Scaling properties of self-expanding surfaces

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Scaling properties of self-expanding surfaces are studied with a comparison to those of self-flattening surfaces [Phys. Rev. E **66**, 040602(R) (2002)]. The evolution of self-expanding surfaces is described by a restricted solid-on-solid type monomer deposition-evaporation model in which both deposition at the globally lowest site and evaporation at the globally highest site are suppressed. We find numerically that equilibrium surface fluctuation has a scaling behavior with a roughness exponent $\alpha \simeq 1$ in one dimension (1D). In contrast, 2D equilibrium surfaces show the same dynamical scaling behavior with $\alpha = 0$ (log) and dynamic exponent $z \simeq 5/2$ as 2D self-flattening surfaces. Stationary roughness can be understood analytically by relating the self-expanding growth model to self-repelling random walks. In the case of nonequilibrium growing/eroding surfaces, self-expanding dynamics cause the fluctuation of surfaces to be characterized by $\alpha \simeq 1$ in both 1D and 2D.

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Dynamical scaling properties for fluctuating surfaces under thermal white noise have been studied extensively by use of the scaling ansatz [1]

$$W = L^{\alpha} f(t/L^{z}) = \begin{cases} L^{\alpha}, & t \gg L^{z}, \\ t^{\beta}, & t \ll L^{z}, \end{cases} \tag{1}$$

where W is the root-mean-square fluctuation of surface heights and $\beta = \alpha/z$. Dynamical scaling properties of such kinetic roughenings are now well documented and classified, like the Edwards-Wilkinson (EW) universality class [2], the Kardar-Parisi-Zhang (KPZ) universality class [3], etc. [1].

Recently we have introduced a global mechanism to suppress surface fluctuations in addition to ordinary local surface tension [4]. We call it a *self-flattening* (SF) mechanism [5] to reduce the growth (erosion) probability at the globally highest (lowest) point on the surface. The SF model is physically related to the various dynamic evolution models with global constraints, such as multiparticle-correlated surface evolution models [6], dissociative dimer models [7,8], even-visited random walks [7], self-attracting walks [9], random walks with static traps [10], and the motion of the step on a vicinal surface where its motion is bounded by two neighboring steps [11]. Physically, the partition function [5,12] for equilibrium SF surfaces is

$$Z = \sum_{\text{RSOS conf.}} e^{-\kappa S} (S \equiv h_{\max} - h_{\min} + 1), \tag{2}$$

where the summation is over all height configurations satisfying the restricted solid-on-solid (RSOS) condition, and $h_{\max}$ ($h_{\min}$) is the globally maximum (minimum) height for a given configuration. SF dynamics is a sort of Metropolis-type evolution [5,12] based on the partition function (2), where deposition (evaporation) at the site with $h = h_{\max}$ ($h_{\min}$) increases S by one unit, and these attempts are accepted with Boltzmann-type probability $e^{-\kappa}$ ($\kappa > 0$). This global type suppression makes the equilibrium surface less rough, with $\alpha \simeq 1/3$ in one dimension (1D) instead of the normal random walk value $\alpha = 1/2$.

Other phases are also expected from the partition function (2) apart from the SF phase for $\kappa > 0$. For $\kappa = 0$, equilibrium surfaces belong to the EW class [2,4] and nonequilibrium growing/eroding surfaces belong to the KPZ class [3]. For $\kappa < 0$, S should have a tendency to expand itself, and the *self-expanding* (SE) mechanism dominates. A 1D equilibrium surface can be mapped to the time trajectory of a walker by identifying the height $h(x)$ at each column x with the position $n(t)$ at the step $t = x$. In this mapping, the EW class for $\kappa = 0$ corresponds to the normal random walk and this correspondence explains why $\alpha = 1/2$ for the EW class. The SF phase for $\kappa > 0$ then corresponds to the so-called self-attracting (timid) random walks [9], in which the walker tends to visit previously visited sites, and the correspondence also explains $\alpha = 1/3$ [5]. The SE phase for $\kappa < 0$ is then equivalent to the self-repelling walks [9] that visit a new site more heavily than a previously visited site. In the surface evolution sense a new site means a new height which is not in a given surface configuration, and the increase of S is more favored in the next evolution step. A 2D SE surface which deals with the membrane fluctuation is completely different from a 2D walk model which deals with polymer fluctuations. 2D SE surfaces could be physically related to self-avoiding membranes [13].

