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Nonlinear conserved current model with negative diffusion

Jin Min Kim*

Department of Physics and Interdisciplinary Research Center in Physical Science, Hallym University, Chunchon, Kangwondo, 200-702, Korea

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A discrete growth model following a nonlinear equation $\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda \nabla (\nabla h)^3 + \eta$, where ν_2 is negative and η is the random noise of the deposition, has been introduced. For negative ν_2, the standard deviation of the surface height increases as $t^{1/4}$ in $d = 1 + 1$ being consistent with the Edwards and Wilkinson universality class. The λ nonlinearity balances negative ν_2 such that the effective ν_2 becomes positive. Time dependent surface current measurement on a tilted substrate shows how ν_2 is renormalized. A possible mechanism for the nonlinear equation in real molecular beam epitaxial growth is also discussed.

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Recently, there have been considerable efforts in the study of rough surfaces of various growth models [1]. Among them, the class of models known as "conserved" models, which conserve the total numbers of particles after being deposited, has been extensively studied as a possible description of real molecular beam epitaxy (MBE) growth [2]. There are some attempts [3, 4] to classify the conserved growth models, with each universality class corresponding to a particular continuum growth equation for the coarse grained height variable $h(x, t)$ which describes the growing interface as a function of the lateral surface coordinate x and time t. In real MBE growth, a particle does not easily step down at a step edge due to the Schwoebel effect [5], which behaves like a negative surface diffusion. In this paper, we present a simple discrete growth model following a continuum equation that has both negative diffusion and a cubic nonlinearity to mimic a realistic MBE growth surface. Since the surface structure of many growth processes is self-affine, most efforts have concentrated on measuring the surface fluctuations. The surface width W is defined as the standard deviation or the root mean square fluctuation of the surface height. In a finite system of lateral size L, the width W starting from a flat substrate scales as [6]

$$\begin{aligned} W(t) &\sim L^\alpha f(t/L^z) \\ &\sim t^\beta, \quad t \ll L^z, \\ &\sim L^\alpha, \quad t \gg L^z, \end{aligned} \tag{1}$$

where the scaling function $f(x)$ is x^β for $x \ll 1$ and is constant for $x \gg 1$. The exponents β and z are connected by the relation $z\beta = \alpha$.

The conserved current model without overhangs and vacancies in growth is described by a continuum equation for the surface current $\mathbf{j}$:

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = -\nabla \cdot \mathbf{j}(\mathbf{x}, t) + \eta(\mathbf{x}, t) \tag{2}$$

where $h(\mathbf{x}, t)$ is the height of the film and $\eta(\mathbf{x}, t)$ is a *nonconserved*, uncorrelated random noise

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

Here we consider a cubic nonlinear current $\mathbf{j}$

$$\mathbf{j}(\mathbf{x}, t) = -\nu_2 \nabla h + \nu_4 \nabla^3 h - \lambda (\nabla h)^3. \tag{4}$$

A possible candidate for the λ term is a knockout process [7] which can suppress the Schwoebel effect. Then the conserved continuum equation becomes [4]

*Electronic address: JMKIM@sun.hallym.ac.kr

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda \nabla (\nabla h)^3 + \eta(\mathbf{x},t). \quad (5)$$

For $\nu_2 > 0$, it belongs to the Edwards and Wilkinson (EW) universality class [8] with $\alpha = (3-d)/2$ and $z = 2$ for substrate dimension $d-1$.

