Partition functions and Metropolis-type evolution rules for surface growth models with constraints

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We study dynamical scaling properties of the surface growth model with the Metropolis-type evolution rule from a partition function $Z=\Sigma_{\{h(\vec{r})\}}\Pi_{h=h_{min}}^{h_{max}}\frac{1}{2}(1+z^{n_h})$, where z is a fugacity-like quantity and n_h is the number of sites with height h in a surface configuration $\{h(\vec{r})\}$. The partition function describes a 2-particle correlated growth model when $z=-1$ and a self-flattening growth model when $z=0$. For one-dimensional equilibrium surfaces, the scaling properties for $z\geqslant -1$ except $z=1$ are all one phase with roughness exponent $\alpha=1/3$ and growth exponent $\beta\simeq 0.22$. For the growing (eroding) surfaces, there exists a phase transition at $z=0$ from the grooved phase ($\alpha=1$) for $-1\leqslant z<0$ to the ordinary Kardar-Parisi-Zhang phase ($\alpha=1/2$) for $z>0$.

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In equilibrium statistical mechanics, the partition function plays the decisive role in finding the macroscopic properties of thermodynamic systems. In contrast, successful theories based on a partition function for nonthermodynamic systems, such as surface growth [1], are scarce except for Edwards-Wilkinson-type thermal roughening [2,3]. In this paper, we show that some of the recently developed growth models with global constraints [4–6] can be unified through a partition function. By using a Metropolis-type evolution rule established directly from the partition function, scaling properties for equilibrium surfaces of the models are shown to belong to the same universality class and a sharp phase transition is shown to exist for the growing (eroding) surfaces. Our study is important because several different growth models can be explained from one partition function.

Dynamical scaling theories for fluctuating surfaces under thermal white noise have been studied extensively because of the theoretical and experimental importance of the long time, large scale surface morphology [1]. The dynamical scaling hypothesis used in these studies is

$$W=L^{\alpha}f(t/L^{z_W}), \tag{1}$$

where W is a root-mean-square fluctuation of surface heights. α and z_W are the roughness and dynamic exponents, respectively. In the hypothesis, $W(t;L)$ increases as t^{β} initially ($t\ll L^{z_W}$) and saturates to L^{α} for $t\gg L^{z_W}$, where $\beta=\alpha/z_W$. Most of these theories have used the Langevin-type equations and the discrete growth models [1], which originate from the evolution rules considering only local surface morphology.

Recently, several surface growth models in which global or nonlocal constraints are taken into consideration have been suggested and studied. Among them, the first suggested model was the Q-mer-type surface growth model [6], where particles can deposit and evaporate only in the Q-mer form of equal heights. The surface width W of one-dimensional (1D) equilibrium Q-mer models with the system size L diverges as $W\sim L^{\alpha}$ with $\alpha\simeq 1/3$ instead of the conventional random-walk value $\alpha=1/2$. The Q-mer model is related to Q-visited random walks (RWs) and the localization models for the Lifschitz tail [6]. To resolve the sector (or initial-morphology dependent) problems [6,7] in the Q-mer models, the Q-particle (QP) correlated model [4] was subsequently suggested, which is believed to have the true one-to-one correspondence to Q-visited RWs. Another kind of model with the global constraints is the self-flattening (SF) surface growth [5], in which the growth (erosion) rate at the globally highest (lowest) site is reduced or suppressed. The 1D equilibrium SF model also has $\alpha=1/3$. The 1D equilibrium SF model can be mapped onto a self-attracting walk [8] and to the survival of random walks with static traps [9], even though the higher-dimensional SF models cannot be mapped directly to walk models [5]. In this paper, we show that these growth models with global constraints can be unified through the unique form of a partition function (or generating function) Z.

We think about the surface configurations described in terms of integer height variables $\{h(\vec{r})\}$ on a D-dimensional hypercubic lattice. They are subject to the restricted solid-on-solid (RSOS) constraint, $h(\vec{r}+\hat{e}_i)-h(\vec{r})=0,\pm 1$ with $\hat{e}_i$ a primitive lattice vector in the ith direction ($i=1,\ldots,D$). Then Z which unifies the growth models [5,6] is