In this Brief Report, we want to investigate the scaling properties of SE surfaces ($\kappa < 0$) by using a Metropolis-type evolution rule from the partition function (2). In our model we assume that the height $h(\vec{r})$ at site $\vec{r}$ on a D-dimensional hypercubic lattice has only integer values. The RSOS constraint $|h(\vec{r} + \hat{e}_i) - h(\vec{r})| \leq 1$ is always imposed, where $\hat{e}_i$ is a primitive lattice vector in the ith direction ($i = 1, \ldots, D$). The evolution rule for SE dynamics is as follows. First, select a site $\vec{r}$ randomly. Next, deposit a particle $h(\vec{r}) \rightarrow h(\vec{r}) + 1$ with probability p or evaporate a particle $h(\vec{r}) \rightarrow h(\vec{r}) - 1$ with probability $q = 1 - p$. Equilibrium surfaces are the surfaces for $p = q = 1/2$, while nonequilibrium surfaces are

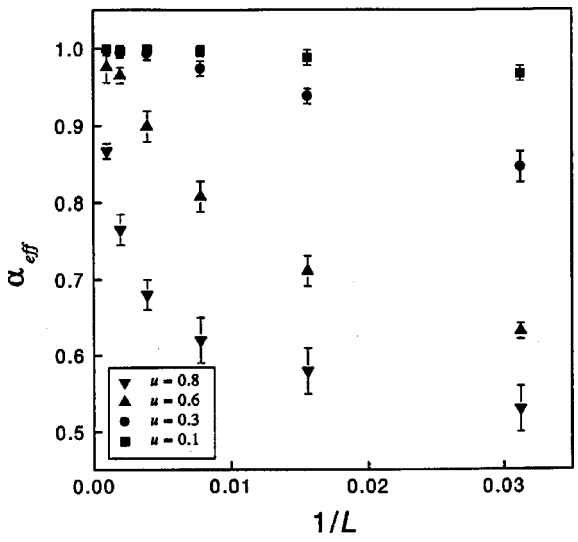

FIG. 1. Effective exponent α_{eff} versus $1/L$ for 1D self-expanding equilibrium surfaces. All data for various values of u converge to 1 rather nicely in the $L\to\infty$ limit. System sizes used are $L=2^5,\ldots,2^{11}$.

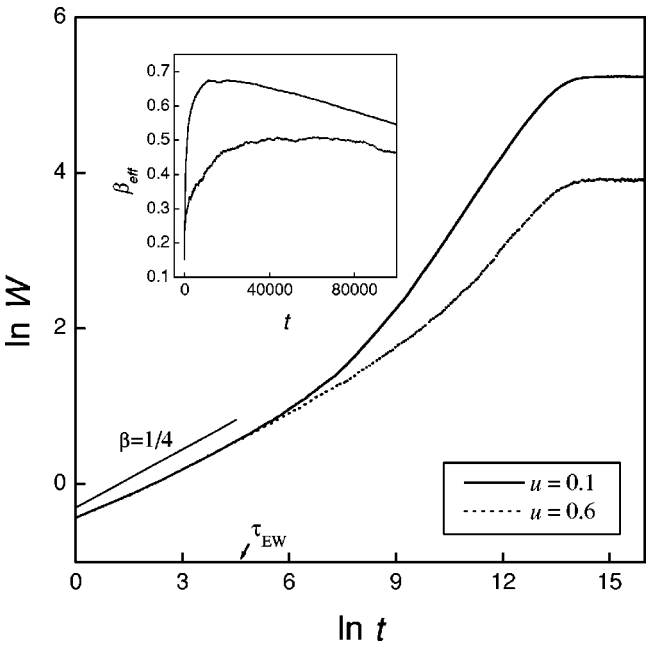

FIG. 2. Plots of $\ln W$ against $\ln t$ for 1D self-expanding equilibrium surfaces at $u=0.1$ and $u=0.6$. System size used is $L=2^{11}$. The solid line represents the relation $W\simeq t^{\beta}$ ($\beta=1/4$). W for $t<\tau_{\text{EW}}$ follows EW behavior ($\beta=1/4$) fairly well. In the inset, we plot β_{eff} versus t for 1D self-expanding equilibrium surfaces.

those for $p\neq q$. For the SE mechanism, we need a slight variation of the evolution rule at the extremal heights $h_{\max}$ and $h_{\min}$: both the deposition attempt $h_{\min}\to h_{\min}+1$ at $h=h_{\min}$ and the evaporation attempt $h_{\max}\to h_{\max}-1$ at $h=h_{\max}$ are accepted only with probability u. At $u=1$, the ordinary RSOS model [14] is recovered.

