# Roughness of two-dimensional surfaces with global constraints

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We study dynamical scaling properties of the two-dimensional surface growth models with global constraints. These include the growth model from a partition function $Z=\Sigma_{\{h(\vec{r})\}}\Pi_{h=h_{min}}^{h_{max}}\frac{1}{2}(1+z^{n_h})$, multiparticle-correlated surface growth models and dissociative $Q$-mer growth models. The equilibrium surfaces of all the models except the dimer model show the same dynamical scaling behavior $W^2(L,t)=(1/2\pi K_G)\ln[L\ g(t/L^{z_W})]$ with $z_W=2.5$ and $K_G=0.916$, whereas the surface in the dimer model has a correction to the scaling. The growing (eroding) surfaces have two phases. The models with $z\geqslant 0$ show the normal Kardar-Parisi-Zhang scaling behavior. In contrast the models with $-1\leqslant z<0$ and multiparticle-correlated growth model manifest grooved surface structures with $\alpha=1$. The growing surfaces of $Q$-mer models form rather complex facets.

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Recently there have been some studies on surface growth models with global constraints. They are dissociative $Q$-mer models [1–3], $Q$-particle-correlated growth (QP) models [4], self-flattening (SF) surfaces [5], and self-expanding (SE) surfaces [6]. Some of these models have shown to be unified through the partition function [7]

$$Z=\sum_{\{h(\vec{r})\}}\prod_{h=h_{min}}^{h_{max}}\frac{1}{2}(1+z^{n_h}), \tag{1}$$

where the summation is that over all possible surface height configurations $\{h(\vec{r})\}$ and $n_h$ is the number of sites to satisfy $h(\vec{r},t)=h$ in $\{h(\vec{r})\}$. The partition function (1) for $z=0$ is equal to that of SF growth model [5] in which the growing (eroding) at the globally highest (lowest) column is suppressed. $Z$ with $z=-1$ is exactly equal to $Z$ of the two-particle-correlated growth (2P) model [4] with the global evenness constraint. The ordinary restricted solid-on-solid (RSOS) model [8] corresponds to the case $z=1$. In the $Q$-particle-correlated model (QP model) only the simultaneous deposition (or evaporation) of $Q$ particles at the randomly chosen $Q$ columns of equal heights takes place. QP models have been suggested to resolve the so-called sector-dependent (or initial-morphology-dependent) problem of the dissociative dimer growth model [2]. In the $Q$-mer models particles can deposit (or evaporate) only in the $Q$-mer form of equal heights.

Recent studies on these models in one spatial dimension have shown that scaling properties of these models cannot be classified as the well-known classes such as the Edward-Wilkinson (EW) class [9] or Kardar-Parisi-Zhang (KPZ) class [10]. The one-dimensional (1D) equilibrium surfaces of all QP models [4], $Q$-mer models of $Q\geqslant 3$, SF model [5], and growth models from Eq. (1) with $z\geqslant -1$ [7] have been shown to scale as $W_s[\equiv W(t\gg L^{z_W})]\simeq L^{\alpha}(\alpha=1/3)$. However the dimer model, which has nonergodicity, has been shown to have $\alpha$ somewhat smaller than 1/3 [4]. The growing (eroding) 1D surfaces of QP models [4] and the models from Eq. (1) with $z<0$ [7] have been shown to form a certain groove-type morphology with $\alpha=1$. Especially the growing 1D surfaces of the $Q$-mer models have a special faceted structure [2,4]. In contrast, the growing surfaces of the models from Eq. (1) with $z\geqslant 0$ [7] show the KPZ scaling behavior ($\alpha=1/2$).