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

where the summation is over all possible surface height configurations with the RSOS constraint, and n_h is the number of sites $\vec{r}$ which satisfy the relation $h(\vec{r},t)=h$ in the configuration $\{h(\vec{r})\}$. Of course, z in Eq. (2) is an analog of *fugacity* or *chemical potential* in equilibrium statistical mechanics. In $z\to 0$ limit, each term inside the product in Z is equal to 1/2 if $n_h\neq 0$ or to 1 otherwise. Then $Z(z=0)=\Sigma_{\{h(\vec{r})\}}\exp(-\beta S)$ with $S=h_{max}-h_{min}+1$ and $\beta=\ln 2$. $Z(z=0)$ is exactly the same as the partition function Z_{SF} of the SF growth model [5]. When $z=-1$, Z becomes nonzero only when all n_h are even. Z with $z=-1$ is exactly equal to Z of the 2-particle (2P) correlated growth model [4] because only the height configurations obeying the global evenness conservation law have nonzero contribution to Z. Of course, the ordinary RSOS-type behavior [10] recovers when $z=1$.

The dynamical scaling properties for the 2P (QP) growth models ($z=-1$) [4] and SF growth model ($z=0$) [5] are as follows. For the equilibrium surfaces when the deposition attempt probability p is the same as the evaporation probability q ($p=q=1/2$), $\alpha=1/3$ for the both 1D QP and SF models. The growth exponent β has been found to be $\beta=0.22$ (or 2/9) for the SF model and $\beta\simeq 0.2$ for the 2P model. For $z=1$, the scaling behavior should be the ordinary RSOS behavior with $\alpha=1/2$ and $\beta=1/4$ [3] for equilibrium surfaces. The scaling property of the growing ($p=1-q>1/2$) or eroding ($q=1-p>1/2$) surface in the QP model is quite different from the equilibrium surfaces [4]. The growing (eroding) surface for the QP model ($z=-1$) shows the grooved structure with $\alpha=1$ [4]. In contrast, the SF model still shows the ordinary RSOS [10] behavior with $\alpha=1/2$ and $\beta=1/3$.

So the natural interesting questions concerning the equilibrium surfaces are the scaling properties of the models with $-1<z<0$, $0<z<1$, and $z>1$. From the properties of the QP (2P) model ($z=-1$) and SF model ($z=0$), we easily expect that all the models with $-1\leqslant z\leqslant 0$ have the same phase with $\alpha=1/3$. However, the scaling property for $0<z<1$ and $z>1$ cannot be predicted easily from the known results of the SF and 2P models. It is also very interesting to know at what value of z the transition from the grooved phase to the normal RSOS behavior occurs for the growing (eroding) surfaces.

It is thus the purpose of our paper to study the dynamical scaling properties of the model with $z\geqslant -1$ by using the Metropolis-type evolution rules based on the generalized partition function (2). From this study, we show that all of the phases of equilibrium ($p=q=1/2$) surfaces for $z\geqslant -1$ are the same as those with $\alpha=1/3$ and $\beta=0.22(2/9)$, except for $z=1$. An analytic explanation based on the partition function (2) is given for the existence of the same phase with $\alpha=1/3$. We also show that the growing (eroding) surfaces for $-1\leqslant z<0$ are the grooved phases ($\alpha=1$), whereas the growing (eroding) surfaces for $z\geqslant 0$ show the ordinary RSOS scaling behavior ($\alpha=1/2$).

We now explain the Metropolis-type evolution rule based on the partition function (2) in detail. First evaluate the weight

$$w(\{h(\vec{r})\})=\prod_{h=h_{min}}^{h_{max}}\frac{1}{2}(1+z^{n_h}) \tag{3}$$

in a given height configuration $\{h(\vec{r})\}$. Next choose a column $\vec{x}$ randomly. Then decide the deposition attempt $h(\vec{x})\to h(\vec{x})+1$ with probability p or the evaporation attempt $h(\vec{x})\to h(\vec{x})-1$ with probability q. Then calculate $w(\{h'(\vec{r})\})$ for the new configuration $\{h'(\vec{r})\}$ from the decided deposition (evaporation) process. Then the acceptance parameter P is defined by $P\equiv w(\{h'(\vec{r})\})/w(\{h(\vec{r})\})$. If $P\geqslant 1$, then the new configuration is accepted unconditionally. If $P<1$, the new configuration is accepted only when $P\geqslant R$, where R is a generated random number with $0<R<1$. Any new configuration is rejected if it would result in the violation of the RSOS constraint.