When $\nu_2 = 0$, one of the simplest conserved equation is the Mullins-Herring curvature driven linear equation, which is obtained by putting both ν_2 and λ as zero in Eq. (5): $\frac{\partial h(\mathbf{x},t)}{\partial t} = -\nu_4 \nabla^4 h(\mathbf{x},t) + \eta(\mathbf{x},t)$. This equation can be solved exactly giving $\alpha = (5-d)/2$ and $z = 4$, i.e., $\beta = (5-d)/8$. Since the Mullins equation allows very high steps [9, 10, 3], one expects some nonlinear effects in real MBE growth [4, 11]. Among them, the λ term is the most relevant fourth order term. For $\lambda > 0$, the equation becomes $\frac{\partial h(\mathbf{x},t)}{\partial t} = -\nu_4 \nabla^4 h + \lambda \nabla (\nabla h)^3 + \eta(\mathbf{x},t)$. The exponent values $\beta = 3/10$ and $\alpha = 3/4$ in $d = 1+1$ [in general dimensions $\beta = (5-d)/2(3+d)$ and $\alpha = (5-d)/4$ [4]] were suggested by both the scaling argument and the dimensional analysis. However, direct numerical integration of the equation shows that the λ term generates a positive effective ν_2 and the equation belongs [12] to the Edwards and Wilkinson universality class. This is also supported by a recent renormalization group analysis [13, 14].

Consider a negative ν_2 case which mimics Schwoebel barriers [5] reflecting an atom at a descending step. Is there any negative ν_2^* which exactly cancels the contribution from the λ term so that the effective ν_2 becomes zero? To answer the question, we present a simple discrete growth model following the continuum Eq. (5), especially for $\nu_2 \leq 0$ in $d = 1+1$. When $\nu_2 = 0$, our model shows EW behaviors supporting the above results that the $\lambda \nabla (\nabla h)^3$ term behaves like a surface tension $\nabla^2 h$ term [12–14]. For negative ν_2, we find that the model also belongs to the EW class. The λ nonlinearity suppresses any negative ν_2 so that the effective ν_2 becomes positive. Hence we claim that the equation with positive λ belongs to the EW universality class even for negative ν_2.

We introduce a simple discrete growth model following Eq. (5). The general growth rule of our model is to randomly select a site i on a $d-1$ dimensional substrate, and calculate local currents $\hat{\jmath}$ for both positive direction and negative direction following the continuum equation. As an example for $\nu_4 = \lambda = 0$, the local current is defined as $\hat{\jmath}(k,i) = \nu_2[h(k) - h(i)]$ in d=1+1 where k is either $i+1$ or $i-1$ and we add a particle on site k where $\hat{\jmath}(k,i)$ is negative. If both $\hat{\jmath}(i+1,i)$ and $\hat{\jmath}(i-1,i)$ are positive, a particle is added on site i. In case both $\hat{\jmath}(i+1,i)$ and $\hat{\jmath}(i-1,i)$ are negative, we add a particle on either site randomly. In general we calculate the local current $\hat{\jmath}$ by

$$\begin{aligned}\hat{\jmath}(k,i) = \nu_2[h(k) - h(i)] - \nu_4[h(k+1) + h(k-1) \\ -2h(k) - h(i+1) - h(i-1) + 2h(i)] \\ +\lambda[h(k) - h(i)]^3. \quad (6)\end{aligned}$$

When $\nu_2 > 0$ and $\nu_4 = \lambda = 0$, the growth rule is the same as that of Family's model [15]. A dropped particle is allowed to diffuse to the nearest neighbor site whose height is lower than that of the dropped site. If there are two lower sites, one is chosen randomly. If $\nu_2 < 0$ and $\nu_4 = \lambda = 0$, a dropped particle is diffused to the higher site resulting in unstable growth. Our model is a generalization of the model to the arbitrary surface currents given in Eq. (4). Since the local particle movement is approximately proportional to the surface current, the discrete model follows the continuum equation very well. The advantage of our model is that it can generate the λ nonlinear term [16]. Also the model is flexible enough to be adjustable for continuous values of the various coefficients ν_2, ν_4, and λ in the continuum equation, allowing one to study crossover behaviors.

