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Width distribution for random-walk interfaces

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Roughening of a one-dimensional interface is studied under the assumption that the interface configurations are continuous, periodic random walks. The distribution of the square of the width of interface, w^2, is found to scale as $P(w^2)=\langle w^2\rangle^{-1}\Phi(w^2/\langle w^2\rangle)$ where $\langle w^2\rangle$ is the average of w^2. We calculate the scaling function $\Phi(x)$ exactly and compare it both to exact enumerations for a discrete-slope surface evolution model and to Φ's obtained in Monte Carlo simulations of equilibrium and driven interfaces of chemically reacting systems.

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Interfaces (invariably called surfaces, reaction fronts, active zones, etc.) play an important role in our understanding of a large number of physical, chemical, and biological processes. Apart from practical importance such as, e.g., the quality of a growing crystal being determined by the properties of its moving surface, interest in interfaces stems also from the realization that pattern formation in the wake of a moving front is a rather general phenomenon [1]. Two-dimensional equilibrium systems as well as nonequilibrium steady states frequently display rough interfaces and there are many examples where the width w (defined as the root mean square fluctuation in the position of the interface) is proportional to the (length)$^{1/2}$ of the interface. The $w\sim$(length)$^{1/2}$ scaling is a basic feature of random walks and the connection actually runs deeper since random-walk models [2,3] (and their generalizations to higher dimensions [4]) have been very successful in describing various features of interfaces. Our aim here is to return to this "old but perennially alive topic of *random walks*" [3] and derive the probability distribution $P(w^2)$ for interfaces describable by such walks. We do this because w^2 is one of the simplest and certainly the most investigated quantity in the theory of growing surfaces [5]. The way of achieving a more detailed description is usually the investigation of static and dynamic structures factors. Here we suggest that another path for detailed characterization of the surface is the study of the distribution of the width and, as a first step along this path, we calculate $P(w^2)$ for random-walk interfaces. The results show that $P(w^2)$ contains a single scale which is the average $\langle w^2\rangle$, and so the probability distribution is obtained in terms of a universal scaling function $P(w^2)=\langle w^2\rangle^{-1}\Phi(w^2/\langle w^2\rangle)$. We then calculate this scaling function Φ for a discrete-slope surface-evolution model as well as for the interfaces emerging in Monte Carlo (MC) simulations of catalytic reactions. In both cases, we find excellent agreement (without using any adjustable parameters) with the random-walk results.

We turn now to the derivation of the main result. As a continuum model for a one-dimensional fluctuating surface, consider Brownian paths $\{h_t\}$ in the time interval $0\leq t\leq T$ and require the paths to be periodic with period T. The correspondence between a path $\{h_t\}$ and a surface configuration is given by identifying h_t as the height of the surface over a substrate of length T with t being the coordinate along the substrate. The surface roughness of a configuration $\{h_t\}$ is characterized by the square of the width of the surface, w^2, defined as the mean square of height fluctuations:

$$w^2(\{h_t\})=\overline{h_t^2}-\overline{h_t}^2, \tag{1}$$

where the average $\bar{f}$ of a function $f(h_t)$ in a configuration $\{h_t\}$ is defined as

$$\bar{f}(\{h_t\})=\frac{1}{T}\int_0^T dt\, f(h_t). \tag{2}$$

The calculation of the probability density $P(w^2)$ for the random variable w^2 is done by writing $P(w^2)$ as a path integral [6,7]:

$$P(w^2)=\mathcal{N}\int \mathcal{D}[h]\,\delta(w^2-[\overline{h_t^2}-\overline{h_t}^2])\exp\left(-\frac{T}{2}\overline{\dot{h}_t^2}\right), \tag{3}$$

where $\int\mathcal{D}[h]$ stands for sum over all periodic paths, $\mathcal{N}$ is a normalization constant, and $\dot{h}_t=dh_t/dt$. It should be noted that the above expression could have been the starting point of our discussion had we assumed that the interface was a random Gaussian surface [4].

