PHYSICAL REVIEW E VOLUME 50, NUMBER 5 NOVEMBER 1994

Width distribution of curvature-driven interfaces: A study of universality

M. Plischke and Z. Rácz*
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6

R. K. P. Zia
Center for Stochastic Processes in Science and Engineering and Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061
(Received 12 July 1994)

One-dimensional interfaces with curvature-driven growth kinetics are investigated. We calculate the steady-state distribution $P(w^2)$ of the square of the width of the interface w^2 and show that, as in the case for random-walk interfaces, the result can be written in a scaling form $\langle w^2\rangle P(w^2) = \Phi(w^2/\langle w^2\rangle)$, where $\langle w^2\rangle$ is the average of w^2. The scaling function $\Phi(x)$ is found to be distinct from that of random-walk interfaces, but, as our Monte Carlo simulations indicate, this function is universal for curvature-driven growth. It is argued that comparison of scaling functions can be a useful method for distinguishing between universality classes of growth processes.

PACS number(s): 05.50.+q, 05.70.Ln, 64.60.Cn

I. INTRODUCTION

The simplest quantitative characteristic of an interface is its width w, defined as the root-mean-square fluctuation of the interface around its average position. For rough interfaces, the average width $\langle w\rangle$ diverges as the size L of the system goes to infinity and one usually observes scaling with time t and L in the form $\langle w\rangle \sim L^{\zeta} f(t/L^z)$. This scaling form and the associated critical exponents provide a useful framework for analyzing and classifying interfaces formed in various equilibrium and nonequilibrium processes [1,2]. A problem with $\langle w\rangle$, however, is that crossover effects are often quite pronounced and this makes it difficult to extract the critical exponents ζ and z. This problem is somewhat reduced by characterizing interfaces in terms of the static and dynamic structure functions which are the Fourier transforms of the spatial fluctuations. The virtue of these functions is that the important long-wavelength modes can be separated and studied in detail. The precise determination of the critical exponents, and thus the classification of growth processes, however, remains a difficult task and it is desirable to develop alternative methods for their analysis.

Recently, it has been suggested [3] that an interesting and potentially useful characteristic of a surface is the steady-state distribution of its width (or its width squared) $P(w^2)$. For one-dimensional random-walk interfaces, $P(w^2)$ has been calculated and the results show that $P(w^2)$ contains a single length scale which is the quantity $\langle w^2\rangle^{1/2}$. As a consequence, the probability distribution can be written in a scaling form

$$P(w^2) = \langle w^2\rangle^{-1}\Phi(w^2/\langle w^2\rangle) \quad . \tag{1}$$

It turns out that $\Phi(x)$ is a universal function in the sense that a number of surface evolution models, which are expected to be in the "random-walk" universality class, produce the same function Φ.

The scaling form (1) is not surprising; it follows from dimensional analysis provided there is only a single scale $\langle w^2\rangle$ for w^2. The universality of Φ, however, is not quite obvious. In order to understand it, we have to view rough surfaces as finite-size systems at a critical point and, furthermore, we should note that w^2 can be considered to be a macroscopic quantity since it diverges as the size of the system goes to infinity. Then the universality of Φ may follow from the fact that the distribution of macroscopic quantities at an (equilibrium) critical point (e.g., the distribution of the magnetization in an Ising model at the critical temperature [4]) is described in terms of scaling functions which are universal. Provided the above analogy with equilibrium critical points is correct, one can, in principle, proceed to create a directory of Φ's and classify surfaces by their scaling functions. It should be remarked that this approach is not without experimental implications. In a recent experiment, Tong *et al.* [5] measured the height distribution of a growing surface in an atomic force microscope study of molecular-beam epitaxial growth. Thus experimental techniques are available for measuring $P(w^2)$ and thus deducing Φ.

