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Conserved Noise Restricted Curvature Model

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Abstract A restricted curvature model with conservation of total number of particles is introduced. The surface width W of the model grows as t^{β} at the beginning with $\beta \approx 0.25$ and becomes saturated at L^{α} for $t \gg L^{z}$ with $\alpha \approx 1.5$, where L is the system size. The conservation law leads to a new universality class following sixth-order linear equation with conservative noise. The relation between our model and the equation is discussed.

Keywords Restricted curvature model · Mullins Herring equation · Scaling law · Restricted solid-on-solid model · Surface roughness · Volume conservation · Sixth-order linear equation · Conservative noise

1 Introduction

Recently, there have been a number of studies on the surface of the growth phenomena [1–5]. Considerable theoretical effort has been focused on the study of roughening surfaces for various growth equations and many growth models which describe different growth phenomena [1–20]. Some universality classes have been identified for growth models with each universality class corresponding to a particular continuum equation.

For most surface models with stochastic dynamics such as growth, evaporation or diffusion, it is known that the surface configurations show scaling behavior. An interesting quantity of the dynamic process is the kinetically rough self-affine surface structure. The interface width, which characterizes the roughness of the interface, is defined as the standard variation of the height:

$$W^2(L,t) \equiv \left\langle \frac{1}{L} \sum_{x=1}^{L} [h(x,t) - \bar{h}(t)]^2 \right\rangle, \tag{1}$$

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where L is the system size. The mean height $\bar{h}$ of the surface is defined as $\bar{h}(t) = \frac{1}{L}\sum_{x=1}^{L} h(x,t)$, and $\langle A \rangle$ is the sample average of A. The scaling hypothesis is that in a finite system of lateral size L, starting from a flat substrate, the mean square fluctuation W^2 of the surface height scales as [10]

$$W^2(L,t) \sim \begin{cases} L^{2\alpha} g(t/L^z), & \\ t^{2\beta} & (t \ll L^z), \\ L^{2\alpha} & (t \gg L^z), \end{cases} \tag{2}$$

where α and β are the roughness and growth exponents respectively. The dynamic exponent z has a relation $z = \alpha/\beta$ [1–3].

The growth processes are mostly constituted with deposition and evaporation of particles, and surface diffusion of adatoms. The stochastic nature of deposition flux generates a nonconservative noise, where the total volume is not conserved. Among them, there is a simple restricted curvature (RC) model, which has a restriction on the local curvature [11]. Here, we explain RC model briefly for completeness [11]. The growth rule of the equilibrium RC model is to randomly select a site on one dimensional substrate and then take a random action between deposition or evaporation (within the solid on solid condition) with equal probability, provided the restriction on the local curvature $|\nabla^2 h| \leq N$ is obeyed at both the selected site and the nearest-neighbor sites, where N is a preassigned fixed positive integer. If this RC condition is not satisfied, the corresponding deposition or evaporation event is forbidden. No relaxation or hopping of the deposited atom is allowed in the model. Thus, the model is analogous to the restricted solid on solid model [12, 13], except that the restriction is on the local curvature $\nabla^2 h$ rather than on the height difference. It is known that the equilibrium RC model can be described by the fourth-order linear equation given by [11]

$$\frac{\partial h(x,t)}{\partial t} = \nu \nabla^4 h(x,t) + \eta(x,t), \tag{3}$$

where $\eta(x,t)$ is an uncorrelated Gaussian noise. This equation can be solved exactly giving $\alpha = (5-d)/2$, $z = 4$ and $\beta = (5-d)/8$, where d is the total dimensions [14–16].

The activation of adatoms through the surface diffusion also creates some randomness, and the surface diffusion itself generates a conservative noise, leading to the smoothening surface. It would be interesting to consider a discrete model describing a conserved surface dynamics. One can imagine surface atoms diffusing due to thermal excitation where the total number of atoms is conserved. The diffusion of adatoms generates a conservative noise which leads to smoothening of the surface. Actually at a certain experimental configurations such as Pb island on Si(111) surface, the total mass of Pb atoms at stable heights is conserved for a quite long time where surface diffusion is allowed [8]. There have been a few trials to describe conserved surface fluctuation without deposition or evaporation of particles. Actually different exponents and universality classes are expected for the equation with a conservative noise [17–19]. In this work, we study the restricted curvature model with conserved noise. We explain the model and present our numerical simulation results in Sect. 2. We summarize our work in Sect. 3.

