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Universality classification of restricted solid-on-solid type surface growth models

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We consider the restricted solid-on-solid (RSOS) type surface growth models and classify them into dynamic universality classes according to their symmetry and conservation law. Four groups of RSOS-type microscopic models—asymmetric (A), asymmetric-conserved (AC), symmetric (S), and symmetric-conserved (SC) groups—are introduced and the corresponding stochastic differential equations (SDEs) are derived. Analyzing these SDEs using dynamic renormalization group theory, we confirm the previous results that A-RSOS, AC-RSOS, and S-RSOS groups belong to the Kardar-Parisi-Zhang class, the Villain–Lai–Das Sarma class, and the Edwards-Wilkinson class, respectively. We also find that SC-RSOS group belongs to a new universality class featuring the conserved-cubic nonlinearity.

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Universality is one of the most important features in modern theory of critical phenomena because various models can be classified purely in terms of their collective behavior into classes insensitive to details of microscopic structure and interactions. The theory of critical phenomena and universal behavior are quite well understood in equilibrium systems [1]. We can use renormalization group (RG) theory to classify the different systems into universality classes. The different universality classes are characterized only by a small set of basic features—spatial dimensionality, dimensionality, and symmetry of the order parameter, and whether the interactions are long or short range. The situation is not so clear in the framework of nonequilibrium systems because there is no general theory available to describe nonequilibrium systems. Most of the known results are based on numerical simulations. However, the concept of universality appears to be relevant although we do not completely understand how the universality classes are characterized in nonequilibrium systems. Again, the basic ingredients affecting the universality classes may be the collective behavior of systems, spatial dimensionality, symmetries, and conservation laws.

In this paper, we address the issue of how to classify the restricted solid-on-solid (RSOS) type nonequilibrium surface growth models into different dynamic universality classes by concentrating on the symmetry and the conservation law. Kinetic surface roughening of nonequilibrium surface growth has been investigated using various discrete models and continuous equations [2]. Comprehension of nonequilibrium surface growth plays an important role in understanding and controlling many interesting interface processes, such as vapor deposition [3], crystal growth [4], and molecular beam epitaxy (MBE) [5]. During the MBE growth process, the solid-on-solid growth condition is applied without defects, such as overhangs and vacancies. Various discrete models describing the kinetic properties of the MBE surface growth process have been proposed and studied by intensive numerical simulations.

While the generic nonequilibrium surface growth models that allow for overhangs and vacancies are theoretically accepted to belong to the Kardar-Parisi-Zhang (KPZ) universality class [6], there is no such consensus for classifying growth models of the MBE growth processes. We investigate the several variants of RSOS-type growth models and classify these models into universality classes according to their symmetry and conservation law. First, we introduce discrete models satisfying the RSOS constraint. These models are named depending on local growth rules: asymmetric-RSOS model (A-RSOS), asymmetric-conserved-RSOS model (AC-RSOS), symmetric-RSOS model (S-RSOS), and symmetric-conserved-RSOS model (SC-RSOS). Symmetric models have growth rules which preserves height-inversion symmetry and conserved models have growth rules in which the trial move (adsorption or desorption) is not rejected, keeping the particle flux conserved. We apply a hard-core bosonic field theoretical formalism developed by the authors for these models and derive corresponding stochastic differential equations (SDEs) for each surface growth model [7,8]. We then analyze these SDEs using the dynamic RG theory and classify models into their universality classes.

The RSOS model is one of the simplest microscopic growth models [9]. It describes the growth of simple cubic surfaces, in which the height difference between any nearest neighbor pair does not exceed some value (the RSOS constraint). We limit ourselves to the case wherein the height difference between two nearest neighbors is not larger than 1. For ease of explanation, we introduce some nomenclatures. If a site satisfies the RSOS constraint after the height increase (decrease) by 1, we call the site "adsorptive (erosive)." For example, a site m whose height satisfies $|(h_m-1)-h_{m\pm1}|\leq 1$ in a one-dimensional lattice is erosive, and so forth. A site is "active," if a site is either adsorptive or erosive. The model we are describing has two parameters, p and l. p is the probability with which adsorption occurs at an arbitrarily chosen site and l is the search range (see below). The growth algorithm for a one-dimensional system is as follows:

(i) We choose a site m randomly.