Of course, nonequilibrium systems have provided us with many surprises and the equilibrium arguments used above may have only a limited validity. Thus the universality of Φ should be checked by working out concrete examples. This is what we shall do below by calculating Φ for a ($d = 1$)-dimensional deposition-surface-diffusion model in which the diffusion current depends only on the curvature of the surface [6,7]. The result is then compared to Φ's obtained from Monte Carlo (MC) simula-

*Permanent address: Institute for Theoretical Physics, Eötvös University, 1088 Budapest, Puskin u. 5-7, Hungary.

tions of discrete models with curvature-driven kinetics [8–10] that are expected to belong to the same universality class. We find good agreement between theoretical and "experimental" results and thus provide evidence for the universality of Φ.

Finally, we have also considered the Wolf-Villain model [11] for which ζ, if measured in the most naive fashion, is equal to that of the curvature-driven models ($\zeta = 3/2$). Indeed, for some time, it was believed that these models were in the same universality class. Closer examination [12] revealed, however, that the Wolf-Villain model has a rather peculiar scaling behavior and it does not appear to belong to the universality class of models with curvature-driven kinetics. Our simulations support this view: The Φ obtained for the Wolf-Villain model is distinct from that of the curvature-driven models.

II. MODEL AND THE CALCULATION OF THE WIDTH DISTRIBUTION

A simple and much studied model of surface growth occurring through deposition coupled to surface diffusion is a linear Langevin equation [6,7] which, in the $d = 1$ case, is

$$\frac{\partial h(x,t)}{\partial t} = -\nu \frac{\partial^4 h(x,t)}{\partial x^4} + \eta(x,t) \quad . \tag{2}$$

Here $h(x,t)$ is the height of the surface at time t above a substrate of linear dimension L. The coordinate x is measured along the substrate $0 \leq x \leq L$ and periodic boundary conditions $h(x+L,t) = h(x,t)$ are assumed. The first term on the right-hand side with $\nu > 0$ provides a simplified description of surface diffusion while the second term (η) is a nonconserved noise resulting from the fluctuations of the deposition rate. As usual, η is assumed to be Gaussian white noise with correlations of the form

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

The model defined by (2) and (3) can be solved exactly and the the critical exponents $\zeta = 3/2$ and $z = 4$ are known. Furthermore, the steady-state distribution of configurations $\{h(x)\}$ can also be calculated [13] since the model satisfies detailed balance (this can be explicitly seen after rescaling lengths by ν/Γ). As a result, one finds a quadratic effective Hamiltonian in the probability distribution

$$\mathcal{P}(\{h\}) = \mathcal{N} \exp\left[-\frac{\nu}{2\Gamma}\int_0^L \left(\frac{\partial^2 h}{\partial x^2}\right)^2 dx\right] \quad , \tag{4}$$

where $\mathcal{N}$ is a normalization factor and $h \equiv h(x)$. The effective Hamiltonian depends only on the curvature of the surface, hence the name "curvature-driven" kinetics.

Once $\mathcal{P}(\{h\})$ is known, we can calculate $P(w^2)$ by repeating the steps in the derivation of $P(w^2)$ for random walk interfaces [3]. First, the square of the width of the surface w^2 in a configuration $\{h\}$ is defined as

$$w^2(\{h\}) = \overline{h^2} - \overline{h}^2 \quad , \tag{5}$$

where we introduced the average $\overline{f}$ of a function $f(h)$ in a given configuration $\{h\}$ as the integral

$$\overline{f}(\{h\}) = \frac{1}{L}\int_0^L dx\, f(h)\,. \tag{6}$$

Next, we express the probability density $P(w^2)$ as a path integral $\int \mathcal{D}[h]$ over all periodic paths [14,15]

$$P(w^2) = \int \mathcal{D}[h]\,\delta\left(w^2 - [\overline{h^2} - \overline{h}^2]\right)\mathcal{P}(\{h\}) \,, \tag{7}$$

and, in order to eliminate the δ function, we introduce the generating function for the moments of $P(w^2)$

$$G(\lambda) = \int_0^\infty dz\, P(z)e^{-\lambda z} \quad . \tag{8}$$

Substituting (4) into (7) and evaluating the integral (8), we find that $G(\lambda)$ is a Gaussian functional integral

$$G(\lambda) = \mathcal{N}\int \mathcal{D}[h]\,\exp\left[-\frac{\nu L}{2\Gamma}\overline{(\Delta h)^2} - \lambda\left(\overline{h^2} - \overline{h}^2\right)\right] \,. \tag{9}$$