Compared to the studies in one-dimension, these models on higher-dimensional substrates have not intensively been studied yet. Recently Lee and den Nijs [11] numerically found that $W_s$ for the two-dimensional (2D) equilibrium surface in the dissociated dimer model scales as $W_s^2\simeq[1/(2\pi K_G^A)]\ln L$ with an anomalous value $K_G^A=0.988$ instead of the conventional logarithmic behavior $W_s^2\simeq[1/(2\pi K_G^0)]\ln L$ with the equilibrium RSOS value $K_G^0=0.916$ [12]. They [11] argued that the numerical result $K_G^A>K_G^0$ could be an intrinsic property of the globally constrained models or the partition function Eq. (1). They also argued from an analytic theory that $W_s$ for the models from Eq. (1) could scale $W_s^2\simeq\ln[L/(\ln L)^{1/4}]$, which could explain the anomalous behavior of $W_s$ with $K_G^A$ of the dimer model. However, the anomalous behavior can be found only in the dimer model as we shall see, and the dimer model has been shown not to be described by Eq. (1) with $z=-1$ due to the sector-dependent problem [3,4]. Furthermore, if one believed such a theoretical argument, the SF model (or the model with $z=0$) should have such correction as $\ln(\ln L)$. In reality, a 2D SF surface [5] has been shown to satisfy the dynamic scaling relation $W^2(L,t)=(1/2\pi K_G)\ln[L\ g(t/L^{z_W})]$ with $z_W=2.5$ and $K_G=K_G^0=0.916$, and has no numerical evidence for the scaling correction. An analytic theory [13] based on the SF partition function $Z\rightarrow\Sigma_{\{h(\vec{r})\}}\exp(-\beta S)$ with $S=h_{max}-h_{min}+1$ also suggested the possibility of the absence of the correction in two dimensions. So the reported results on 2D surfaces of the globally constrained models until now are somewhat confusing and thus there needs to be a study to resolve the contradicting situation.

Another motivation for the study is as follows: In the 1D SF point $z=0$ in the parameter space of $z$ was shown to act as a stable fixed point in the sense of renormalization group (RG) transformations [7,11]. This result was shown not directly by the RG theory, but numerically and by analytic arguments based on the partition function (1). This result

 

means that the growth models from Eq. (1) with $z \geqslant -1$, except for $z=1$, belong to the same universality class. In this sense it is very important to show all the models except for $z=1$ in two dimensions satisfy the same scaling behavior. If they belong to the same universality class, then the SF point $z=0$ is also the stable fixed in two dimensions. If this is the case, the robustness of the 2D scaling with $z_W=2.5$ and $K_G=0.916$ will strongly support an exact RG theory for globally constrained models with $z=0$ as a stable fixed point in future studies.

In this paper, we want to study 2D globally constrained growth models in a comprehensive and unified way. First 2D equilibrium surfaces of growth models from Eq. (1) with $z \geqslant -1$, which include SF and 2P models as special cases, are studied to show that the dynamical scaling with $z_W=2.5$ and $K_G=0.916$ robustly holds for any physically relevant $z(z \geqslant -1)$ except for $z=1$. Two-dimensional equilibrium surfaces of QP models and $Q$-mer models with $Q \geqslant 3$ are also studied to show the same scaling behavior. However, the dimer model shows the anomalous behavior $K_G^A=0.988$, which should come from the sector-dependent behavior as in a 1D case. Compared to the equilibrium surfaces, studies on 2D growing (eroding) surfaces of the SF model and the SE model have been reported [5,6]. We also need a comprehensive and unified study of 2D nonequilibrium surfaces, which can give a unified picture for the various globally constrained models.