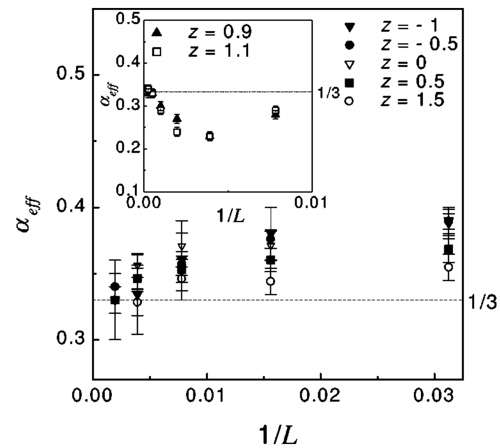

FIG. 1. Effective exponents α_{eff} versus $1/L$ for the equilibrium surfaces of the model with $z=-1,-0.5,0,0.5,1.5$. Used system sizes are $L=2^5,2^6,\ldots,2^{10}$. All data for various values of z converge to 1/3 rather nicely in the $L\to\infty$ limit. The inset shows the same plot for $z=0.9$ and 1.1. The data in the inset are shown for the system sizes $L=2^7,2^8,\ldots,2^{13}$.

By using the Metropolis-type evolution rule, we perform numerical simulations, starting from a flat surface on the 1D substrate of linear size L with the lateral periodic boundary condition. To measure the surface fluctuation W of Eq. (1) for a given z, we run simulations for $L=2^5,\ldots,2^{13}$ and average the data for W over at least 300 independent samples.

First, we show the results for the equilibrium surfaces ($p=q$). In order to extract the saturation-regime property, the data for W for $t\gg L^{z_W}$ are analyzed to obtain $W_s(L)=W(t\gg L^{z_W})$. For the estimation of exponent α, we introduce effective exponents

$$\alpha_{eff}(L)=\ln[W_s(mL)/W_s(L)]/\ln m, \tag{4}$$

where m is an arbitrary constant (here, we set $m=2$). Effective exponents for $z=-1$, -0.5, 0, 0.5, and 1.5 are obtained by using systems with sizes up to $L=2^{10}$. The results are plotted in Fig. 1. For small system sizes up to $L=2^7$, our data show relatively large corrections to scaling as expected. However, the asymptotic estimates seem to be independent of z. We estimate $\alpha\simeq 1/3$ for all z in the systems with $L\geqslant 2^8$. Since the model with $z=1$ is exactly equal to the ordinary RSOS model with $\alpha=1/2$, we also investigate the models with z close to 1. For this, α_{eff} for $z=0.9$ and $z=1.1$ is evaluated by using systems up to $L=2^{13}$. The results are displayed in the inset of Fig. 1. We also find large corrections to the scaling up to $L=2^{10}$, but find $\alpha\simeq 1/3$ for $L\geqslant 2^{11}$. Since the model based on the partition function (2) cannot be physically defined for $z<-1$, the result in Fig. 1 strongly supports the fact that all the equilibrium surfaces for $z\geqslant -1$, except for $z=1$, have the same phase with $\alpha=1/3$. In Fig. 2, we also display the early-time ($t\ll L^{z_W}$) dynamical behavior for the equilibrium surfaces for the same z's in Fig. 1. The data in Fig. 2 are obtained from the simulation in the system with $L=2^{12}$. The growth exponent β is obtained by a simple fitting of the relation $W\simeq t^{\beta}$ to the data.

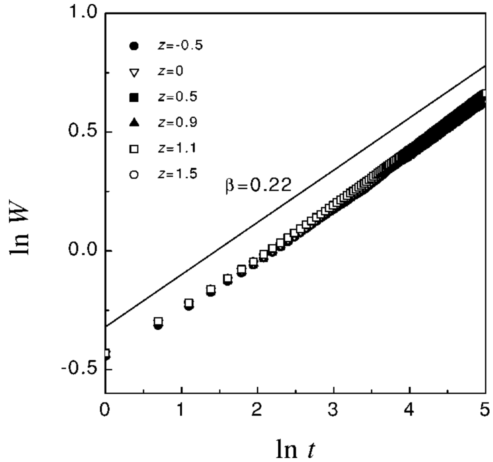

FIG. 2. Plots of $\ln W$ against $\ln t$ for $z=-0.5,0,0.5,0.9,1.1,1.5$ for the equilibrium surfaces. The used system size is $L=2^{12}$. The straight line denoted by $\beta=0.22$ represents the relation $W \simeq t^{0.22}$.