This functional integral can be calculated by expressing h in terms of a Fourier series $h(x) = \sum_n c_n \exp(2\pi i n x/L)$ and then evaluating the product of Gaussian integrals over the coefficients c_n. As a result, $G(\lambda)$ is obtained in closed form

$$G(\lambda) = \prod_{n=1}^{\infty}\left(1 + \frac{\sigma\lambda}{4\pi^4 n^4}\right)^{-1} = \frac{\sqrt{\sigma\lambda}}{\cosh[(\sigma\lambda)^{1/4}] - \cos[(\sigma\lambda)^{1/4}]} \quad , \tag{10}$$

where $\sigma = \Gamma L^3/(2\nu)$ and where we have used the identity $k\pi\prod_{n=1}^{\infty}(1 + k^2/n^2) = \sinh(k\pi)$ in deriving the second equality.

The average of w^2 can now be calculated as the first moment of $P(w^2)$ and one finds

$$\langle w^2\rangle = -\left.\frac{dG}{d\lambda}\right|_{\lambda=0} = \frac{\sigma}{360} = \frac{\Gamma}{720\nu}L^3 \quad . \tag{11}$$

The well known exponent $\zeta = 3/2$ can be read off from the above equation and, furthermore, it follows from $\langle w^2\rangle \sim \sigma$ that $G(\lambda)$ is a function only of the product $\langle w^2\rangle\lambda$. Consequently, $\langle w^2\rangle$ is the only scale for w^2 and $P(w^2)$ has the scaling form discussed in the Introduction

$$P(w^2) = \int_{-i\infty}^{i\infty}\frac{d\lambda}{2\pi i}\,G(\lambda)\,e^{w^2\lambda} = \frac{1}{\langle w^2\rangle}\Phi\left(\frac{w^2}{\langle w^2\rangle}\right) \quad . \tag{12}$$

The last step is to evaluate the scaling function $\Phi(x)$ by collecting the residues of $G(\lambda)\,e^{w^2\lambda}$ at the simple poles

$\lambda = -(n\pi)^4/(90\langle w^2\rangle)$, where $n = 1, 2, \ldots$. The resulting sum can be written in a form that is easily calculated numerically

$$\Phi(x) = \frac{2\pi^5}{45} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}\, n^5}{\sinh(\pi n)} \exp\left(-\frac{\pi^4}{90} n^4 x\right) . \quad (13)$$

Figure 1 shows $\Phi(x)$ together with the corresponding scaling function for random-walk interfaces. One can see that the two scaling functions are different and easily distinguishable.

In the case of random-walk interfaces, simple expressions of large- and small-x asymptotics describe the entire function $\Phi(x)$ very well. The large-x asymptotics of $\Phi(x)$ is simple in the present case too [it is just given by the first term of the sum (13)] and it approximates Φ well starting already at $x \approx 0.25$:

$$\Phi(x) \approx \frac{2\pi^5}{45 \sinh(\pi)} \exp\left(-\frac{\pi^4}{90} x\right) , \quad x \geq 0.25 . \quad (14)$$

The small-x asymptotics, which is obtained by calculating the integral (12) using the method of stationary phase, however, has only a small range of validity:

$$\Phi(x) \approx \left(\frac{2^8 3^7 5^5}{\pi^3 x^{11}}\right)^{1/6} \exp\left[-\frac{3}{2}\left(\frac{45}{4x}\right)^{1/3}\right] , \quad x \leq 0.03. \quad (15)$$

Having completed the calculation of Φ, we turn now to various discrete, curvature-driven surface-evolution models and test the idea of universality of Φ by comparing their scaling functions to the result obtained above.