In this paper, all the models are defined on a 2D square lattice. The surface height configurations $\{h(i,j)\}$ are imposed to satisfy the RSOS condition $|h(i\pm1,j\pm1)-h(i,j)| \leqslant 1$ [8]. Details of the growth models from the the partition function (1) [7] are as follows. First, a site $(i,j)$ is randomly selected. Then we decide the deposition (evaporation) attempt $h(i,j) \rightarrow h(i,j)+1 (h(i,j) \rightarrow h(i,j)-1)$ with the probability $p(q=1-p)$. Next, the weights $w(\{h(\vec{r})\})=\Pi_{h=h_{min}}^{h_{max}} \frac{1}{2}(1+z^{n_h})$ before the deposition (evaporation) attempt and $w(\{h'(\vec{r})\})$ after the attempt are calculated. We can then define the acceptance probability $P_a$ as $P_a \equiv w(\{h'(\vec{r})\})/w(\{h(\vec{r})\})$. The new configuration is accepted only if $P_a$ is larger than a random number $R(0<R<1)$.

In the 2D $Q$-particle-correlated (QP) growth model $Q$ sites $\{\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_Q\}$ are randomly selected. These sites do not need to be adjacent to one another. If all the heights $\{h(\vec{r}_k)\}$ are not the same, the $Q$ sites are discarded and a new set of $Q$ sites is randomly selected until $\{h(\vec{r}_k)\}$ are the same. Then simultaneous deposition (evaporation) of $Q$ particles, $h(\vec{r}_k) \rightarrow h(\vec{r}_k)+1 (h(\vec{r}_k) \rightarrow h(\vec{r}_k)-1)$, is attempted with the probability $p(q=1-p)$. The QP model includes the $Q$-mer model as a special case. In the $Q$-mer model only $Q$ sites adjacent to one another are selected. Otherwise, $Q$-mer models are the same as the corresponding QP models. In this paper we mainly think of dissociative dimer and trimer growth models. We also consider the dimer model with monomer diffusion along the surface, in which the diffusion to a new terrace is forbidden [2] for the global evenness constraint. In the dimer model with the diffusion, the hopping of a monomer to a nearest neighbor is attempted with the probability $r(=1-p-q)$, where $p(q)$ is the probability of a dimer deposition (evaporation).

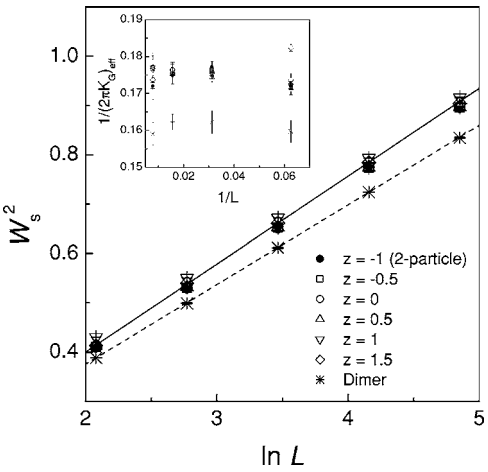


FIG. 1. Plots of $W_s^2$ against $\ln L$ for the growth models from partition function (1) with $z=-1$ ($2P$ model), $-0.5$, 0, 0.5, 1, 1.5, and for the dimer model. The slope of a straight-line fit yields the same value of $K_G \simeq 0.916(5)$ for all $z$. The slope for the dimer model gives $K_G=K_G^A \simeq 0.989(6)$. The inset shows the plot of the effective slope $[1/(2\pi K_G)]_{eff}$ against $1/L$.

To investigate the scaling property of the surfaces, we measure the root-mean-square surface fluctuation $W$ as function of time $t$ and system size $L$. All simulations are started from the flat surface $\{h(i,j)=0\}$ and a periodic boundary condition is always imposed. We run simulations for the system sizes $L=2^3,\ldots,2^7$. $W$ is obtained by averaging over at least 300 independent runs for each system size.

We report the results for the equilibrium surfaces ($p=q=1/2$). Before explaining the numerical results, let us remember that the ordinary RSOS model is well known to satisfy the dynamical scaling

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

where $K_G=K_G^o=0.916$ and $z_W=2$ [12]. The results for $W_s$ are first explained.