The Laplace transform of the probability density determines the generating function for the moments of $P(w^2)$:

$$G(\lambda)=\int_0^\infty d\zeta\, P(\zeta)e^{-\lambda\zeta}, \tag{4}$$

and one finds that $G(\lambda)$ is the following Gaussian functional integral:

$$G(\lambda)=\mathcal{N}\int \mathcal{D}[h]\exp\left[-\frac{T}{2}\overline{\dot{h}_t^2}-\lambda(\overline{h_t^2}-\overline{h_t}^2)\right]. \tag{5}$$

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This functional integral can be calculated by standard methods [7]. For periodic paths, we write h_t in terms of a Fourier series

$$h_t = \sum_{n=-\infty}^{\infty} c_n e^{2\pi i n t/T}, \quad c_{-n} = c_n^*, \tag{6}$$

and Eq. (5) reduces to a product of Gaussian integrals over the coefficients c_n:

$$G(\lambda) = \mathcal{N} \cdot \int \mathcal{D}[c] \exp\left[-\sum_{n=1}^{\infty} \left(\frac{(2\pi n)^2}{T} + 2\lambda \right) |c_n|^2 \right]. \tag{7}$$

The integration with respect to the homogeneous mode c_0 generates an (infinite) constant which can be absorbed into the normalization factor, and the remaining integrals over the real and imaginary parts of c_n $(n=1,2,\ldots)$ give

$$G(\lambda) = \prod_{n=1}^{\infty} \left(1 + \frac{2\lambda T}{(2\pi n)^2} \right)^{-1} = \frac{\sqrt{\lambda T/2}}{\sinh(\sqrt{\lambda T/2})}. \tag{8}$$

Note that we have obtained an expression which is similar to the partition function of the harmonic oscillator [7]. This is expected from the form of Eq. (5); differences are due to the boundary conditions. The moments of $P(w^2)$ can now be calculated and one finds the average of w^2 as

$$\langle w^2 \rangle = -\left. \frac{dG}{d\lambda} \right|_{\lambda=0} = \frac{T}{12}. \tag{9}$$

Comparing now (8) and (9), we can see that $G(\lambda)$ is a function of the product $\langle w^2 \rangle \lambda$ only and thus the inverse Laplace transform of $G(\lambda)$ yields $P(w^2)$ in a scaling form:

$$P(w^2) = \int_{-i\infty}^{i\infty} \frac{d\lambda}{2\pi i} G(\lambda) e^{w^2 \lambda} = \frac{1}{\langle w^2 \rangle} \Phi\left(\frac{w^2}{\langle w^2 \rangle} \right). \tag{10}$$

The inverse Laplace transform and, consequently, the scaling function $\Phi(x)$, can be easily calculated since $G(\lambda)$ has only simple poles at $\lambda = -2(n\pi)^2/T$ $(n=1,2,\ldots)$. Collecting the contributions from the poles, we find

$$\Phi(x) = \frac{\pi^2}{3} \sum_{n=1}^{\infty} (-1)^{n-1} n^2 \exp\left(-\frac{\pi^2}{6} n^2 x \right). \tag{11}$$

Finite-sum approximants to the above expression converge quickly for any finite $x>0$ since significant contributions come only from the first $1/\sqrt{x}$ terms. For $x \geq 1.5$, the sum is dominated by the first term

$$\Phi(x) \approx \frac{\pi^2}{3} \exp\left(-\frac{\pi^2}{6} x \right), \quad x \geq 1.5 \tag{12}$$

and Fig. 1 shows that the large-x asymptotics is indeed indistinguishable from the "exact" result [obtained by retaining 10^3 terms in (11)] in this regime. It is remarkable that $\Phi(x)$ is very well approximated by a simple analytical form in the $0 \leq x \leq 1.5$ interval as well, using the method of stationary phase. In calculating the integral (10), the path of integration may be chosen as a parabola $[\mathrm{Re}\lambda = a(1-y^2), \mathrm{Im}\lambda = 2ay]$ where $-\infty < y < \infty$ and $a = 3\langle w^2 \rangle / (2w^2)$. As a result, one finds the following $x \to 0$ asymptotics:

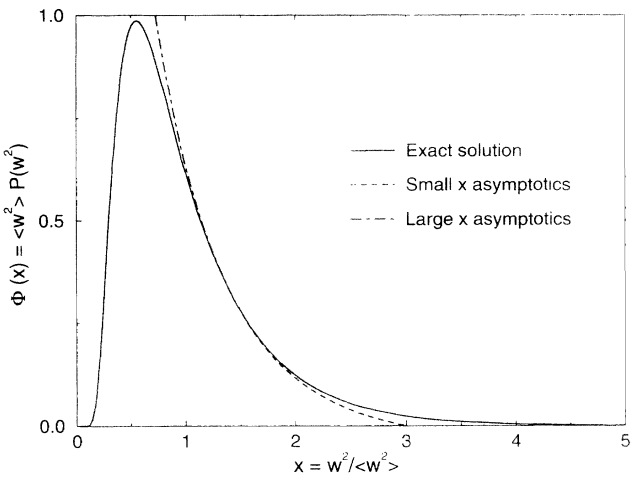

FIG. 1. Scaling function for the width distribution of periodic random walks given by Eq. (11). Small- and large-argument asymptotes, Eqs. (12) and (13), are also shown.

