Effect of symmetry on volume conserving surface models

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(Received 19 January 1999)

We study the effect of symmetry on volume conserving models without deposition and evaporation. By using the master equation approach, we identify two types of stochastic continuum equation with a conservative noise, depending on the symmetry of hopping rate in diffusion rules. In the model with symmetric hopping rate, a Laplacian term is essentially absent from the continuum equation. The dynamic scaling of this model is thus determined by the nonlinear fourth order equation with a conservative noise. When the symmetry is broken, a Laplacian term may be present, so the asymptotic scaling behavior is governed by the Laplacian term with nonzero coefficient. We verify this result by investigating a simple discrete model analytically.
[S1063-651X(99)08806-6]

PACS number(s): 05.40.−a, 68.35.Ct, 05.10.Gg

I. INTRODUCTION

For the past decade the kinetic roughening of nonequilibrium surface growth has attracted much interest theoretically and experimentally. The kinetic roughening properties of surfaces can be classified into universality classes by obtaining the critical exponents, which determine the asymptotic scaling behavior of the surface on a large length scale and in a long time limit. For surface growth, various discrete models and stochastic continuum equations have been studied by the use of computer simulations, symmetry arguments, renormalization-group analyses, and direct numerical integrations [1]. One can establish the correspondence between a continuum equation and a discrete model numerically or analytically. Many studies are devoted to numerical simulations of discrete models and compare the scaling exponents which obtain with corresponding continuum equations. In the analytical approaches, the continuum equation is derived from the dynamic rule of a given discrete model, mostly based on the master equation description proposed by Vvedensky *et al.* for a solid-on-solid model with Arrhenius hopping dynamics [2]. This master equation approach has been successfully applied to the derivation of continuous stochastic equations for many discrete models, including the restricted solid-on-solid (RSOS) model [3], the Wolf-Villain model and Das Sarma–Tamborenea model [4,5], the conserved RSOS model [6], the ballistic model [7], and the erosion model [8]. However, this method fails for an unrestricted SOS diffusion model with Glauber dynamics [9]. Uncertainty in the regularization process is also discussed [4].

The growth process of all discrete models mentioned above is constituted by the deposition of particles, inherently generating a nonconservative noise. There are few attempts to describe the surface reconstruction when no particles are deposited from external sources. Without deposition flux, the surface could be reconstructed by thermal fluctuations or by some external agent such as an electric field [10]. A recent study of the surface electromigration induced by an alternating electric field explicitly shows the smoothening effect of surfaces by a net downhill current [11]. Two types of discrete model for the volume conserving surface fluctuations have been studied. In the model a surface diffusion is driven, not by equilibrium fluctuations, but rather by some external agent. One is a conservative variant of the RSOS model [12,13] and another is the mobility-restricted diffusion model [14,15]. Numerical simulations have shown that these models are described by the continuum equations with a conservative noise, $\eta_c(x,t)$, which has the following properties:

$$\langle \eta_c(x,t)\rangle = 0,$$
$$\langle \eta_c(x,t)\,\eta_c(x',t')\rangle = -D_c\nabla^2\delta(x-x')\,\delta(t-t'). \tag{1}$$

The integral of the conservative noise over the entire surface remains at zero at every moment so that the volume conservation requirement is automatically satisfied.

In this Brief Report, we study the volume conserving surface model, in which no particles are deposited but only a self-diffusion occurs on the surface. By using the master equation approach, we obtain two kinds of stochastic continuum equations corresponding to discrete models. We show that the symmetry in hopping rate plays a crucial role in the determination of continuous stochastic equations. We also consider a simple discrete model to verify the effect of symmetry in hopping rate.