(ii) With probability p, the adsorption is tried. The erosion will be attempted with probability $q=1-p$.

(iii) Check if site m is active.

(iv) If site m is active, the height at site m is changed by the dynamics determined at step (ii). If site m is not active, we search for an active site in the interval from $m-l$ to $m+l$. If an active site is found in this interval, the height at the nearest active site from m is changed. (If there are two active sites having the same distance from m, site to be updated is decided with equal probability). If an active site is not found within this interval, the trial move is rejected and the system remains unchanged.

(v) After the dynamics (adsorption, desorption, or rejection), time is increased by $1/L$, where L is the system size.

The model with $l=0$ and $p=1$ corresponds to the original RSOS model [9] and the model with $l=\infty$ and $p=1$ corresponds to the conserved-RSOS (C-RSOS) model [10]. Recently, the models with nonvanishing finite l for $p=1$ were shown to belong to the same universality class as the RSOS model by the authors [8,11]. If $p\neq 1$, then the role of desorption is problematic. It has been argued [12] that erosion generates the surface tension term. This implies that if $p\neq 1$, the system may be described by SDE with a tension term. In what follows, we show that this is not the case. Hence, we classify the variants of the RSOS model introduced above into four groups according to the conservation and the symmetry. We name each group as follows ($q=1-p$): A-RSOS model with finite l and $p\neq q$, AC-RSOS model with infinite l and $p\neq q$, S-RSOS model with finite l and $p=q$, and SC-RSOS model with infinite l and $p=q$.

The model introduced can be mapped onto the reaction-diffusion system of two-species hard-core particles, since the height difference between two neighbors is restricted to be -1, 0, and 1. The step up (step down) is mapped to an A (B) particle and if two neighbors have equal height, a particle vacuum is located between two sites [11]. According to this mapping, the dynamics with the search range l and adsorption (erosion) probability p (q) can be described by the master equation in the form of the (imaginary time) Schrödinger equation $\partial/\partial t|\Psi;t\rangle=-\hat{\mathcal{H}}|\Psi;t\rangle$ for the state vector $|\Psi;t\rangle\equiv\Sigma_{\mathcal{C}}P(\mathcal{C};t)|\mathcal{C}\rangle$, where $P(\mathcal{C};t)$ is the probability with which the system is in state $\mathcal{C}$ at time t, the sum is over all possible states, and $\hat{\mathcal{H}}(=\Sigma_n\hat{\mathcal{H}}_n)$, called a Hamiltonian, is an evolution operator given by

$$\mathcal{H}_n=p(\hat{I}-\hat{A}_n-\hat{D}_n)\hat{\Pi}_n^{\mathrm{A}}+q(\hat{I}-\hat{E}_n-\hat{\mathcal{E}}_n)\hat{\Pi}_n^{\mathrm{E}}, \qquad (1)$$

where

$$\Pi_n^{\mathrm{A}}=\hat{I}+\frac{1}{2}\sum_{j=1}^{2l}\left(\prod_{k=1}^{j}\hat{A}_{n+k}+\prod_{k=1}^{j}\hat{A}_{n-k}\right),$$

$$\Pi_n^{\mathrm{E}}=\hat{I}+\frac{1}{2}\sum_{j=1}^{2l}\left(\prod_{k=1}^{j}\hat{E}_{n+k}+\prod_{k=1}^{j}\hat{E}_{n-k}\right), \qquad (2)$$

and

$$\hat{A}_n=\hat{a}_n^\dagger\hat{a}_n+\hat{b}_{n+1}^\dagger\hat{b}_{n+1}-\hat{a}_n^\dagger\hat{a}_n\hat{b}_{n+1}^\dagger\hat{b}_{n+1},$$

$$\hat{E}_n=\hat{b}_n^\dagger\hat{b}_n+\hat{a}_{n+1}^\dagger\hat{a}_{n+1}-\hat{b}_n^\dagger\hat{b}_n\hat{a}_{n+1}^\dagger\hat{a}_{n+1},$$

$$\hat{D}_n=(\hat{a}_n^\dagger+\hat{b}_n)(\hat{a}_{n+1}+\hat{b}_{n+1}^\dagger),$$

$$\hat{\mathcal{E}}_n=(\hat{b}_n^\dagger+\hat{a}_n)(\hat{b}_{n+1}+\hat{a}_{n+1}^\dagger). \qquad (3)$$