Figure 1 shows $W_s^2$ for the growth models with $z=-1$, 0.5, 0, 0.5, 1, 1.5. From the slope of the linear fit of $W_s^2$ to $\ln L$ and the relation $W_s^2=(1/2\pi K_G)\ln L$, we find that $K_G \simeq 0.916(5)$ for all $z$, which is nearly the same as $K_G^o$. In contrast the slope of the linear fit of $W_s^2$ to $\ln L$ for the dimer model yields $1/(2\pi K_G^A)=0.161(1)[K_G^A=0.989(6)]$, which is the same result as Ref. [11]. For more accurate estimation we use the effective slope $[1/(2\pi K_G)]_{eff}=[W_s^2(2L)-W_s^2(L)]/[\ln(2L)-\ln(L)]$. The effective slopes are displayed in the inset of Fig. 1. From the data in the inset, we can estimate the limiting value of $[1/(2\pi K_G)]_{eff}$ in the limit $L \rightarrow \infty$ as 0.176(5) for various $z$ and 0.159(3) for the dimer model. Even considering the measurement errors in the inset, the effective slopes for various $z$ are completely different from that for the dimer model. From $K_G^A \neq K_G^o$ for the dimer model, they argued that there is a correction term $\ln(\ln L^{1/4})$ [11]. However there should be no such correction for $z \neq 1$, since $K_G$ for various $z$ is nearly the same as $K_G^o$. We find the leading corrections for $z \neq 1$ are small constants. Effective

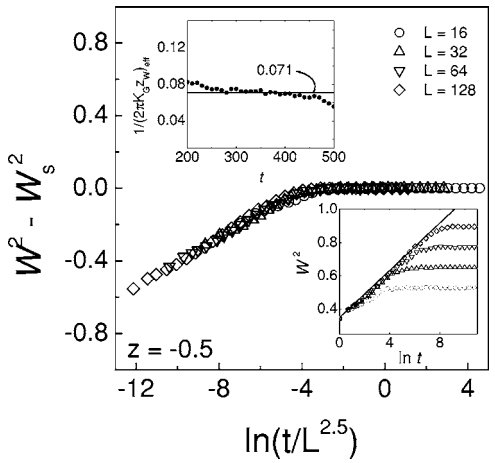


FIG. 2. The data collapse of $W(L,t)$ for the models with $z=-0.5$ (main figure). The lower inset shows the plot of $W^2$ against $\ln t$ for $z=-0.5$. The straight line in the lower inset means the linear fit of $W^2(t \ll L^{z_W})$ to $\ln t$. From the fit, $1/(2\pi K_G z_W)=0.071(2)$ is obtained. The upper inset shows the plot of effective slope $[1/(2\pi K_G z_W)]_{eff}$ against $t$.

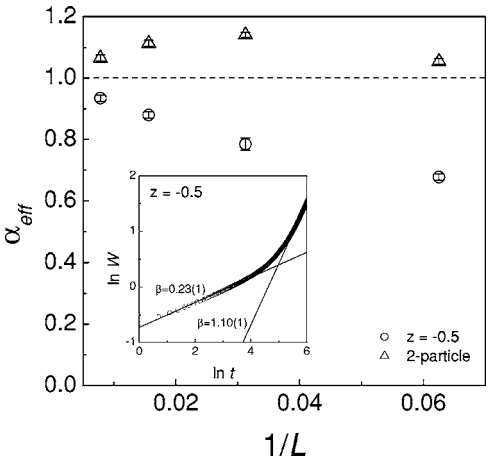


FIG. 3. Effective roughness exponents $\alpha_{eff}$ vs $1/L$ for the model with $z=-0.5$ (circles in the main plot) and the 2P model ($z=-1$) (triangles in the main plot). The asymptotic values of $\alpha_{eff}$ for both models in the limit $L \to \infty$ are nearly close to 1. The early-time behaviors of $W(t)$ on the substrate with $L=2^7$ for the model with $z=-0.5$ is shown in the inset.