III. MONTE CARLO SIMULATIONS

We shall present here MC results for Φ for the following three models of deposition coupled to surface diffusion: (i) the "$n = 2$ model" of Siegert and Plischke [8], (ii) the "larger-curvature model" introduced independently by Kim and Das Sarma [9] and by Krug [10], and (iii) the "larger-coordination model" of Wolf and Villain [11]. The first two models are expected to belong to the universality class of the curvature-driven growth since the diffusion (hopping) of particles depends only on the local curvature of the surface. The third one, however, has been shown to display scaling behavior more complex than that following from the continuum description of curvature-driven growth. Thus we expect that the Φ's for models (i) and (ii) are given by Eq. (13), while model (iii) should display a distinct scaling function.

The above models are all solid-on-solid type models with a given rate of deposition of particles of height one. The differences are in the way the diffusion on the surface is modeled. In the $n = 2$ model [8], the hopping of particles satisfies detailed balance and, furthermore, the energy functional is a quadratic function of height differences $E(\{h\}) = \sum_i [h(i) - h(i+1)]^2$, where i denotes the sites along the substrate. A hopping rate that satisfies detailed balance for the process $h(i) \to h(i) - 1$ and $h(i+1) \to h(i+1) + 1$ is given, e.g., by $W = \tau^{-1}[\exp(\beta\Delta E) + 1]^{-1}$, where ΔE is the change of energy due to change in the position of the particle, β is the inverse temperature, and τ is the parameter which determines the rate of diffusion with respect to the rate of deposition. For a quadratic energy function, ΔE due to a hop from i to $i+1$ is proportional to $h(i+2) - 3h(i+1) + 3h(i) - h(i-1)$, which is nothing but the discretized version of the spatial derivative of the curvature. Thus the rate of hopping and, consequently, the diffusion of particles are driven by the local curvature of the surface. Of course, if diffusion were the only dynamics, then the noise would be *conserved* and the system would evolve to an equilibrium state with $\mathcal{P}(\{h\}) \sim \exp[-\beta E(\{h\})]$, so that the width distribution would be that of the random-walk interfaces [3]. This model, however, also involves the deposition of particles which provides a *nonconserved* noise. The curvature-driven deterministic dynamics combined with nonconserved noise is then expected to give rise to an effective Hamiltonian $H_e \sim \sum_i [h(i+1) - 2h(i) + h(i-1)]^2$ even though the underlying Hamiltonian is just $H \sim \sum_i [h(i) - h(i+1)]^2$. As can be seen from Fig. 2, the simulation of this model indeed produces a width distribution that is practically identical to the theoretical curve given by Eq. (13).

In the larger-curvature model [9,10], the deposition and the diffusion are coupled in the sense that a site i is randomly chosen for deposition, but then the cur-

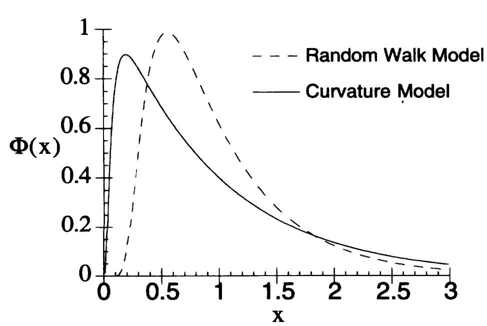

FIG. 1. Comparison of scaling functions for the width distribution of periodic random walks and for the curvature-driven model as given by Eq. (13).

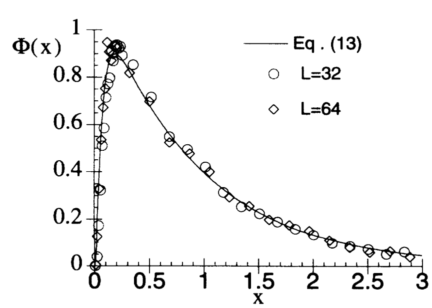

FIG. 2. Scaling functions for the curvature-driven model and for the "$n = 2$ model" of Siegert and Plischke with substrate sizes $L = 32$ and 64. Note that no fitting parameters are used in collapsing the curves.