II. DERIVATION OF STOCHASTIC CONTINUUM EQUATIONS

According to the master equation approach [2], the continuous stochastic Langevin equation is written as

$$\frac{\partial h(x,t)}{\partial t} = K_i^{(1)}(h(x,t)) + \eta(x,t), \tag{2}$$

where $K_i^{(1)}$ is the first moment of the transition matrix $W(\mathbf{H},\mathbf{H}')$, η represents the noise with zero mean, and the noise covariance is given by the second transition moment

$$\langle \eta(x,t)\,\eta(x',t')\rangle = K_{ij}^{(2)}(h(x,t))\,\delta(t-t'). \tag{3}$$

Equations (2) and (3) describe the evolution of height $h(x,t)$ at site x as a function of height difference between neighboring sites and determine the dynamics of the model. Once the explicit form of the transition matrix $W(\mathbf{H},\mathbf{H}')$ between the configuration **H** and the configuration **H**′ of the surface is obtained from the dynamic rule of a discrete model, the corresponding continuum equation and the noise covariance can be derived explicitly.

In the volume conserving surface models, the total number of particles existing on the surface is always conserved without deposition and evaporation. Whenever the position of a particle changes, any decrease of the height at one site must be accompanied by an increase of the same height at another site on the surface. If we allow one particle movement only, the change of height is given by one unit lattice spacing a. This is always true for any volume conserving surface model so that the transition matrix has the following form:

$$W(\mathbf{H},\mathbf{H}')=\frac{1}{\tau}\sum_i\,[w_i^+\delta(h_i',h_i-a)\delta(h_{i+1}',h_{i+1}+a)+w_{i+1}^-\delta(h_i',h_i+a)\delta(h_{i+1}',h_{i+1}-a)]\times\prod_{j\neq i,i+1}\delta(h_j',h_j), \tag{4}$$

where τ is the time scale and the nearest neighbor hopping is assumed. The w_i^+ (w_i^-) and w_{i+1}^- (w_{i-1}^+) are hopping rates from site i to site $i+1$ $(i-1)$, and from site $i+1$ $(i-1)$ to site i, respectively. These hopping rates depend on the morphology of the surfaces, more explicitly, on the height difference between two hopping sites and also on the diffusion rules of a given model. From Eq. (4), we obtain the first and second moments of $W(\mathbf{H},\mathbf{H}')$ as follows:

$$K_i^{(1)}=\frac{a}{\tau}(w_{i+1}^- - w_i^- - w_i^+ + w_{i-1}^+), \tag{5}$$

$$K_{ij}^{(2)}=aK_i^{(1)}\delta_{i,j}-\frac{a^2}{\tau}[(w_i^+ + w_j^-)(\delta_{i+1,j}-\delta_{i,j})+(w_j^+ + w_i^-)(\delta_{i-1,j}-\delta_{i,j})], \tag{6}$$

where $\delta_{i,j}$ is the Kronecker delta. The above form of the transition matrix and its moments is a general one for volume conserving surface models. Consequently, by obtaining the hopping rates $w_i^\pm$ for a certain discrete model, we can derive the discrete Langevin equation explicitly.

We now show that the corresponding continuous stochastic equations for the volume conserving surface models depend on the symmetry of hopping rate. As in Ref. [4], we suppose that the height difference can be replaced by a smooth function in the limit of lattice constant $a\to 0$ as follows:

$$h_{i\pm1}(t)-h_i(t)=\sum_{k=1}^{\infty}\left.\frac{(\pm a)^k\partial^k h}{k!\quad \partial x^k}\right|_{x=ia}. \tag{7}$$

Since the hopping rates, $w_i^\pm$, depend on the height difference between two hopping sites, we can regard $w_i^\pm$ as a continuous function of height differences, $h_{i\pm1}-h_i$, described by Eq. (7). We thus express $w_i^\pm$ as a sum of products of various space derivatives of $h(x)$,

$$w_i^\pm=\sum_{n=0}^{\infty}C_n(x)(\mp a)^n. \tag{8}$$

Other hopping rates from site $i\pm1$ to site i, w_{i+1}^- and w_{i-1}^+, can be obtained by the Taylor expansion as follows:

$$w_{i\pm1}^\mp=\sum_{k,n=0}^{\infty}\frac{\partial^k C_n(x)}{\partial x^k}\frac{(\pm a)^{k+n}}{k!}, \tag{9}$$

where $C_n(x)$ denotes all combinations of any possible nth space derivatives; for example, $C_0=\text{const}, C_1=\boldsymbol{\nabla}h, C_2=[\nabla^2 h,(\boldsymbol{\nabla}h)^2], C_3=[\nabla^3 h,(\boldsymbol{\nabla}h)^3,\boldsymbol{\nabla}(\boldsymbol{\nabla}h)^2]$, $C_4=[\nabla^4 h,(\boldsymbol{\nabla}h)^4,\nabla^2 h(\boldsymbol{\nabla}h)^2,\boldsymbol{\nabla}(\boldsymbol{\nabla}h)^3]$, etc.

From Eqs. (5), (8), and (9), we finally obtain the following continuum equation

$$\frac{\partial h(x,t)}{\partial t}=\frac{2a}{\tau}\sum_{\substack{n=2\\ n:\text{even}}}^{\infty}\sum_{k=1}^{n-1}\frac{\partial^k C_{n-k}(x)}{\partial x^k}\frac{a^n}{k!}+\eta_c(x,t), \tag{10}$$

where the noise covariance is also obtained from Eqs. (6), (8), and (9) as follows:

$$\langle\eta_c(x,t)\eta_c(x',t')\rangle=-D_c\nabla^2\delta(x-x')\delta(t-t'), \tag{11}$$

with $D_c=2C_0a^5/\tau$, up to $O(a^5)$. This form of the noise covariance demonstrates that the continuum equation for the volume conserving model is indeed given, not by a nonconservative white noise, but rather by a conservative noise. The resulting continuum equation has several terms such as $\nabla^2 h,\nabla^4 h,\nabla^2(\nabla h)^2$, and $\nabla(\nabla h)^3$ up to the fourth order. Note that the nonlinearity, $(\nabla h)^2$, is essentially absent. If the coefficient of the Laplacian term is positive, the Laplacian term determines the asymptotic scaling behavior of the model.

For the model with a *symmetric* hopping rate, in which a particle at one site hops to another site with equal probability, i.e., $w_i^+=w_i^-$, $w_{i+1}^+=w_{i+1}^-$, and $w_{i-1}^+=w_{i-1}^-$, the hopping rates are given by

$$w_i^\pm=\sum_{\substack{n=0\\ n:\text{even}}}^{\infty}C_n(x)a^n,$$
$$w_{i\pm1}^\pm=\sum_{\substack{k,n=0\\ n:\text{even}}}^{\infty}\frac{\partial^k C_n(x)}{\partial x^k}\frac{a^{k+n}}{k!}(\pm1)^k. \tag{12}$$

In this case, we finally obtain the following continuum equation

$$\frac{\partial h(x,t)}{\partial t}=\frac{2a}{\tau}\sum_{\substack{n=4\\ n:\text{even}}}^{\infty}\sum_{\substack{k=2\\ k:\text{even}}}^{n-2}\frac{\partial^k C_{n-k}(x)}{\partial x^k}\frac{a^n}{k!}+\eta_c(x,t), \tag{13}$$

with the same noise covariance as Eq. (11). This continuum equation has $\nabla^4 h$ and $\nabla^2(\boldsymbol{\nabla}h)^2$ terms as the lowest order. The well-known Laplacian term $\nabla^2 h$ and the nonlinearity $\boldsymbol{\nabla}(\boldsymbol{\nabla}h)^3$, associated with the Edwards-Wilkinson (EW) universality class, is essentially absent. The model with a symmetric hopping rate thus is described by the fourth order continuum equation with a conservative noise.