Our estimate is $\beta=0.22(1)\simeq 2/9$ regardless of the value z. The best estimation of β for the 2P model ($z=-1$) from Ref. [4] was $\beta\simeq 0.20$. The results in Fig. 2 also support the fact that all the models for $z>-1$, except $z=1$, have the same dynamical behavior of $\beta=2/9$, even though the estimated β value for $z=-1$ seemed to be somewhat smaller than 2/9. The sector (or initial-morphology) dependence is checked for the models with $z>-1$, but it is found that the results in Figs. 1 and 2 are not varied by changing the initial surface configuration. As mentioned in the introductory part, the QP models [4] have no sector (or initial-morphology-dependent) problem, whereas the Q-mer models have the problem [6,7]. Since the models considered here are deeply related to the 2P models, the models show no sector dependence.

The scaling behaviors in Fig. 1 can be analytically understood from the partition function because the equilibrium surface has no external bias. The partition function (2) can be expanded as

$$Z=\sum_{\{h(\vec{r})\}}(1/2)^S\left[1+\sum_{h=h_{min}}^{h_{max}} z^{n_h}+\cdots+z^L\right], \tag{5}$$

where $S=h_{max}-h_{min}+1$ and $L=\Sigma_h n_h$. Then in the limit $z\to\infty$,

$$Z=z^L\sum_{\{h(\vec{r})\}}(1/2)^S=z^L Z_{SF}, \tag{6}$$

where Z_{SF} is simply the partition function for the SF surface growth. Equation (6) thus implies that the models for $z\gg 1$ have the same scaling behavior as the SF model. For $|z|\ll 1$, Z in Eq. (5) can be written as

$$Z\simeq\sum_{\{h(\vec{r})\}}e^{-\beta S}\left[1+\sum_{h=h_{min}}^{h_{max}} z^{n_h}\right] \tag{7}$$

and the most dominant (relevant) term in Z is Z_{SF}. We thus expect the SF scaling behavior for $|z|\ll 1$. The simulation

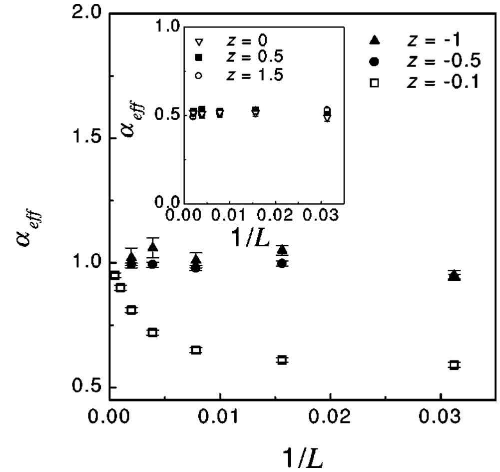

FIG. 3. α_{eff} versus $1/L$ for the growing surfaces ($p=1$) of the model with $z=-1,-0.5,-0.1$. The inset shows the same plot for $z=0,0.5,1.5$. The data for $z=-0.1$ are taken from the system sizes up to $L=2^{12}$ and other data are from the system sizes up to $L=2^{10}$.

results and the analytic arguments in Eqs. (6) and (7) strongly support the following renormalization group (RG) flows in the phase space of z. The $z=1$ fixed point for the ordinary RSOS behavior is the unstable fixed point. For $z>1$, the RG flow is directed to the $z=\infty$ fixed point, which represents the scaling behavior governed by the partition function (6), or coincidentally the SF behavior. For $|z|<1$, the RG flow is directed to $z=0$, which represents the SF behavior itself [see Eq. (7)]. This analytic argument supports the phase diagram in which all of the phases for $z\geq -1$, except the singular point $z=1$, are the same phase with $\alpha=1/3$ as the SF growth with $z=0$. This theoretical argument based on the partition function explains the existence of a phase with $\alpha=1/3$ for $z\geq -1$. However, the evolution dynamics, especially the results $\beta\simeq 2/9$ and $z_W\simeq 3/2$, can hardly be explained from the partition function itself, even though the SF model [5] has numerically been shown to have $\beta\simeq 2/9$ and $z_W\simeq 3/2$. Further analytical study to explain the common dynamical behavior $\beta\simeq 2/9$ for models with $z\geq -1$ is left for future research.