slopes for the trimer model, QP models and the dimer models with monomer diffusion are also estimated. Effective slopes for the trimer model, the three-particle (3P) model, and dimer model with monomer diffusion, which are not shown for simplicity, are almost the same as those in the inset of Fig. 1. They are also completely different from that for the dimer model, especially the dimer model with monomer diffusion, which has better ergodic behavior than the simple dimer model and has $K_G=0.916(5) \simeq K_G^o$. The results for $W_s$ suggest that $W_s$ for the growth model from partition function (1), QP models, and $Q$-mer models with $Q \geqslant 3$ all show the same scaling behavior. However, $W_s$ only for the dimer model shows the anomalous behavior. The anomalous behavior is sure to come from the sector-dependent behavior as in one dimension [3,4] and is not the intrinsic property of the global evenness constraint or of the partition function (1). This conclusion is strongly supported by the fact that the dimer model with monomer diffusion never shows such anomalous behavior.

Next we want to report the results for the dynamical behavior of the equilibrium surfaces. The time dependence of $W(L,t)$ of the model with $z=-0.5$ is shown in the lower inset of Fig. 2. By assuming the dynamical scaling ansatz (2) and by comparing the slope $1/(2\pi K_G z_W)$ of $W^2(t \ll L^{z_W})$ to $1/(2\pi K_G)$ of $W_s^2$, we can decide the dynamical exponent $z_W$. From the slope of the linear fit of $W^2(t)$ to $\ln t$, $1/(2\pi K_G z_W) \simeq 0.071$ is obtained. For more accurate estimation we also measured the effective slope $[1/2\pi K_G z_W]_{eff} = [W^2(3t) - W^2(t)]/[\ln(3t) - \ln(t)]$, which was shown in the upper inset of Fig. 2. After initial transients, the stabilized time zone for $[1/(2\pi K_G z_W)]_{eff}=0.071$ is found. From the result $1/(2\pi K_G z_W)=0.071(2)$, the estimated $z_W$ is $z_W = 2.5(1)$, which is clearly distinct from the normal EW value of $z_W=2$. We also check the dynamical scaling relation of Eq. (2) by plotting $W^2 - W_s^2$ against $t/L^{z_W}$ with $z_W=2.5$. As shown in main plot in Fig. 2, the data collapse well to the scaling function (2) with $K_G=0.916$ and $z_W=2.5$. We also find that $z_W$'s for the models with various $z$, the QP model, the dimer model with monomer diffusion, and the trimer model satisfy $z_W=2.5(1)$.

Now we discuss growing (eroding) surfaces ($p \neq q$). Here we mainly discuss the results for $p=1$. It is well known that the monomer-type growth model belongs to the Kardar-Parisi-Zhang (KPZ) universality class [8,10]. The KPZ class in two dimensions means the scaling behavior $W(L,t) = L^{\alpha} f(t/L^{z_W})$ with $\alpha \simeq 2/5$, $z_W = \alpha/\beta \simeq 1/4$ [8,10]. According to the recent studies [14,15] the exponents may not be exact fractional numbers in two dimensions. We find that $W(L,t)$ for $p=1$ in the growth model with $z=0$, 0.5, 1, 1.5 is found to satisfy the known KPZ behavior as shown in Ref. [5]. This result means that the dynamical scaling behavior of the growing (eroding) surfaces for the models with $z \geqslant 0$ is the same as that of the ordinary RSOS model ($z=1$).

