Exact derivation of the Kardar-Parisi-Zhang equation for the restricted solid-on-solid model

Kwangho Park and ByungNam Kahng
Department of Physics, Kon-Kuk University, Seoul 133-701, Korea
(Received 3 August 1994)

We derive the Kardar-Parisi-Zhang (KPZ) equation exactly for a discrete model, the restricted solid-on-solid (RSOS) model introduced by Kim and Kosterlitz [Phys. Rev. Lett. **62**, 2289 (1989)] by using the master-equation approach. It is confirmed that the RSOS model belongs to the KPZ universality class and the coefficient λ of the nonlinear term is negative for the RSOS model.

PACS number(s): 61.50.Cj, 05.40.+j

Recently, there have been many studies in the field of nonequilibrium surface growth. A number of discrete models and continuous equations for growth phenomena have been introduced and studied [1]. One of the most interesting features in the nonequilibrium surface growth is the nontrivial scaling behavior of the dynamical interface width, i.e.,

$$W(L,t)=\left\langle \frac{1}{L^{d'}}\sum_i (h_i-\bar{h})^2\right\rangle \sim L^{\alpha} f(t/L^z) , \qquad (1)$$

where h_i is the height of site i of the substrate. $\bar{h}$, L, and d' denote the mean height, system size, and the dimension of the substrate, respectively. The symbol $\langle\ \rangle$ stands for the statistical average. The scaling function, $f(x)\rightarrow$const for $x\gg 1$, and $f(x)\sim x^{\beta}$ for $x \ll 1$ with $\beta=\alpha/z$. The exponents α, β, and z are called the roughness, the growth, and the dynamical exponents, respectively.

The simplest nonlinear equation describing a growing surface with lateral growth effect was introduced by Kardar, Parisi, and Zhang [2],

$$\frac{\partial h(x,t)}{\partial t}=\nu\nabla^2 h(x,t)+\frac{\lambda}{2}[\nabla h(x,t)]^2+\eta(x,t) , \qquad (2)$$

where $\eta(x,t)$ is the Gaussian white noise satisfying

$$\langle \eta(x,t)\eta(x',t')\rangle = 2D\delta^{d'}(x-x')\delta(t-t') . \qquad (3)$$

Associated with the KPZ equation, a lot of discrete models have been introduced; for example, the restricted solid-on-solid (RSOS) model [3], the Eden model [4], the ballistic deposition model [5], and the deposition-evaporation model [6]. Among these stochastic models, the RSOS model exhibits a surprisingly good scaling behavior even in a small system size, and it exhibits fast convergent behavior toward a steady state. The physical reason for this effect could originate from the fact that the restricted condition reduces the random growth process, which leads to surface diffusion and tends to smooth the surface. Since the numerical solution of the RSOS model in one dimension is consistent with the analytic result of the KPZ equation, and the scaling behavior of the numerical solution in higher dimensions behaves consistently with the result from the Flory type argument [7], it may be said that the RSOS model is a good stochastic model corresponding to the KPZ equation, but any direct derivation of the continuous equation from the RSOS model is absent, to our knowledge. In this Brief Report, we derive the KPZ equation from the RSOS model exactly by using the master-equation approach introduced by Vvendensky *et al.* [10]. Originally this method was introduced to derive the continuous equation for the Arrhenius hopping in the molecular beam epitaxial (MBE) growth. However, since the MBE surface contains deep valleys and steep cliffs, it is rather ambiguous to take a continuous limit in the height difference between the nearest-neighbor columns, even in the limit of a unit lattice constant $a\rightarrow 0$. But in the RSOS model, the height difference is at most as small as the unit lattice constant, so that the regularization from discrete to continuous variables as $a\rightarrow 0$ is much more manifest. On the other hand, the direct derivation of the continuous KPZ equation from a discrete model exists only for the deposition-evaporation model of Plischke, Rácz, and Liu [6], to our knowledge, and any other derivation is absent. Thus we think it worthwhile to consider the exact derivation of the KPZ equation from the RSOS model in this Brief Report.

The derivation process mainly consists of the two steps. First, we derive the discrete Langevin equation for the RSOS model by setting up a master equation and by using the Fokker-Planck formalism. Second, we change the discrete equation into the continuous one by taking the limit of the lattice constant $a\rightarrow 0$. We begin the first step by considering a birth and death type of master equation,

$$\frac{\partial P(H;t)}{\partial t}=\sum_{H'} W(H',H)P(H';t)-\sum_{H'} W(H',H)P(H;t) , \qquad (4)$$

where $H=\{h_i\}$ denotes the configuration of the heights and $P(H;t)$ is the probability distribution of having the configuration H at time t. $W(H',H)$ is the transitional probability from the state H to the state H'. Next, we define the transition moments of $W(H',H)$ as

$$K_i^{(1)}=\sum_{H'} (h_i'-h_i)W(H',H) ,$$

$$K_{i,j}^{(2)}=\sum_{H'} (h_i'-h_i)(h_j'-h_j)W(H',H) ,$$

$$\vdots$$

$$K_{i_1,i_2,\ldots,i_p}^{(p)}=\sum_{H'}\prod_{j=1}^{p} (h_{i_j}'-h_{i_j})W(H',H) . \qquad (5)$$