As in Ref. [11], we use an integer to indicate the location of particles and a half integer for the height configuration. The role of the rejection operator $\hat{A}_n(\hat{E}_n)$ is to check if the site $n+1/2$ is not adsorptive (erosive), that is, if the site $n+1/2$ is adsorptive (erosive) in a configuration $|\mathcal{C}\rangle$, $\hat{A}_n(\hat{E}_n)|C\rangle=0$, and otherwise $\hat{A}_n(\hat{E}_n)|C\rangle=|C\rangle$. The adsorption (erosion) operator $\hat{D}_n(\hat{\mathcal{E}}_n)$ describes the configuration change after a successful adsorption (erosion). $\hat{a}_n(\hat{b}_n)$ is the annihilation operator of an $A(B)$ particle at site n and $\hat{a}_n^\dagger(\hat{b}_n^\dagger)$ is the corresponding creation operator, satisfying the mixed commutation relations [7],

$$\hat{a}_n\hat{a}_n^\dagger=\hat{b}_n\hat{b}_n^\dagger=\hat{I}_n-\hat{a}_n^\dagger\hat{a}_n-\hat{b}_n^\dagger\hat{b}_n, \quad \hat{a}_n\hat{b}_n=\hat{a}_n^\dagger\hat{b}_n^\dagger=0. \qquad (4)$$

All operators at different sites commute with each other.

We apply the method recently introduced by us to find the SDEs for the above microscopic model [7,11]. This procedure is very similar to that in Ref. [11]. Thus, we briefly sketch the procedure in this paper (the detailed calculation may be found elsewhere [13]). We first derive the lattice version of the SDEs for densities a_n and b_n of particle species A and B. We find the Kramers-Moyal coefficients via the commutation relations between the Hamiltonian and the number operators by deriving the time evolutions of the one-point and two-point correlation functions of the number operators $\hat{a}_n^\dagger\hat{a}_n$ and $\hat{b}_n^\dagger\hat{b}_n$ using the Hamiltonian in Eq. (1), and comparing with the formal time evolutions of the correlation functions obtained from the Kramers-Moyal coefficients using the Fokker-Planck equation. We obtain the Fokker-Planck equation with the Kramers-Moyal coefficients in terms of densities from these commutation relations. These coefficients describe the time evolution of the probability of finding the system in a certain state with given densities. Once the Fokker-Planck equation is known for the system, the corresponding SDEs for densities can be derived following the standard method [14–16]. Next, we introduce two quantities ρ_n and S_n defined as

$$\rho_n=a_n+b_n, \quad S_n=a_n-b_n, \qquad (5)$$

which are step density and slope, respectively. The step density saturates fast due to the mass term present in the SDE for the step density S_n. As a result, the step density in the stationary state becomes a slave field of the slope, and takes the form

$$\rho=\rho_0+\mu_0\partial S+\theta_0 S^2+\lambda_0\partial S^3+\cdots, \qquad (6)$$

where ρ_0, μ_0, θ_0, and λ_0 are appropriate functions of p, q, and l to be determined. The SDE for the slope gives the SDE for the height field h of the surface via $S=\nabla h$ in one dimension. Following the *figurization* described in Ref. [11] and performing continuum limit, we obtain the continuum SDE for the height field.

The SDE for the A-RSOS model is the KPZ equation [6,8]

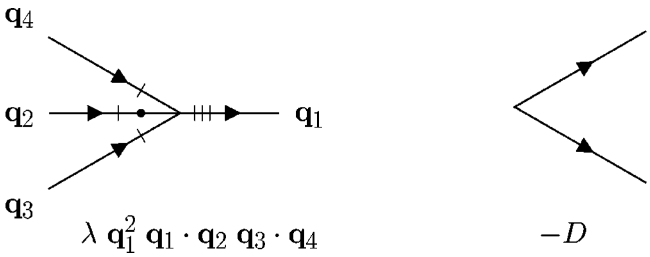

FIG. 1. Vertices for DRG calculation.