Physically, SE dynamics is simply Metropolis type evolution with the partition function (2) with $\kappa<0$ to reach equilibrium. Deposition (erosion) at $h_{\min}$ ($h_{\max}$) which decreases S by 1 is accepted with the Boltzmann type probability $u=e^{-|\kappa|}$. Any other attempts are always accepted, because $u=e^{|\kappa\Delta S|}>1$. In contrast, SF dynamics [5] suppresses deposition (erosion) attempt at $h_{\max}$ ($h_{\min}$), which increases S.

To see the scaling properties of SE surfaces, we perform numerical simulations, starting from a flat surface of linear size L with periodic boundary conditions. We measure the surface width W. First we report the numerical results for equilibrium surfaces ($p=q$). In 1D, we run simulations for $L=2^5,\ldots,2^{11}$ and various u. Numerical data are obtained after averaging over at least 300 independent samples. In order to extract the stationary property, we should estimate $W_s(L)$ [$\equiv W(L,t\to\infty)$]. For efficient estimation of α, we introduce an effective exponent

$$\alpha_{\text{eff}}(L)=\ln[W_s(2L)/W_s(L)]/\ln 2. \tag{3}$$

$\alpha_{\text{eff}}(L)$ for various u are plotted in Fig. 1. Close to $u=1$, our data show large corrections to scaling as expected, due to the presence of the EW fixed point ($\alpha=1/2$) at $u=1$. However, the asymptotic estimates seem to be independent of u. We obtain $\alpha=1.00(1)$ for all u.

For the early-time dynamical behavior, we show $W(L,t)$ for $u=0.6$ and $u=0.1$ in Fig. 2. To see whether W grows algebraically as $W\sim t^{\beta}$, we introduce another effective exponent β_{eff},

$$\beta_{\text{eff}}(t)=\frac{\ln W(t)-\ln W(t/10)}{\ln t-\ln(t/10)}. \tag{4}$$

$\beta_{\text{eff}}(t)$ for $u=0.1$ and 0.6 are plotted in the inset of Fig. 2. After initial EW behavior ($\beta=1/4$), β_{eff} seems to vary continuously until the saturation regime begins. Unlike SF growth models, a stabilized time zone of β_{eff} for both $u=0.1$ and $u=0.6$ hardly exists. This result means that W of 1D SE surfaces does not seem to follow the power law $W\simeq t^{\beta}$.

To see the time-dependent behavior more carefully we study the time evolution of the surface configuration. Figure 3(a) shows the time evolution of 1D equilibrium SE surfaces for $u=0.5$ in a typical simulation sample. Initially the configurations are nearly the same as those in other growth models which satisfy the scaling law (1). But soon W grows rapidly and surfaces form groove structures like those at $t=(25,100,500)\times 10^4$. The more specific structure of the groove is shown in the inset of Fig. 3(a), which is a snapshot of the surface configuration when W has the maximal value among the fluctuating W's in the saturation regime ($t\gg 1$). The grooved structure is very similar to the surface morphology of other growth models with $\alpha=1$ like the multiparticle-correlated surface growth model [6,12] and conserved RSOS (CRSOS) model [15]. The CRSOS model is a stochastic model which is believed to follow a Lai–Das Sarma–Villain (LSV) equation [16,17]. Recently, a similar phenomenon to our case, i.e., rapid unstable growth, was found in a study of the discretized LSV equation [18]. However, the rapid growth for the discretized LSV equation originated from the nonlinear term in the LSV equation. Furthermore, the rapid