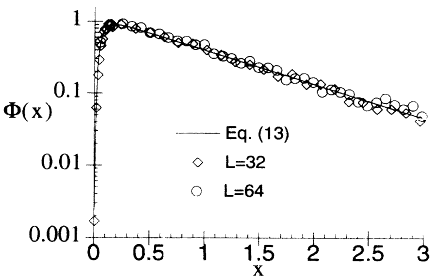

FIG. 3. Comparison of scaling functions of the curvature-driven model and of the "larger-curvature" model of Kim and Das Sarma and of Krug for a system of sizes $L = 32$ and 64. In order to demonstrate better the collapse of the theoretical and MC curves at small Φ (at small probabilities), we present the data on a semilog plot.

vatures at sites $i - 1$, i, and $i + 1$ are examined and the deposited particle moves to the site with the largest curvature. Since, by construction, diffusion depends on curvature only, one expects and indeed finds [9] that, by measuring the critical exponents, this model belongs to the universality class of curvature-driven interfaces. Our simulations further confirm this fact; Fig. 3 shows that the scaling function for the larger-curvature model follows the theoretical curve (13) over the measured range of probabilities.

The Wolf-Villain model [11] is also a model where the "diffusion" immediately follows the deposition of the particle. If the randomly chosen deposition site is i, then the particle may move in the next step to either $i-1$ or $i+1$ provided the move increases the coordination number of the particle. The coordination number (the number of nearest-neighbor sites which are occupied) cannot be expressed through the curvature of the surface alone. Consequently, the continuum description of this model may contain nonlinear terms which are relevant perturbations to the $\partial^4 h/\partial x^4$ term in Eq. (2). Recent studies [11,12] point in this direction and indeed we find (see Fig. 4)

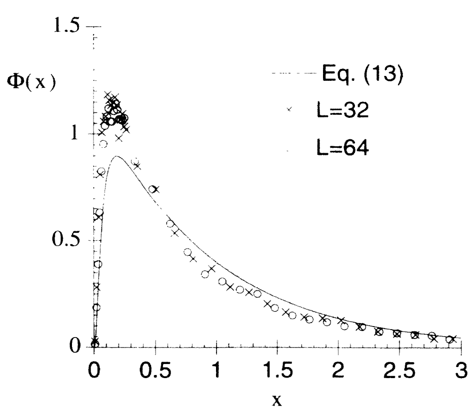

FIG. 4. Comparison of scaling functions for the curvature-driven model and for the Wolf-Villain model with a system sizes $L = 32$ and 64.

that the scaling function of the width distribution is distinct from the corresponding Φ of the curvature-driven surfaces. Thus the assumption of universality of the scaling function Φ is consistent with the view that the Wolf-Villain model is in a universality class that is different from that of the curvature-driven surfaces.

IV. FINAL REMARKS

The results presented in Sec. III in conjunction with the evidence coming from random-walk interfaces [3] provide strong support for our suggestion that $\Phi(x)$ can be used to distinguish universality classes of growing interfaces. As with every method, however, when trying to implement it, one encounters problems of principle as well as practical difficulties.