Our simulations are performed from a flat substrate with periodic boundary conditions in $d-1$ substrate dimensions. The time t corresponds to the number of Monte Carlo steps. We first test our model for $\nu_2 = \lambda = 0$ and obtain the known result $\beta = 3/8$ in $d = 1+1$ very accurately. As usual, the surface width $W^2(t) =$

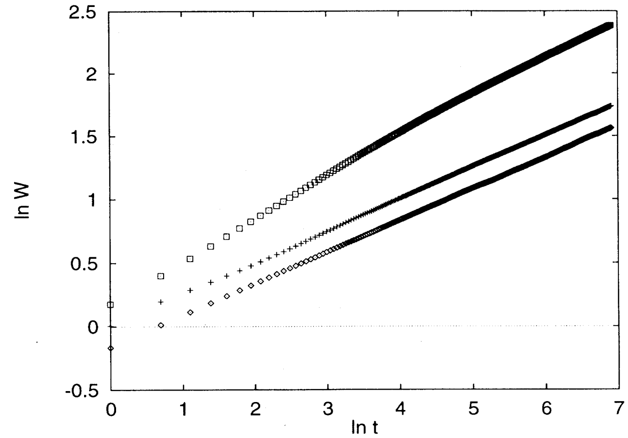

FIG. 1. Surface width W as a function of time in log-log plot for various values of ν_2 and ν_4 with $\lambda = 1$. The data are, at the top, $\nu_2 = -1$ and $\nu_4 = 0.5$ where 0.5 is added to ln W to avoid overcrowding; $\nu_2 = -3$ and $\nu_4 = 0$ (middle); and the bottom data are for $\nu_2 = -1$ and $\nu_4 = 0$ ($\beta \approx 0.25$).

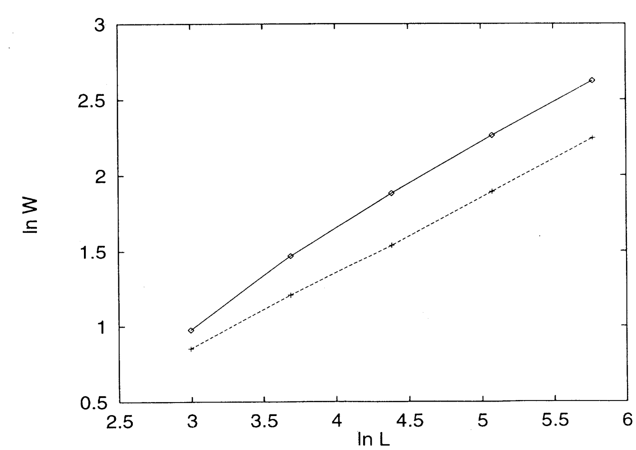

FIG. 2. Saturation surface width W as a function of L in log-log plot for $\nu_2 = -3$, $\nu_4 = 0$, and $\lambda = 1$ (bottom) and $\nu_2 = -1$, $\nu_4 = 1$, and $\lambda = 1$ (top).

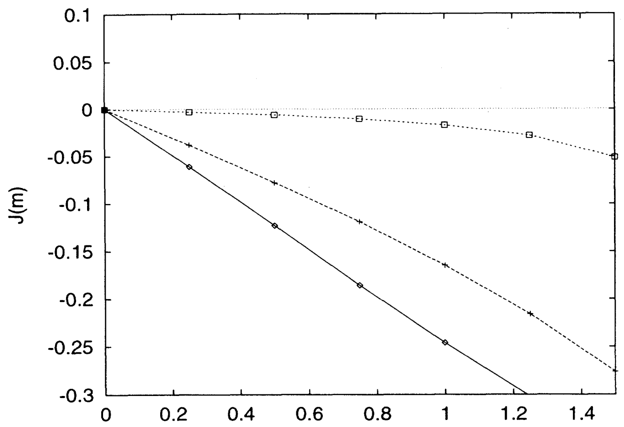

FIG. 3. Surface current $J(m)$ in the saturated regime as a function of slope m for various values of ν_2 and ν_4 with $\lambda = 1$. The data are for $\nu_2 = -3$, $\nu_4 = 1$, and $\lambda = 1$ (top); $\nu_2 = -3$, $\nu_4 = 0$, and $\lambda = 1$ (middle); $\nu_2 = 0$, $\nu_4 = 1$, and $\lambda = 1$ (bottom).