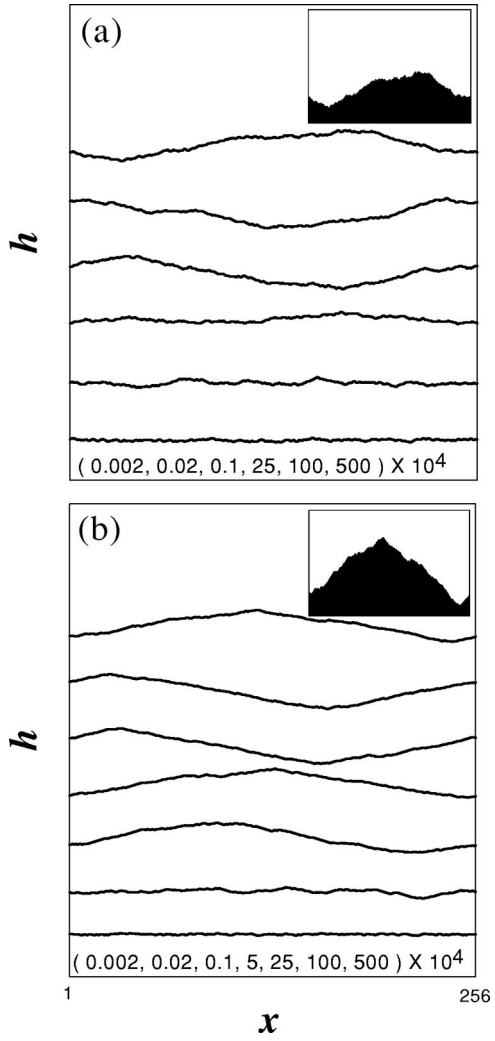

FIG. 3. (a) Time evolution of 1D equilibrium SE surface for $u=0.5$ in a typical simulation sample. Typical surface configuration with a maximal W is shown in the upper right corner. Used system size is $L=2^8$. (b) The same figure for the 1D nonequilibrium growing SE surface for $u=0.5$. The numbers in the bottom of each figure denote Monte Carlo times when each configuration is taken.

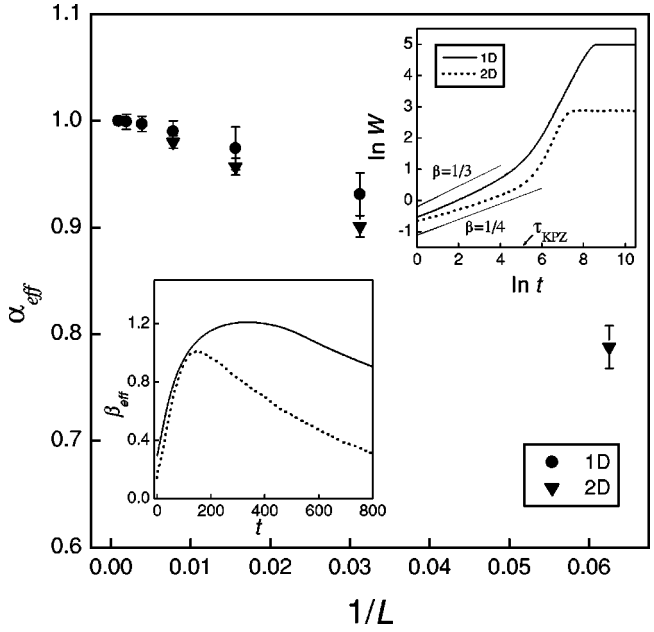

FIG. 4. Plots of α_{eff} against $1/L$ in 1D and 2D nonequilibrium growing surfaces at $p=1$ and $u=0.5$. All the data converge to 1 in the $L\to\infty$ limit. System sizes used are $L=2^5,\ldots,2^{11}$ in 1D and $L=2^4,\ldots,2^8$ in 2D. The upper inset shows the early-time behavior of W. Solid lines represent the early-time KPZ behaviors with $\beta=1/3$ in 1D and $\beta=1/4$ in 2D. For $t<\tau_{\text{KPZ}}$ W for both 1D and 2D nonequilibrium surfaces follows the KPZ behavior fairly well. We plot β_{eff} against t for the nonequilibrium growth in the lower inset.

growth was found to induce instability, so that W seems to grow indefinitely and thus never saturates. In contrast, the time-dependent behavior of the SE surfaces is quite different as shown in Figs. 2 and 3(a). Initially, when the SE mechanism is still immature, the growth follows 1D EW behavior $W\simeq t^{1/4}$. This EW behavior is clearly seen in the time region $t<\tau_{\text{EW}}$ in Fig. 2, where $W(t)$ for $u=0.6$ is nearly the same as that for $u=0.1$. For $t>\tau_{\text{EW}}$, the SE mechanism becomes mature and makes $W(t)$ behave differently from the power-law behavior $W\simeq t^{\beta}$. But the SE mechanism makes W saturate as shown in Figs. 2 and 3(a) to satisfy $W_s\simeq L$. This means the SE mechanism never induces unstable growth.

Stationary properties of 1D SE surfaces can be understood analytically. The 1D SE surface can be mapped to self-repelling walks [9] that tend to visit a new site with heavier weights. Since the mean number of sites $\langle S\rangle$ of L-step self-repelling walks scales linearly with L [9], a 1D SE surface is also expected to show the scaling behavior $W\simeq\langle S\rangle\simeq L$. The dynamical behavior for $t>\tau_{\text{EW}}$ that deviates from $W\simeq t^{\beta}$ is from the SE mechanism. The dynamical behavior directly from the SE mechanism is hard to understand analytically, because the continuum equation for SE dynamics must contain a global type nonlinear term. Further study in this direction is left for future research into SF dynamics [5].