Next, we consider nonequilibrium growing/eroding surfaces ($p\neq q$). We run simulations for $p=1$ in the system sizes $L=2^5,\ldots,2^{12}$. α_{eff} for $z=-1,-0.5,-0.1$ is shown in the main figure of Fig. 3 and that for $z=0,0.5,1.5$ is shown in the inset of Fig. 3. As can be seen from Fig. 3, α for $z<0$ is quite different from that for $z\geq 0$. For $z\geq 0$, we estimate that $\alpha\simeq 0.50(1)$, which are consistent with the results for the ordinary RSOS model [10]. However, $\alpha\simeq 1$ is estimated for $z<0$ as in the 2P (QP) model with $z=-1$ [4]. Even for small negative z (or $z=-0.1$), α_{eff} approaches 1 in the limit $L\to\infty$, even though there exists a large correction to the $\alpha=1$ scaling behavior in systems with small L. We also investigated the time-dependent behavior of $W(t)$. For $z>0$ we get $\beta\simeq 0.32(1)$, which is the ordinary RSOS behavior [10]. In contrast, the different time-dependent behavior of W is found as shown in Fig. 4. In Figs. 4(a)–4(c), a typical time evolution of the surface for $z<0$ in a simulation

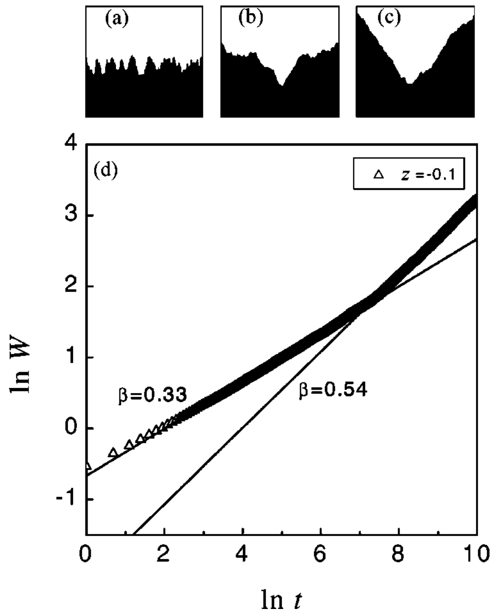

FIG. 4. (a)–(c) Typical time evolution of the surfaces for $z=-0.5$ in a simulation sample. The used system size is $L=2^8$. (a) The morphology at the initial stage of growth; (b) that around the time at which a valley bottom is formed; (c) that after the fully developed grooved is formed; (d) the time dependence of W in the early-time regime for $z=-0.1$.

sample is shown. At the initial stage of growth, the morphology of the surface is like that in Fig. 4(a) as in the ordinary RSOS model. But after some time, the valley bottom is formed and localized as in Fig. 4(b). Then the grooved structure, such as in Fig. 4(c), eventually appears as in the 2P model [4]. The formation of the valley bottom and the grooved structure is believed to have come from the mechanism similar to the evenness constraint of the 2P model [4,6] with $z=-1$. A sort of stochastic evenness constraint [6] seems to be effective for $z<0$, even though the constraint becomes weaker as $z\to 0^-$. This kind of the time-dependent behavior can also be seen from the early-time behavior of W as shown in Fig. 4(d). Initially, $W(t)$ follows the ordinary power-law behavior with $W(t)\simeq t^{\beta}$. After the time in which the valley bottom is formed, a sort of unstable growth with quite large value of β occurs before $W(t,L)$ becomes the saturated value $W_s(L)$. The growing (eroding) surfaces thus have the phase transition (or the sudden crossover) at $z=0$. The transition, of course, occurs from the grooved phase ($\alpha=1$) for $-1\leqslant z<0$ to the ordinary RSOS behavior ($\alpha=1/2$) for $z\geqslant 0$.

The growing (eroding) biases, except the effects from the partition function, definitely have physical roles for the nonequilibrium growing/eroding ($p\neq q$) surfaces. So it is hard to understand the existence of $\alpha=1$ phase for $z<0$ and the ordinary RSOS phase for $z\geqslant 0$ directly from the partition function. An analytic understanding of these characteristics of nonequilibrium surfaces is also left for future research.

In summary, we studied the scaling properties of the growth model described by the Metropolis-type evolution rule based on the partition function (2). For the equilibrium surfaces, the scaling properties for $z\geqslant -1$ are all one phase with $\alpha=1/3$ and $\beta=0.22$. For the growing (eroding) surfaces, there exists a phase transition at $z=0$ from the grooved phase ($\alpha=1$) to the ordinary RSOS behavior ($\alpha=1/2$).

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