$\langle [h(x,t) - \langle h(x,t)\rangle]^2\rangle$ increases as $t^{2\beta}$ for early times and eventually saturates when the parallel correlation $t^{1/z}$ is of the order of the lateral system size L. To determine the growth exponent β, we measure $W(t)$ as a function of time for a system size $L = 100\,000$, averaging over 30 independent runs with $\lambda = 1$ ($d = 1+1$). Figure 1 shows three different cases for negative ν_2: $\nu_2 = -1$, $\nu_4 = 0$, and $\lambda = 1$; $\nu_2 = -3$, $\nu_4 = 0$, and $\lambda = 1$; $\nu_2 = -1$, $\nu_4 = 0.5$, and $\lambda = 1$. Through the relation $W(t) \sim t^\beta$ for early times $t \ll L^z$, we obtain

$$\beta = 0.25 \pm 0.01, \quad d = 1+1 \tag{7}$$

for the three cases. Even for $\nu_2 = -3$, β remains 1/4. When $\nu_4 = 0.5$, $\beta > 0.25$ at the beginning, and then it approaches 1/4 with time. Nonzero ν_4 only increases the initial transient regime.

To measure the roughness exponent α describing the saturation of the interface fluctuation, we use the relation $W(L) \sim L^\alpha$ for system size L in the steady state regime $t \gg L^z$. We have used system sizes $L = 20, 40, 80, 160$, and 320 in $d = 1+1$. From the log-log plot of $W(L)$ and size L, we get

$$\alpha = 0.50 \pm 0.02, \quad d = 1+1 \tag{8}$$

for $\nu_2 = -3$, $\nu_4 = 0$, and $\lambda = 1$ as shown in Fig. 2. In the case $\nu_2 = -1$, $\nu_4 = 1$, and $\lambda = 1$, α approaches 1/2 with L slowly. This is due to the nonzero ν_4 which produces a finite correlation of the slope ∇h. Through the relation $z = \alpha/\beta$, we get $z \approx 2$. Our numerical results are in good agreement with $\beta = 1/4$ and $\alpha = 1/2$ implying that the equation belongs to the EW universality class.

Recently Krug, Plischke, and Siegert [17] have suggested a method to determine the surface diffusion coefficient in various growth models by measuring the surface current $J(m)$ as a function of m, which is the slope of the tilted surface. The surface current is measured by counting the number of diffusion jumps in between the uphill direction and the downhill direction. If the net current is in the uphill direction, $J(m)$ is positive. By expanding J as a function of m, the effective ν_2 can be given as $\nu_2^{eff}(t) = -\frac{\partial J}{\partial m}(m=0,t)$. We calculate the surface current $J(m,t)$ as a function of both time and surface slope m in the simulation of deposition onto tilted substrates. As shown in Fig. 3, ν_2^{eff} is positive in the saturated regime for $\nu_2 = 0$, $\nu_4 = 1$, and $\lambda = 1$, supporting the recent numerical and analytical results [12, 13]. Even for $\nu_2 = -3$, the effective ν_2 remains positive, being consistent with the EW model. Nonzero ν_4 does not change the sign of ν_2^{eff} but only reduces the magnitude of it. Figure 4 shows the time dependent surface current $J(m,t)$ for $m = 1$, $\nu_2 = -3$, $\nu_4 = 1$, and $\lambda = 1$. The surface current J is positive at the beginning due to negative ν_2 and slowly becomes negative as $\langle(\nabla h)^2\rangle$ increases. In the saturated regime ($t \to \infty$), the current remains negative and constant. This time dependent surface current shows explicitly how ν_2 is renormalized with time (in other words with the correlation length scale). For small m, we expect

$$\nu_2^{eff}(t) = -J'(m=0,t) \approx \nu_2 + 3\lambda\langle(\nabla h)^2\rangle(t) \tag{9}$$

where the $\langle(\nabla h)^2\rangle$ term is obtained by linearizing Eq. (5) around a tilt slope m. For negative ν_2, $\langle(\nabla h)^2\rangle$ grows with time and then saturates producing a positive effective ν_2.