The 2D equilibrium SE surface is found to satisfy the dynamic scaling relation

$$W^2(L,t)=\frac{1}{2\pi K_G}\ln[Lg(t/L^z)] \tag{5}$$

with $z=2.5$ and $K_G=0.916$, where $W_s^2\simeq(1/2\pi K_G)\ln L$, and $W^2(t\ll L^z)\simeq(1/2\pi K_G z)\ln t$. These scaling properties of 2D SE surfaces are exactly the same as those of 2D SF surfaces [5]. In particular, the logarithmic behavior of W_s^2 with the same K_G ($K_G^0=0.916$) [19] is very surprising in that it occurs for both SE and SF surfaces, even though the SE mechanism is physically the completely reverse of the SF mechanism. Furthermore, we find no L-dependent corrections to the logarithmic scaling as in the dimer model [20]. The common dynamical scaling behavior of both 2D SE and SF surfaces also means that EW-like logarithmic behavior of W_s^2 is very robust against both SE and SF mechanisms. Recently, a theory has been suggested for the stationary properties of general SF surfaces [21]. In that theory, the SF mechanism is argued to induce no L-dependent corrections

when W_s without the SF mechanism is logarithmic ($\alpha = 0$). The theory also seems to hold for the SE mechanism in 2D.

We now discuss the simulation results for nonequilibrium growing/eroding SE surfaces ($p \neq q$). We report the numerical results for $p=1$ and $u=0.5$. The system sizes used are $L=2^5, \ldots, 2^{11}$ in 1D and $L=2^4, \ldots, 2^8$ in 2D. In Fig. 4, we plot α_{eff} against $1/L$. From Fig. 4, we can estimate $\alpha \simeq 1$ for both 1D and 2D surfaces. The result, $\alpha \simeq 1$, for the nonequilibrium 1D and 2D surfaces is the same as that for 1D equilibrium surfaces. This fact tells us that the SE mechanism is apparently enhanced by external bias of the growth (or erosion), so that nonequilibrium SE surfaces in 2D as well as 1D satisfy $\alpha=1$. This kind of enhanced SE behavior can also be seen from the early-time dynamical behavior. As one can see from the inset for the time dependence of $W(L,t)$ and the inset for β_{eff} of Fig. 4, the early-time dynamical behaviors of nonequilibrium SE surfaces in both 1D and 2D are qualitatively very similar to that of 1D SE equilibrium surfaces (see Fig. 2). Initially, when the SE mechanism is still immature, the nonequilibrium growth follows KPZ behaviors, $W \simeq t^{1/3}$ in 1D and $W \simeq t^{1/4}$ in 2D. This KPZ behavior is clearly seen in the time region $t < \tau_{\text{KPZ}}$ as shown in the upper inset of Fig. 4. For $t > \tau_{\text{KPZ}}$, the SE mechanism with the effect of external bias of growth makes $W(t)$ grow more rapidly and makes $W(t)$ behave differently from the power-law behavior $W \simeq t^{\beta}$, as in the 1D equilibrium case. The time evolution of nonequilibrium surface configurations as shown in Fig. 3(b) is also very similar to that of 1D SE equilibrium surfaces [Fig. 3(a)]. From Figs. 3(b) and 4 we can see that the SE mechanism appears to be enhanced by external bias of growth. The scaling behavior of SE growing surfaces is nearly the same in both 1D and 2D.

In summary, we studied the scaling properties of self-expanding surfaces in 1D and 2D. Scaling behavior with $\alpha \simeq 1$ distinct from the EW class is shown for 1D equilibrium surfaces. The result can be understood analytically from mapping to 1D self-repelling walks. The dynamical behavior of 1D SE equilibrium surfaces deviates from the power-law behavior $W \simeq t^{\beta}$ and shows an anomalously rapid growth of W before W saturates. In contrast, the SE mechanism in 2D does not change the EW stationary property. Furthermore, W of 2D equilibrium SE surfaces shows the same scaling behavior (5) as 2D SF surfaces. In both 1D and 2D, nonequilibrium SE surfaces show nearly the same dynamical behavior as the 1D equilibrium SE surface. The nonequilibrium surfaces in both 1D and 2D have the common stationary property $\alpha \simeq 1$.

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