$$\Phi(x) \approx \sqrt{\frac{6}{\pi x^5}} (3-x) e^{-3/(2x)} \{ 1 + O(e^{-6/x}) \}. \tag{13}$$

One can see from Fig. 1 that the leading term in the small-x asymptotics is indistinguishable from the exact scaling function for $x \leq 1.5$. Thus the small- and large-x asymptotics [(13) and (12)] provides us with simple expressions which together describe $\Phi(x)$ very accurately for all $0 < x < \infty$.

We shall now examine various surface-evolution models and compare their scaling functions $\Phi(x)$ to the result obtained above.

First, consider the discrete-slope [8] (or single-step [9]) model which is a solid-on-solid type deposition-evaporation 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 (i.e., the slope of the surface) 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. If the deposition and evaporation rates are equal, the model belongs to the universality class of the Edwards-Wilkinson model [10] while for unequal rates the universality class is that of the Kardar-Parisi-Zhang (KPZ) [11] equation. The steady state, however, is the same in both cases, namely, every state (surface configuration) is equally probable [9]. Since the surface configurations are discretized versions of random walks, it is natural to start our comparisons with this model.

After taking the $L \to \infty$ limit and rescaling both the coordinates and the heights appropriately, the surface configurations become continuous random walks. Thus it would not be surprising to get good agreement between the $\Phi(x)$'s for large L's. What is surprising is that Fig. 2 shows excellent agreement with the continuum result already for $L=32$. We

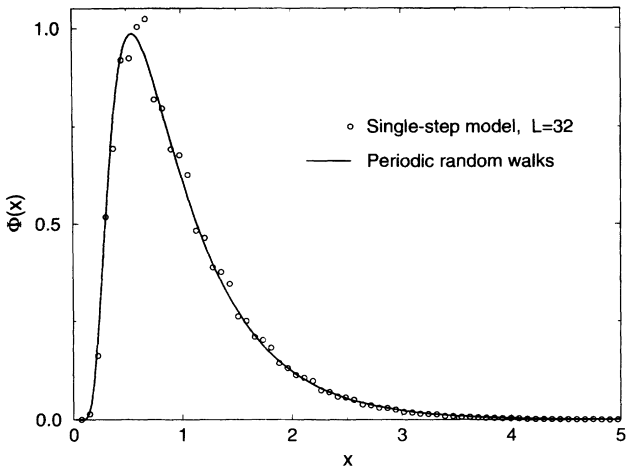

FIG. 2. Scaling function for the finite ($L=32$) single-step model as compared with the result for the periodic random-walk model.

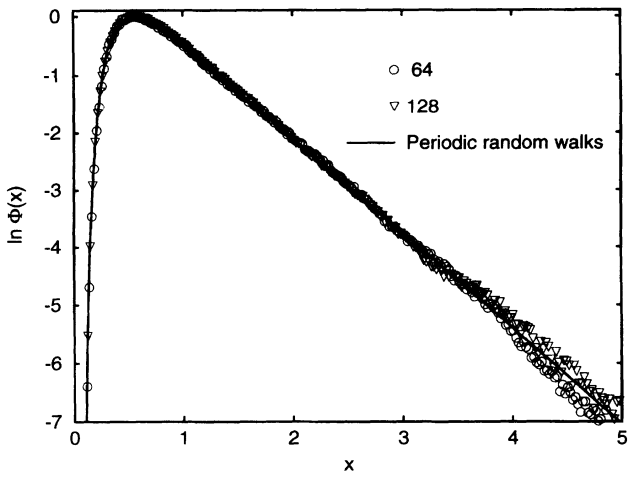

FIG. 3. Comparison of scaling functions for the catalytic reaction model ($p=\frac{1}{2}$, standing interface) and the periodic random-walk model.

have chosen $L=32$ because it was the largest L where $\Phi(x)$ could be calculated exactly by enumerating all the states (without requiring an excessive amount of computer time). Similar results can be obtained for $L<32$ but the fluctuations become larger since the finite number of possible values of w^2 becomes more prominent.