From the point of view of principle, we see the following limitation. It is known from the theory of critical phenomena that there can be many dynamic universality classes associated with a single static class [18]. The reason for this is the decoupling of dynamics and statics due to the detailed balance condition satisfied by any dynamics in the equilibrium state. Thus equilibrium distributions provide information only about the static universality classes. In nonequilibrium systems, however, dynamics and steady-state properties are coupled nontrivially and, consequently, $P(w^2)$ carries information about the dynamics. The coupling of statics and dynamics in surface evolution models emerges in the form of scaling laws connecting the static ζ and the dynamic z exponents (it appears that most surface evolution models presently under study satisfy such scaling laws; see [2,11,19]). This is crucial if we want to distinguish universality classes in growth processes by using the steady-state distribution function. It may happen, however, that the system is effectively an equilibrium system and then the information about the dynamics is lost in Φ. An example is the Kardar-Parisi-Zhang (KPZ) model [16], which, in $d = 1$ dimension, satisfies detailed balance. As a consequence, its $P(w^2)$ is equal to that of the Edwards-Wilkinson model [17], although these two models are in different universality classes. This feature of the KPZ equation does not exist in $d = 2$ or higher dimensions, but, unfortunately, this is not known *a priori* about other processes. Perhaps a conservative viewpoint here would be that Φ can be used at least to distinguish static universality classes of surface growth. The question of what the circumstances are when the dynamics is also encoded in Φ and how to decode that information remains to be investigated. The problem discussed above can, of course, be bypassed by studying the *time-dependent* width distribution. The price one pays is that the calculational difficulties increase significantly.

From a practical point of view, the problem with Φ is that its calculation by analytical means seems to be highly nontrivial for any process for which nonlinear terms are relevant in the Langevin description. This difficulty can be overcome by using MC simulations both in producing the directory of Φ's and in comparing scaling functions. In principle, one should also be able to develop renormalization-group methods for calculating Φ.

The above problems notwithstanding, we believe that the calculation of the width distribution provides us with a new and interesting tool in the investigations of interfaces. Application of the above ideas to two-dimensional interfaces and to the analysis of experimental results will be described in a separate presentation [20].

ACKNOWLEDGMENTS

Z.R. is grateful for hospitality extended to him during his stay at Simon Fraser University. R.K.P.Z. thanks the Isaac Newton Institute (Cambridge, U.K.), where some of this research was accomplished. We thank J. Shore for helpful discussions and for critical reading of the manuscript. This work was partly supported by the NSERC of Canada and by the Division of Materials Research of the U.S. National Science Foundation.

[1] F. Family and T. Vicsek, J. Phys. A **18**, L75 (1985).
[2] For a recent review, see J. Krug and H. Spohn, in *Solids far from Equilibrium: Growth, Morphology and Defects*, edited by C. Godrèche (Cambridge University Press, Cambridge, England, 1991).
[3] G. Foltin, K. Oerding, Z. Rácz, R. Workman, and R.K.P. Zia, Phys. Rev. E **50**, 639 (1994).
[4] K. Binder, Z. Phys. B **34**, 119 (1981); A.D. Bruce, J. Phys. C **14**, 3667 (1981).
[5] W.M. Tong, R.S. Williams, A. Yanase, Y. Segawa, and M.S. Anderson, Phys. Rev. Lett. **72**, 3374 (1994).
[6] W.W. Mullins, J. Appl. Phys. **28**, 333 (1957).
[7] J. Villain, J. Phys. I **1**, 19 (1991).
[8] M. Siegert and M. Plischke, Phys. Rev. E **50**, 917 (1994).
[9] J.M. Kim and S. Das Sarma, Phys. Rev. Lett. **72**, 2903 (1994).
[10] J. Krug, Phys. Rev. Lett. **72**, 2907 (1994).
[11] D.E. Wolf and J. Villain, Europhys. Lett. **13**, 389 (1990).
[12] M. Schroeder, M. Siegert, D.E. Wolf, J.D. Shore, and M. Plischke, Europhys. Lett. **24**, 563 (1993); M. Plischke, J.D. Shore, M. Schroeder, M. Siegert, and D.E. Wolf, Phys. Rev. Lett. **71**, 2509 (1993).
[13] C.W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, New York, 1983).
[14] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1971), Vol. II.
[15] R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965); H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics* (World Scientific, Singapore, 1990).
[16] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).
[17] S.F. Edwards and D.R. Wilkinson, Proc. R. Soc. London Ser. A **381**, 17 (1982).
[18] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
[19] P. Meakin, P. Ramananlal, L.M. Sander, and R.C. Ball, Phys. Rev. A **34**, 5091 (1986).
[20] Z. Rácz and M. Plischke (unpublished).