Then it is straightforward to show that the above master equation is turned into the form of the Kramers-Moyal partial differential equation [8] with the transition moments,

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial h_i}(K_i^{(1)}P)+\frac{1}{2}\frac{\partial^2}{\partial h_i\partial h_j}(K_{i,j}^{(2)}P)+\cdots+\frac{(-1)^p}{p!}\prod_{j=1}^{p}\frac{\partial}{\partial h_{i_j}}(K_{i_1,i_2,\ldots,i_p}^{(p)}P)+\cdots . \quad (6)$$

All the terms after $p>2$ may be neglected in Eq. (6) due to higher order. Then Eq. (6) reduces to the following Fokker-Planck equation:

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial h_i}(K_i^{(1)}P)+\frac{1}{2}\frac{\partial^2}{\partial h_i\partial h_j}(K_{i,j}^{(2)}P) . \quad (7)$$

If the system size is large enough and intrinsic fluctuations in the system are not too big, then it is known that the Langevin equation becomes equivalent to the Fokker-Planck equation [9]

$$\frac{\partial h_i}{\partial t}=K_i^{(1)}+\eta_i , \quad (8)$$

where η_i is the Gaussian white noise such that

$$\langle \eta_i \rangle = 0 , \quad (9)$$

and

$$\langle \eta_i(t)\eta_j(t') \rangle = K_{ij}^{(2)}\delta(t-t') . \quad (10)$$

In order to obtain the discrete Langevin equation for the RSOS model, one has to find out the transition probability $W(H',H)$ explicitly. We follow the method used by Vvedensky *et al.* [10], which was used to derive the continuous equation for the Arrhenius hopping. Note that the RSOS model does not allow overhangs or any vacancies, so that the height h_i of the site i is defined uniquely, and the configuration $H=\{h_i\}$ is also uniquely determined. Since the quantity $W(H',H)$ represents the transition probability from a particular initial surface configuration H to the next surface configuration H', it is related to the deposition process of the RSOS model. The deposition rule of the RSOS model is that a site is selected randomly among substrate sites and the height of the selected site increases by 1, provided that the height difference between the nearest-neighbor columns is less than 1. Thus the diffusion process does not occur, which makes it easier to set up the transition probability explicitly. Also it is important to note that the height difference remains as small as a unit lattice constant through the entire process of growing.

The transition probability for the RSOS model does not vanish only when a height increases by a unit lattice constant a and the others remain unchanged, provided that the restricted condition is held. Then, the transition probability is written as

$$W(H,H')=\frac{1}{\tau}\sum_i\left[\Theta(h_{i+1}-h_i)\Theta(h_{i-1}-h_i)\times\delta(h_i',h_i+a)\prod_{i\neq j}\delta(h_j',h_j)\right] , \quad (11)$$

where τ is the deposition time for a layer. $\Theta(x)$ is the unit step function defined by

$$\Theta(x)=\begin{cases}1 & \text{if } x\geq 0 ,\\ 0 & \text{if } x<0 .\end{cases} \quad (12)$$

Note that, by definition, the case of $x=0$ is included in the case of $x>0$ as an analytic continuation for the range of $x\geq 0$. Then the first and second moments of W for the RSOS model become

$$K_i^{(1)}=\frac{a}{\tau}\Theta(h_{i+1}-h_i)\Theta(h_{i-1}-h_i) , \quad (13)$$

$$K_{i,j}^{(2)}=\frac{a^2}{\tau}\Theta(h_{i+1}-h_i)\Theta(h_{i-1}-h_i)\delta_{ij} . \quad (14)$$

Using these two moments, one can set up the discrete Langevin equation for the RSOS model as proposed in Eq. (8).

Next, we undertake the regularization to obtain the continuous equation from the discrete Langevin equation. In general, a unit step function may be regarded as the limit of $u(\Delta h)\equiv\lim_{n\to\infty}\frac{1}{2}(1+\tanh n\Delta h)$. Since the function of $\tanh x$ is analytic, $u(x)$ can be regarded as an analytic function at least for the range of $x>0$. But since the value of the step function at $x=0$ was defined as the value of the analytic continuation, it must be true that the step function is analytic even at $x=0$. Thus the step function defined in Eq. (12) is analytic for $x\geq 0$.