Consider a Hamiltonian

$$H \sim \int d^{d-1}x \;\; \frac{\nu_2}{2}(\nabla h)^2 + \frac{\nu_4}{2}(\nabla^2 h)^2 + \frac{\lambda}{4}(\nabla h)^4 - \mu h \tag{10}$$

which produces the continuum Eq. (5) up to a constant μ difference via the dynamical Langevin equation approach. The first and third terms on the right hand side restrict the height difference $|\nabla h|$ and the second term controls curvatures. For $\nu_2 = 0$, the fourth order term $\frac{\lambda}{4}(\nabla h)^4$ generates a square term $(\nabla h)^2$ in the effective Hamiltonian in a simple contraction sense [12–14]. If ν_2 is negative and ν_4 is zero, the λ term keeps $\langle(\nabla h)^2\rangle$ finite with the order of $-\nu_2/\lambda$, generating positive ν_2^{eff}

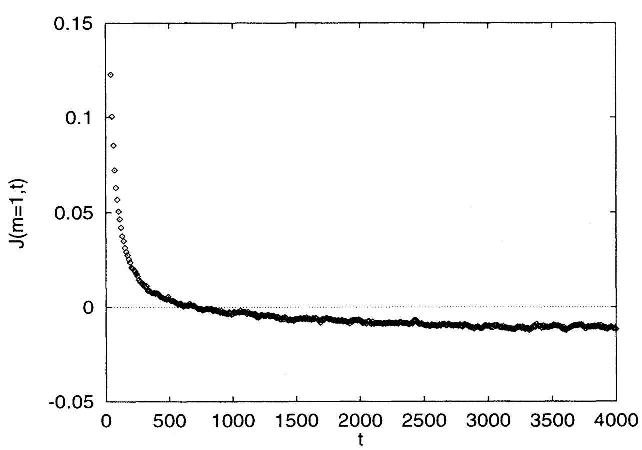

FIG. 4. Surface current $J(m,t)$ as a function of time for $m = 1$, $\nu_2 = -3$, $\nu_4 = 1$, and $\lambda = 1$.

from Eq. (9). So there is no negative ν_2^* which produces $\nu_2^{eff} = 0$. This mean field argument is consistent with the results of the surface current measurement that ν_2^{eff} is positive even for negative ν_2. Both the negative ν_2 term and the positive λ term can be derived from a Hamiltonian $H \sim \int \sqrt{1 - \gamma(\nabla h)^2}$ as the first two terms in a series expansion with the assumption that $\gamma(\nabla h)^2 \leq 1$. Whether γ is positive or negative, the growth model shows the EW universality class. When $\mu = 0$, the Hamiltonian has equilibrium thermodynamic behavior and satisfies detailed balance [18]. If we put $\phi = \nabla h$, the Hamiltonian becomes the standard ϕ^4 theory with a stable double well potential [19]. Some discrete models without incoming particles are well studied in connection with the detailed balance [18]. Imposing the detailed balance is a sufficient condition to reach an equilibrium state. The $-\mu h$ term in the Hamiltonian causes the average surface height to grow with time. It violates the detailed balance due to nonequilibrium dynamics. Since our discrete growth model does not satisfy detailed balance, the model can be described by the Hamiltonian of Eq. (10) with nonzero μ. Also the diffusion of the deposited particles follows [3] the surface current of Eq. (5), which is shown explicitly by the tilt dependent current measurement.

In conclusion, the nonlinear λ term suppresses the Schwoebel effect and leads to downhill current, resulting in positive effective ν_2. With a Schwoebel barrier, if a real MBE growth surface has a finite $\langle(\nabla h)^2\rangle$ value, then there should be a certain term like $\lambda\nabla(\nabla h)^3$ in the continuum equation. By measuring a surface current, we can show how ν_2 is renormalized with time due to the time dependent $\langle(\nabla h)^2\rangle$. In the presence of positive λ, ν_2 becomes irrelevant. It is surprising that the higher order term is more relevant than the lower order term. This is similar to the fact that the Kardar-Parisi-Zhang nonlinearity [20] can overcome negative ν_2 [21]. Our discrete growth model can be generalized to other continuum equations by modifying the growth rule following the local current.

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