We prove analytically that the corresponding continuum equation to the volume conserving surface models can be generally described by either Eq. (10) or Eq. (13), depending on the symmetry of hopping rate in the diffusion rules of the model. The model introduced by Rácz *et al.* [13] satisfies Eq. (10), while the Sun-Guo-Grant model obeys Eq. (13) without the nonlinearity $\nabla^2(\boldsymbol{\nabla} h)^2$ because this model obeys detailed balance and the symmetry $h(x,t)\rightarrow -h(x,t)$. The explicit expression of both equations will be determined through the regularization procedure when the diffusion rules for a model are given.

III. VOLUME CONSERVING MODELS

To identify the result of the preceding section, we investigate a simple discrete model suggested by Krug [14]. The diffusion rule is as follows: A site i is chosen at random. If the surface configuration satisfies the condition

$$h_{i+1}>h_i \quad \text{or} \quad h_{i-1}>h_i, \tag{14}$$

then the particle at site i is regarded as immobile, and a new site is chosen. If it does not, the particle at site i is regarded as a mobile one, no matter what the neighboring configuration is. In this model, any mobile particles are allowed to hop from an existing site to another site. Especially, a particle in a completely flat surface is always regarded as a mobile particle in order to generate a nonequilibrium contribution to the surface diffusion process where no particles are deposited.

As a discrete model for *the symmetric hopping rate*, we allow any mobile particle to hop to one of the nearest neighbors randomly. The hopping rates $w_i^{\pm}$ for this model can be represented by a simple combination of the unit step function $\theta(x)$ as follows:

$$w_i^{\pm}=\frac{1}{2}\,\theta(h_i-h_{i-1})\,\theta(h_i-h_{i+1}). \tag{15}$$

Once hopping rates $w_i^{\pm}$ are written by the step function, the discrete function h_i has to be replaced by a smooth function $h(x,t)$ with $x=ia$ at the macroscopic scale through a regularization procedure. Using the regularization procedure from the literature [2,3,5,6], the step function can be approximated by an analytic shifted hyperbolic tangent function, which is expanded in the Taylor series

$$\theta(x)=1+\sum_{k=1}^{\infty} A_k x^k, \tag{16}$$

where $A_1>0$, $A_3<0,\ldots,$ and $A_2, A_4,\ldots$ are very small and negligible.

Combining Eqs. (5), (15), and (16), we obtain the following continuum equation, up to the fourth order:

$$\frac{\partial h(x,t)}{\partial t}=-K\nabla^4 h+\lambda_{22}\nabla^2(\boldsymbol{\nabla} h)^2+\eta_c(x,t), \tag{17}$$

where the coefficients and the noise covariance are given by

$$K=\frac{a^5}{2\tau}A_1,$$

$$\lambda_{22}=\frac{a^5}{2\tau}(2A_2-A_1^2), \tag{18}$$

$$\langle \eta_c(x,t)\,\eta_c(x',t')\rangle=-\frac{a^5}{\tau}\nabla^2\delta(x-x')\,\delta(t-t'),$$

up to $O(a^5)$. From the fact that $A_1>0$ and A_2 is very small and negligible, we have $K>0$ and $\lambda_{22}<0$. This equation corresponds to the conserved Kardar-Parisi-Zhang equation with a conservative noise [12]. The predicted critical exponents are $\alpha=(2-d)/3$ and $z=(10+d)/3$ for the substrate dimension d [16]. The critical exponents are determined through the surface width $W(L,t)$, which can be described by the dynamic scaling form, $W(L,t)=L^{\alpha}F(t/L^z)$. Here L, α, z, and F are the system size, the roughness exponent, the dynamic exponent ($z=\alpha/\beta, \beta$ is the growth exponent), and the scaling function, respectively. Simulation results for this discrete model are consistent with the predicted values of exponents. See Ref. [14] for $d=1$ and Ref. [15] for $d=2$ and 3.