$$\frac{\partial h}{\partial t}=\nu\nabla^2 h+\lambda(\boldsymbol{\nabla} h)^2+\eta, \tag{7}$$

and the SDE for the AC-RSOS model is the Villain–Lai–Das Sarma (VLD) equation [17]

$$\frac{\partial h}{\partial t}=-\nabla^2[\nu\nabla^2 h+\lambda(\boldsymbol{\nabla} h)^2]+\eta. \tag{8}$$

The extreme asymmetric cases $p=1$, $q=0$ of these models are discussed in Refs. [8,11]. We also find that asymmetric cases with $p\neq q$ belong to the same universality class as the extreme asymmetric case [13]. In the SDE for the S-RSOS model, since the KPZ term violates the up-down symmetry, the coefficient of the KPZ term vanishes and the next relevant term in the SDE is the cubic term $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} h)^3$ which is irrelevant in all dimensions. Thus, the corresponding SDE to the S-RSOS model is the Edwards-Wilkinson (EW) equation [18], in which the nonlinear λ term is absent in the KPZ equation. Finally, the SDE for the SC-RSOS model is found to be

$$\frac{\partial h}{\partial t}=-\nabla^2[\nu\nabla^2 h+\lambda\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} h)^3]+\eta, \tag{9}$$

where $\nu=(8-3\sqrt{2})/2$, $\lambda=(32-9\sqrt{2})/8$, and η is a white noise with correlation $\langle\eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle=2D\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$ with $D=(2\sqrt{2}-1)/4$. This equation is symmetric under the inversion of the height field h, that is, under $h\to -h$, Eq. (9) is invariant, and the cubic term in the equation is marginal in two dimensions. We analyze this equation by deriving the Martin-Siggia-Rose (MSR) action using the conjugate field $\overline{h}$ to the height field h and applying the dynamic renormalization group (DRG) theory [19,20]. The corresponding MSR action is $S=\int dt d\mathbf{x}\mathcal{L}$ with

$$\mathcal{L}=\overline{h}(\partial_t+\nu\nabla^4)h-\lambda\boldsymbol{\nabla}(\nabla^2\overline{h})\cdot(\boldsymbol{\nabla} h)^3-D\overline{h}^2, \tag{10}$$

where we performed the partial integration and dropped the surface term. In Fig. 1, two vertices in the MSR action are depicted. The incoming arrow stands for the height field h, the outgoing arrow for the conjugate field $\overline{h}$, and the line segments on the arrows represent the spatial derivative of the fields.

Using the Wilson DRG method, the flow equations for the parameters ν, λ, and D, to one-loop order are

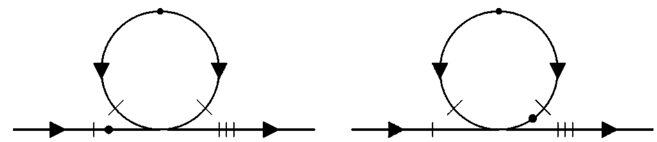

FIG. 2. One-loop contribution to the propagator.

$$\frac{\partial \ln\nu}{\partial\ell}=z-4+\frac{d+2}{d}g, \tag{11a}$$

$$\frac{\partial \ln D}{\partial\ell}=z-2\alpha-d, \tag{11b}$$

$$\frac{\partial \ln\lambda}{\partial\ell}=z+2\alpha-6-\frac{d^2+6d+20}{d(d+2)}g, \tag{11c}$$

where $g\equiv K_d\Lambda^{d-2}\lambda D/\nu^2$ is the expansion parameter and ℓ is the scaling parameter of DRG. The one-loop diagrams contributing to the flow equations are shown in Figs. 2 and 3. Equation (11b) is exact since the SDE (9) consists of the conserved deterministic part and the nonconserved noise.

The fixed point of g is determined by the equation

$$\frac{\partial \ln g}{\partial\ell}=\varepsilon-\frac{3d^2+14d+28}{d(d+2)}g, \tag{12}$$

where $\varepsilon=2-d$. Hence,

$$z=4-\frac{(d+2)^2}{3d^2+14d+28}\varepsilon,\quad \alpha=1+\frac{d^2+5d+12}{3d^2+14d+28}\varepsilon. \tag{13}$$

In one dimension, we find $z=19/5$ and $\alpha=7/5$. For all $d\geqslant 2$, $z=4$ and $\alpha=1$.