In contrast, the growing surface for $z<0$ shows completely different behavior. In order to extract the saturation regime ($t \gg L^{z_W}$) property correctly, we introduce an effective roughness exponent $\alpha_{eff}$ as $\alpha_{eff}(L) = \ln[W_s(2L)/W_s(L)]/\ln 2$. The estimation of $\alpha_{eff}$ for $z=-0.5$ and the 2P model ($z=-1$) is displayed in Fig. 3. From the data in Fig. 3, the asymptotic value of $\alpha_{eff}$ in the limit $L \to \infty$ is estimated as $\alpha_{eff}(\infty)=0.99(2)$ for $z=-0.5$ and $\alpha_{eff}(\infty)=1.01(2)$ for 2P model ($z=-1$). We have also checked $\alpha$ for several other values $z<0$. All obtained results for $z<0$ is $\alpha_{eff}(\infty) \simeq 1$. We also study the early-time behavior of $W(t)$ for $z<0$ on the substrate with the size $L=2^7$, which is displayed in the inset of Fig. 3. Initially $W(t)$ follows the ordinary power-law behavior $W \simeq t^{\beta}$ with $\beta=0.22$–$0.23$. After the initial regime a rapid growth occurs before $W(t)$ reaches the saturated regime. In the morphology study, we also find nearly the same behavior to that on a 1D substrate [4,7]. After the initial regime the grooved structure that makes $\alpha=1$ due to the stochastic evenness constraint appears as in the 1D case

[4,7]. We have also studied the growing surfaces for the 3P model and found almost the same behaviors to those in Fig. 3. The growing surfaces for the $Q$-mer models have been confirmed to show very complex faceted structure as on a 1D substrate [2,4].

In summary, the dynamical scaling behavior of the equilibrium surfaces follows Eq. (2) with $K_G=K_G^0=0.916(5)$ and $z_W=2.5(1)$ very well for all kinds of the growth models with global constraints except for the dimer model. This result means that the scaling relation with $z_W=2.5$, which is distinct from EW-like scaling with $z_W=2$, is very robust against the various global constraints. For growing (eroding) surfaces, the normal KPZ behavior occurs for the growth models with $z\geqslant 0$. The models with $z<0$ and QP models manifest the grooved structure with $\alpha=1$ due to the global constraints.

Possible experimental realizations of dimer ($Q$-mer) models were explained in Ref. [11]. In such a real system the diffusion of an atom within the same terrace can easily happen from the thermal noises. Furthermore if the jumps up or down to a new terrace, which break the modulo-2 conservation at each height level are experimentally suppressed due to the so-called Schwoebel barriers [16], then the dimer model with monomer diffusion is much more easily realized. The 2P model is very close to the dimer model with large-ranged diffusions or with diffusions of a large diffusion constant. The 2P model is thus a more efficient model for dimer model with diffusion.

The anomalous behavior of the dimer models in both one and two dimensions should come from the nonergodic sector-dependent behavior. To form a dimer for deposition or evaporation, one site should be selected from the first sublattice of the base square lattice and the other should be from the second sublattice. This rather special formation of a dimer makes the Fourier-transformed surface heights $\bar{h}(\vec{k})$ with $k_x=2\pi/2$ and $k_y=2\pi/2$ in two dimensions and $\bar{h}(k)$ with $k=2\pi/2$ in one dimension conserve. To break this kind of sector-dependent behavior of the dimer model, one can use the 2P model or the dimer model with monomer diffusion.

The partition function (1) has a symmetry under the transformation $z\rightarrow 1/z$, since $Z(1/z)=\Sigma_{\{h(\vec{r})\}}\Pi_{h=h_{min}}^{h_{max}}\frac{1}{2}[1+(1/z)^{n_h}]=(1/z^L)Z(z)$. The equilibrium property is thus invariant under the mapping $z\rightarrow 1/z$. The model with $z=\infty$ is the same as the SF model with $z=0$. From this partition function symmetry and the argument of the stability of the SF model ($z=0$) in RG transformations [7], we can understand the behavior $W_s=[1/(2\pi K_G^o)]\ln L$ for any $z(\geqslant -1)$.

The global constraints we treated here are a relevant perturbation to the EW fixed point. The continuum equation to describe the constrained models must contain a global-type nonlinear term, which can explain the distinct universality class of the constrained models in both one and two dimensions. The future study in this direction is very important, even though it should be very difficult.

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