As a discrete model for *the asymmetric hopping rate*, we allow a mobile particle to hop only to one of the nearest neighboring sites which has a lower height. In this way, we can break the symmetry in hopping rate. If both heights of the nearest neighbors are lower than that of the selected site, one site is selected randomly among them. From these rules, the hopping rates $w_i^{\pm}$ are given by

$$w_i^{\pm}=\theta(h_i-h_{i\mp1})\,\theta(h_i-h_{i\pm1}) +[1-\theta(h_{i\pm1}-h_{i\mp1})+\tfrac{1}{2}\,\delta(h_{i\pm1}-h_{i\mp1})]. \tag{19}$$

Since the above hopping rates $w_i^{\pm}$ contain a δ function, we will employ another regularization function [4]:

$$\theta(x)=\sum_{k=0}^{\infty} A_k x^k, \tag{20}$$

where $A_0\in(1/2,1)$, $A_1>0$, and $A_2<0$. This choice can distinguish the situations where the argument of the step function is zero.

From Eqs. (5), (19), and (20), we obtain the stochastic continuum equation, up to the fourth order, as follows:

$$\frac{\partial h(x,t)}{\partial t}=\nu\nabla^2 h-K\nabla^4 h+\lambda_{22}\nabla^2(\boldsymbol{\nabla} h)^2 +\lambda_{13}\boldsymbol{\nabla}(\boldsymbol{\nabla} h)^3+\eta_c(x,t), \tag{21}$$

with the same noise covariance as Eq. (18). The coefficients are given by

$$\nu=\frac{4a^3}{\tau}A_0^2A_1,$$

$$K=-\frac{a^5}{6\tau}(8A_0^2A_1-3A_0A_1), \tag{22}$$

$$\lambda_{22}=\frac{a^5}{2\tau}(2A_0A_2-A_1^2-4A_0A_1^2),$$

$$\lambda_{13}=\frac{2a^5}{\tau}(8A_0^2A_3+A_1A_2+4A_0A_1A_2-2A_1^3).$$

By using the conventional regularization function, Eq. (16), we can also obtain the same continuum equation with the coefficients if we let $A_0=1$ in Eq. (22). However, for the model with the asymmetric hopping rate which contains a δ function, the use of regularization function Eq. (20) is proper because the regularization function Eq. (16) does not allow us to define the δ function [4].

Since $A_0 \in (1/2,1)$, $A_1>0$, and $A_2<0$, we have $\nu>0$, $K<0$, $\lambda_{22}<0$, and $\lambda_{13}<0$ so that the dynamic scaling behavior is determined solely by the Laplacian term with a positive coefficient. The model for an asymmetric hopping rate belongs to the same universality class as that of the EW equation with a conservative noise. The critical exponents are given as $\alpha=-d/2$ and $\beta=-d/4$ [17]. Note that the values of the growth (β) and the roughness (α) exponents are negative in all substrate dimensions d, so that the surface is in fact flat. More information for the negative exponents can be found elsewhere [15,18].

IV. SUMMARY

We have studied the effect of symmetry on volume conserving surface models, where the total number of particles is conserved at every moment. We obtained the stochastic continuum equation through the master equation approach. We then showed that the form of continuum equation depends on the symmetry of hopping rate in the stochastic diffusion rules. In the discrete model with symmetric hopping rate, the resulting continuum equation does not possess a Laplacian term, but it is the nonlinear fourth order continuum equation with a conservative noise. If the symmetry in hopping rate is broken, a Laplacian term appears in the corresponding Langevin equation. In this case, if the coefficient of the Laplacian term is positive, the Laplacian term will be relevant so that the asymptotic scaling behavior of the model belongs to that of the EW equation with a conservative noise. As a specific example, we investigated a simple discrete model [14,15] analytically. From the diffusion rules of the model, we explicitly derived two corresponding continuum equations; the conserved Kardar-Parisi-Zhang equation with a conservative noise for the model with symmetric hopping rate, and the Edwards-Wilkinson equation with a conservative noise for the model with asymmetric hopping rate.

ACKNOWLEDGMENTS

This work was supported in part by the Ministry of Education (Grant No. 98-015-D00090), and by the Korea Science and Engineering Foundation (Grant No. 98-0702-05-01-3).

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