefficient, $\Psi(x)$, of the exponential differs significantly from that of the corresponding EW scaling function.

V. FINAL REMARKS

It has been demonstrated previously [3–5] that one can build a ''picture gallery'' of scaling functions for steady-state width distributions and this gallery may be used for distinguishing the static universality classes of growth pro-

cesses. Here we have made the first steps towards building a similar gallery for dynamic scaling functions and we believe that this gallery will be equally instrumental in recognizing dynamical universality classes. At this moment we have results only for the one-dimensional EW and KPZ processes but there does not seem to be any principal difficulty in extending these calculations to other processes and to higher dimensions by using exact solutions, renormalization-group methods, and simulations.

An interesting by-product of our calculation is the result that the early-time width distribution in the EW process is practically identical to the log-normal distribution. Log-normal-like distributions tend to emerge more often in biological and social sciences than in physics [12,13] and they are usually understood in terms of the ''law of proportionate effect'' or on the basis of the assumption that an event occurs only if a large number of independent ''subevents'' take place. In our case, the log-normal distribution is produced by EW dynamics and it appears as a characteristic of the initial roughening of an interface. Whether this generation of log-normal-like distributions was new or it was equivalent to one of the standard derivations remains to be understood.

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