Effects of surface diffusion length on steady-state persistence probabilities

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Abstract. The dependence of the steady-state persistence probabilities \( P^S \) and exponents \( \theta^S \) on surface diffusion length \( l \) for four discrete growth models is investigated. The persistence exponents which describe the decay of the persistence probabilities, the probabilities of the average of all initial height \( h_0 \), are increased as \( l \) is increased for all models. The results of one-dimensional Family ((1+1)-Family) and Das Sarma-Tamborenea ((1+1)-DT) models with kinetically rough film surface show the decrease of the growth exponent \( \beta \) with \( l \). The \( l>1 \) results preserve the relation \( \max[1,1] \beta \theta > 0 \). In contrast, \( \beta \) is observed to increase with \( l \) for the two-dimensional larger curvature ((2+1)-LC) and Wolf-Villain ((2+1)-WV) models with mounded morphology. Our results show that the \( \beta = \max[1-\theta^S,1-\theta^S] \) relation is not valid in \( l>1 \) cases in models with mounded surfaces. The persistence probabilities of a specific value of initial height \( P^S(h_0) \) for \( l>1 \) are found to behave differently between mounded and kinetically rough models.

1. Introduction
One of the first-passage quantities describing dynamics of interface fluctuations of nonequilibrium surface growth is the steady-state persistence probability \( P^S(t) \) [1-4]. This is the probability that the height fluctuations \( \langle h \rangle \) do not cross the initial height value \( h_0 \) within a specific time interval \( t \). The persistence probability exhibits power-law decay behavior with time and the steady-state persistence exponent \( \theta^S \) is calculated from the decay rate. For limited mobility discrete growth models, \( \theta^S \) is related to the growth exponent \( \beta \) which characterizes how the interface width \( W \) scales with time in the early stage [1,2]. This relation makes \( \theta^S \) one of the universal quantities [1,2]. In this work, our results show that the relation does not work in models with mounded morphology. The mounds are obtained in some models when the long surface diffusion length noise reduction technique \( l>1 \) NRT) [5-7] is used. The \( l>1 \) NRT is a computational method used to reach the asymptotic behavior of a
model in shorter time [5-7]. Increasing the diffusion length $l$ in simulation is equivalent to increasing the growth temperature in experiments of thin film fabrication. In this research, we investigate how $P^S(t)$ and $\theta^S$ depend on $l$ and the growth condition when the relation between $\theta^S$ and $\beta$ fails.

2. Theory and discrete growth models

2.1. Steady-state persistence probabilities and exponents

The steady-state persistence probability, average over all values of $h_0$, can be classified into the positive and negative probabilities $\left(P^S_+(t)\right)$. $P^S_+(t)$ is the probability that $h > h_0$ while $P^S_-(t)$ is the probability that $h < h_0$ throughout a specific time interval $t$. $P^S_\pm(t)$ are found to decrease with time as a power-law i.e. $P^S_\pm(t) \sim t^{-\theta^S_\pm}$, where $\theta^S_\pm$ are the positive and negative steady-state persistence exponents. For up-down symmetric models, $\theta^S_\pm$ are equal to each other and relate to the growth exponent ($\beta$) as [1]

$$\beta = 1 - \theta^S_+ = 1 - \theta^S_-.$$  \hspace{1cm} (1)

For the up-down asymmetric models, however, previous study [2] found that $\theta^S_+ \neq \theta^S_-$. The generalized version of equation (1) is [2]

$$\beta = \max(1 - \theta^S_+, 1 - \theta^S_-).$$ \hspace{1cm} (2)

2.2. Discrete growth models with long surface diffusion length

All models studied here are nonequilibrium, solid on solid, discrete growth models. For each model, after randomly deposited on an initially flat substrate, a deposited atom is allowed to move to one of its neighboring sites by model-dependent diffusion rule.

In this research, two types of growth models are studied.

2.2.1. Models with kinetically rough surface. Surface morphologies of these models are kinetically rough without mound feature. Two models in this work are in this category i.e. the one-dimensional Family $((1+1)-$Family) [8] and the one-dimensional Das Sarma-Tamborenea $((1+1)-$DT) [9] models. For the $(1+1)$-Family model, the deposited atoms search for the site that has the local minimum height among the nearest neighboring sites [8]. The morphology of the $(1+1)$-Family model shows smooth surface with up-down symmetry. For the $(1+1)$-DT model, the deposited atoms search among the nearest neighboring sites to find a site with at least one lateral bond [9]. The morphology of the $(1+1)$-DT model shows round tops and deep grooves which reveal that the model is up-down asymmetric.