In our consideration, since the argument of the step function is equal to the height difference between the nearest-neighbor columns, the argument is not greater than the unit lattice constant a. Then one may expand the unit step function in a Taylor series in the limit of $a\to 0$ as

$$\Theta(\Delta h)\approx\left[1+\sum_{k=1}^{\infty}A_k(\Delta h)^k\right] . \quad (15)$$

This regularization is much more reasonable in the RSOS model than in the MBE growth done by Vvendensky [10] because the surface of the MBE growth contains deep valleys and steep cliffs, which yields the height difference between the nearest-neighbor columns larger than 1. However, the height difference in the RSOS model remains at most as small as the unit lattice constant. So the regularization process is much more convincing in the RSOS growth.

The first moment is obtained as

$$K_i^{(1)}\simeq\frac{a}{\tau}[1+A_1(h_{i-1}-h_i)+A_2(h_{i-1}-h_i)^2+\cdots]\times[1+A_1(h_{i+1}-h_i)+A_2(h_{i+1}-h_i)^2+\cdots] . \quad (16)$$

$h_i(t)$ is replaced by a smooth function $h(x,t)$ with $x=ia$, and we expand $(h_{i\pm1}-h_i)$ in powers of a, so that

$$h_{i\pm1}(t)-h_i(t)=\sum_{k=1}^{\infty}\frac{(\pm a)^k}{k!}\frac{\partial^k h(x,t)}{\partial x^k}\bigg|_{x=ia} . \quad (17)$$

Then the first moment is obtained, up to $O(a^3)$, as

$$K_i^{(1)}(x)=\frac{a}{\tau}\left[1+A_1a^2\frac{\partial^2 h}{\partial x^2}+(2A_2-A_1^2)a^2\left[\frac{\partial h}{\partial x}\right]^2\right]+O(a^4)\ . \tag{18}$$

Similarly, the second moment is obtained, up to $O(a^3)$, as

$$K_{ij}^{(2)}=\frac{a^2}{\tau}\delta(x-x')+O(a^4)\ . \tag{19}$$

Thus the resulting continuous equation for the RSOS model is, from Eq. (8),

$$\frac{\partial h(x,t)}{\partial t}=\nu\nabla^2 h(x,t)+\frac{\lambda}{2}[\nabla h(x,t)]^2+F+\eta(x,t)\ , \tag{20}$$

where the coefficients are given by

$$\nu=\frac{A_1}{\tau}a^3\ ,$$
$$\lambda=2(2A_2-A_1^2)a^3\ , \tag{21}$$
$$F=\frac{a}{\tau}\ ,$$

and also the noise is given by

$$\langle\eta(x,t)\eta(x',t')\rangle=\frac{a^2}{\tau}\delta(x-x')\delta(t-t')\ , \tag{22}$$

which is equivalent to the KPZ equation. Since $\tanh x\sim x-x^3/3+\cdots$, $A_1>0$, and $A_2=0$ when the unit step function is regarded as the limit of the hyperbolic tangential function. Then the coefficient $\lambda<0$ in the RSOS model, which confirms the result from the tilt argument. Even though we have derived the KPZ equation in one dimension, it is straightforward to extend it into higher dimensions. Thus we conclude that the RSOS model is equivalent to the KPZ equation in the continuous limit and in the general dimension.

In summary, we have exactly derived the continuous KPZ equation from a stochastic model, the restricted solid-on-solid model, by constructing the master equation, and by changing it into the Langevin equation via the Fokker-Planck formalism. The regularization process from the discrete quantities to the continuous ones has been clearly explained in the RSOS model, which is due to the restriction of the height difference between the nearest-neighbor columns.

This work is supported in part by the KOSEF under Contract No. 941-0200-006-2 and through the SRC program of SNU-CTP, and in part by the BSRI program of the Ministry of Education, Korea.

[1] For a recent review, see, for example, F. Family and T. Vicsek, *Dynamics of Fractal Surfaces* (World Scientific, Singapore, 1991).
[2] M. Kardar, G. Parisi, and Y. Zhang, Phys. Rev. Lett. **56**, 889 (1986).
[3] J. M. Kim and J. M. Kosterlitz, Phys. Rev. Lett. **62**, 2289 (1989).
[4] M. Eden, in *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume IV: Biology and Problems of Health,* edited by J. Neyman (University of California Press, Berkeley, 1961), pp. 223–239.
[5] F. Family and T. Vicsek, J. Phys. A **18**, L75 (1985); P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, Phys. Rev. A **34**, 5091 (1986).
[6] M. Plischke, Z. Rácz, and D. Liu, Phys. Rev. B **35**, 3485 (1987).
[7] H. G. Hentschel and F. Family, Phys. Rev. Lett. **66**, 1982 (1991).
[8] H. A. Kramers, Physica **7**, 284 (1940); J. E. Moyal, J. R. Stat. Soc. B **11**, 150 (1949); R. F. Fox, Phys. Rep. **48**, 179 (1978), Sec. I.5.
[9] R. F. Fox and J. Keizer, Phys. Rev. A **43**, 1709 (1991).
[10] D. D. Vvedensky, A. Zangwill, C. N. Luse, and M. R. Wilby, Phys. Rev. E **48**, 852 (1993).