We also performed the numerical simulations for the SC-RSOS model in one dimension. In Fig. 4, the scaling plot shows the data collapse of the model. The system sizes in the simulations are 64, 90, 128, 256, 360, and 512. Although, the best collapse occurs for $\alpha=1.03$, we cannot exclude the possibility that $\alpha=1$. The calculated α is not decisive in one dimension since Eq. (13) is obtained from the DRG calculation only up to one-loop order. Still, SC-RSOS model is not

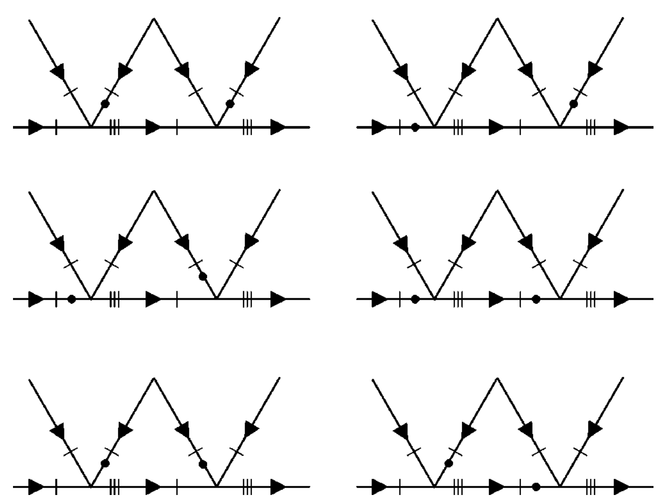

FIG. 3. One-loop contribution to the λ vertex.

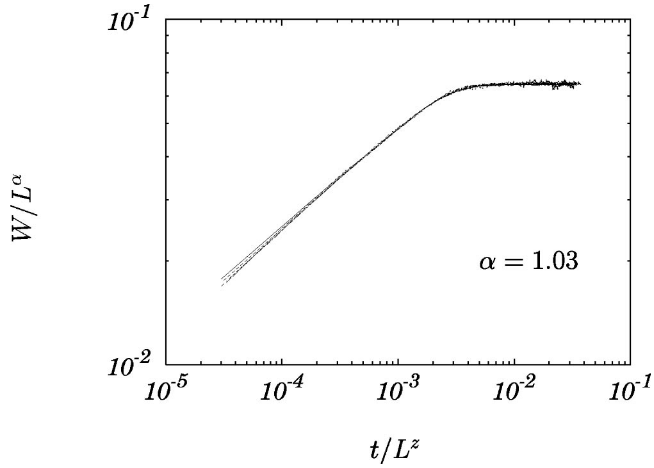

FIG. 4. Log-log plot of the data collapse for Monte Carlo simulation of the SC-RSOS model. The best collapse occurs for $\alpha = 1.03$ and $z = 2\alpha + 1 = 3.06$.

believed to share the same universality class as the VLD equation, because these two systems have different symmetry.

In summary, we studied four different kinds of the RSOS-type microscopic discrete models classified by up-down symmetry and conservation, using both analytical and numerical methods. We confirmed the previous results that the A-RSOS model belongs to the KPZ class, the AC-RSOS model to the VLD class, the S-RSOS model to the EW class. We also derived the stochastic differential equations for the SC-RSOS model analytically and found that the SC-RSOS model belongs to the new class which we call ‘‘conserved cubic’’ (CC) class. The SDE corresponding to the SC-RSOS model of the CC class has the conserved form of the EW term $\nabla^2(\nabla^2 h)$ and the Gaussian noise (not conserved form) similar to the SDE of the VLD class, but it has the conserved form of the cubic term $\nabla^2 \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} h)^3$, which is absent in the EW class, in the KPZ class, and in the VLD class. The conserved cubic term is less relevant than the conserved KPZ term $\nabla^2(\boldsymbol{\nabla} h)^2$ in the VLD equation and is irrelevant in all dimensions in the EW and KPZ equations. In addition to identifying the corresponding SDEs for each microscopic model, we found coefficients of the EW term, the KPZ term, the VLD term, and the CC term. Coefficients of the EW and KPZ terms have been shown to be consistent with the previous numerical study [21]. Verifying the consistency of coefficients of the VLD and CC terms by the numerical study will be a future challenge for the interested.

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