The single-step model is closely related to both the Eden model [8] and the ballistic deposition model [9]. Thus one expects that both of these models display the same scaling of their width distributions. Furthermore, the universal scaling function (11) should already be well approximated for characteristic system sizes ($L\sim 100$) studied in MC simulations.

As a second example, we studied the fluctuations of the interface in a model of catalytic reactions on a surface [12]. Here the interface exists between two reactant species A and B which occupy the sites of a strip of width L on a square lattice. In the initial state, the A (B) particles completely fill the left (right) side of the strip with two columns of sites left empty between the A and B domains. The dynamics consist of the following steps: (i) Particle A or B is chosen with probability p or $1-p$ for attempting an adsorption at a randomly selected empty site; (ii) the particle is adsorbed with probability s^n, where n is the number of nearest neighbor sites occupied by particles of the opposite species and $s<1$; (iii) if the adsorbed particle has nearest neighbors of the opposite species, then it reacts with one of those randomly chosen neighbors and both particles leave the surface.

Extensive simulations of this system have been carried out [12] for $p=\frac{1}{2}$ and various values of s. On the average, the interface does not move for $p=\frac{1}{2}$ and the simulations indicate that the dynamics of fluctuations can be described by the Edwards-Wilkinson equation [10]. For $p\neq\frac{1}{2}$, on the other hand, more particles of one species are adsorbed and, as a result, the interface moves with a uniform velocity. It is expected (but has not been demonstrated) that this case is amenable to analysis in terms of the KPZ equation [11]. If this is true then $P(w^2)$ should be the same for both standing and moving interfaces and their scaling functions should coincide with Φ calculated for the random-walk model. In order to check this point, we have simulated the above catalytic-reaction model for both $p=\frac{1}{2}$ and $p=1$ and have chosen s to be $\frac{1}{2}$. This latter choice was motivated by the observation [Fig. 2(b) of [12]] that the interface is sharp for $s=\frac{1}{2}$ and thus there are no difficulties in defining its position.

The results of our calculations of the steady-state distribution $P(w^2)$ obtained from runs of 3.2×10^6 MC sweeps on strips of width $L=64$ and 128 are displayed in Figs. 3 and 4. In order to emphasize the quality of collapse, we plotted $\ln\Phi(x)$ vs x. It should also be noted that there are *no fitting parameters* in collapsing the MC data and the theoretical scaling function. As one can see, the agreement between the theory and MC data is excellent and we can conclude that the random-walk description of these surfaces works not only on the macroscopic level of width $\sim$(length)$^{1/2}$ scaling but also on the level of distributions of the width.

We conclude by speculating on two obvious extensions of this line of inquiry. One is to consider the distributions of

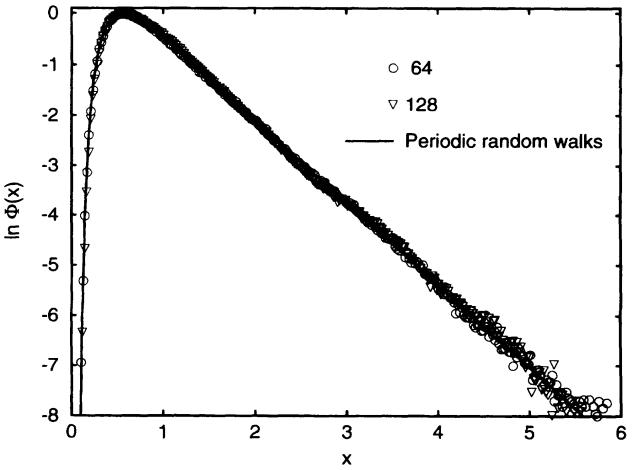

FIG. 4. Comparison of scaling functions for the catalytic reaction model ($p=1$, moving interface) and the periodic random-walk model.

higher powers of the width. In particular, using the generating function approach and considering g as the variable conjugate to w^4, we are led to consider the partition function for an *anharmonic oscillator* $G(\lambda,g)$. This quantity is known to have rich singular structure in g [7], so that we expect $P(w^4)$ to inherit very interesting behavior as well. The other conspicuous generalization is the study of two-dimensional interfaces. In addition to having a different scaling [$w^2 \sim \ln(\text{length})$], there is the possibility of roughening transitions [13], and other types of phase transitions in nonequilibrium surface-evolution models [5]. We hope that the study of width distributions will lead to new insight on a variety of "old" problems.

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