2.2.2. Models with mounded surface. Surface morphologies in asymptotic limit of these models show mounds which can be seen clearly when $l$ is large. Two mounded models used in this study are the two-dimensional larger curvature $(2+1)$-LC [10,11] and the two-dimensional Wolf-Villain $(2+1)$-WV [12] models. For the $(2+1)$-LC model, the deposited atoms move to one of the nearest neighboring sites in which local curvature has the largest value [10,11]. The local curvature of the site $(i, j)$ is $H(i+1, j) + H(i-1, j) + H(i, j+1) + H(i, j-1) - 4H(i, j)$, where $H$ is the height of each site. For the $(2+1)$-WV model, the deposited atoms search for the site in which the number of bonds has the maximum value [12]. The morphology of the $(2+1)$-LC model shows up-down symmetry whereas that of the $(2+1)$-WV model does not.

For models with the $l >1$ NRT, a deposited atom repeats the diffusion rule up to $l$ steps. After that the atom will stick on the final site and a new atom is deposited on the substrate. The value of surface diffusion length studied here are $l = 1, 2, 3, 5$ and 10.
3. Results and discussion

For all models in this work, our results show that the persistence probabilities which have been averaged over all \( h_0 \) decrease more rapidly with increasing \( l \). This finding indicates that the persistence exponents increase with \( l \). For the kinetically rough \((1+1)\)\-Family and \((1+1)\)\-DT models, the growth exponent becomes smaller when \( l \) is increased. Figure 1(a) shows \( P^S_+ (t) \) versus \( t \) plots of the \((1+1)\)\-Family model grown on a substrate with \( L=1000 \) sites for various \( l \). It is clear that \( \theta^S \), which is the magnitude of the slope of the \( P^S_+ (t) \) plot, increases with \( l \). For each \( l \), the plot of \( W \) as a function of time in the inset of figure 1(a) show that \( \beta \), the slope of the \( W \)\-\( t \) plot, decreases as \( l \) is increased. For all values of \( l \), \( \theta^S \) and \( \beta \) satisfy the relation in equation (1). Our results show similar behavior of \( \theta^S \) and \( \beta \) of the \((1+1)\)\-DT model except that \( \theta^S \) is slightly different from \( \theta^S \). For \( l>1 \), equation (2) is not valid showing that neither \( \theta^S \) nor \( \theta^S \) is related to \( \beta \).

![Figure 1](image_url)

Figure 1. \( P^S_+ \) for various \( l \) of (a) \((1+1)\)\-Family and (b) \((2+1)\)\-LC models.

Our data show that effects of \( l \) on the up-down symmetry \(( h \rightarrow -h )\) of models used in this work is weak. The equality of \( \theta^S \) and \( \theta^S \) of the \((1+1)\)\-Family and \((2+1)\)\-LC models is still valid. For the \((1+1)\)\-DT model, our results show explicitly that \( P^S_+ \) and \( P^S_+ \) decay in time with the different rate for every \( l \). For the \((2+1)\)\-WV model with weak asymmetry, \( \theta^S \) and \( \theta^S \) are not very different for all \( l \).

Next, we study effects of \( l \) on \( P^S_+ (h_0) \) which are the persistence probabilities of a specific value of \( h_0 \). For kinetically rough models, larger \( l \) leads to smoother surface and smaller \( W_{sat} \), the saturation
value of $W$ at large time. This means a value of $h_0$ that represents intermediate fluctuation ($h_0 \approx W_{sat}$) in $l=1$ model becomes very strong fluctuation ($h_0 >> W_{sat}$) in large $l$ models. Since strong fluctuation can persist in time longer [4], $\theta_\parallel^S(h_0)$ decrease with increasing $l$. An example is shown in figure 2(a) which is the plots of $P_S^x(h_0 = 6)$ of the (1+1)-Family model for various $l$. In contrast, for mounded models, mound formation in $l>1$ system causes $W_{sat}$ to increase with increasing $l$ (shown in the inset of figure 1(b)). The increase of roughness with $l$ leads to the increase of $\theta_\perp^S(h_0)$ as illustrated in figure 2(b) for the (2+1)-LC model. Note that $W_{sat}$, as well as $\theta_\perp^S(h_0)$, increase only slightly and then become constant for $l \geq 3$. We obtain the same behavior for the (2+1)-WV model.

Figure 2. $P_S^x(h_0)$ for various $l$ of (a) (1+1)-Family and (b) (2+1)-LC models.

4. Conclusion
For all models in this research, $\theta_\parallel^S$ are found to increase with $l$. Effects of $l$ on $\beta$ and $\theta_\parallel^S(h_0)$ are, however, different in mounded and kinetically rough models. With a fixed $h_0$, $\beta$ and $\theta_\parallel^S(h_0)$ of mounded models increase with $l$ whereas those of kinetically rough models decrease when $l$ becomes larger. The relation between $\theta_\perp^S$ and $\beta$ does not work in mounded models when $l>1$. This points to the possibility that the persistence exponent may not be a universal exponent in mounded models with long surface diffusion length.

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