2 The Conserved Noise Restricted Curvature Model

Since the RC model is well described by the linear fourth-order equation [11], it is interesting to study the RC model with surface particle diffusion under the constraint of fixed

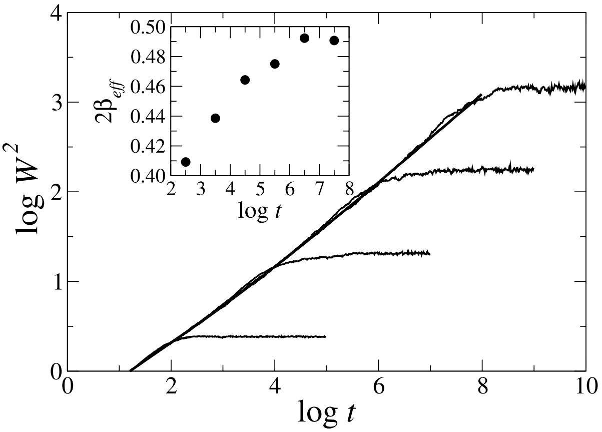


Fig. 1 Interface width $W^2(t)$ versus time in the Conserved Noise Restricted Curvature model for the systems of sizes $L = 8$, 16, 32, 64, and 2×10^4. Effective β is measured as a function of time for the largest system of $L = 2 \times 10^4$ in the *inset*

total number of particles. In this work, we introduce a conserved noise restricted curvature (CNRC) model, which has volume conservation in the RC model. The growth rule of the CNRC model is to randomly select a bond, which is between a nearest-neighbor pair sites x and $x+1$ on a substrate. One particle on the $x+1$ site is moved to the x site with probability 1/2 producing $h(x) \longrightarrow h(x)+1$ and $h(x+1) \longrightarrow h(x+1)-1$, or *vice versa* $h(x) \longrightarrow h(x)-1$ and $h(x+1) \longrightarrow h(x+1)+1$. During each attempt, the total number of particles are conserved automatically. If the restriction on the local curvature $|\nabla^2 h| = |h(x+1)+h(x-1)-2h(x)| \leq N$ on both the pair sites and the nearest neighbor sites is not satisfied, the corresponding local movement of the particle is forbidden, where N is a preassigned integer. There is no deposition or evaporation of particles except local diffusions of surface particles so that the sum of the heights $\sum_x h(x)$ is conserved. The CNRC model is analogous to the restricted curvature (RC) model, except that the total number of particles are conserved.

Our simulation is performed with $N = 3$ in $d = 2$, starting from a flat surface with periodic boundary condition in the substrate. To determine β, the exponent governing the rate of growth of the interface width, we measure $W(t)$ as a function of time for the system size $L = 2 \times 10^4$ as shown in Fig. 1. Through the relation $W(t) \sim t^\beta$ for early times $t \ll L^z$, we obtain

$$\beta = 0.246 \pm 0.005 \quad (d = 2). \tag{4}$$

Since the log-log plot of W^2 has an upward curvature, we calculate effective β, $\beta_{eff} = \frac{d \log w}{d \log t}$ as a function of time as shown in Fig. 1. The effective β increases with t and approaches 0.25. To determine the roughness exponent α describing the saturation of the interface fluctuation, we use the relation $W \sim L^\alpha$ for the system size L in the steady-state regime $t \gg L^z$ and we get

$$\alpha = 1.50 \pm 0.02 \quad (d = 2) \tag{5}$$

as shown in Fig. 2. From the relation $z = \alpha/\beta$, we obtain $z \approx 6.09$. Since the value of z is around 6, it takes a very long time to arrive at the saturated regime. This has forced us to restrict our simulation system size up to $L = 64$. Most of our simulation are performed with preassigned restriction parameter $N = 3$ and $N = 5$. The values of the exponents are found to be independent of N as long as N is larger than three. Note that they are very close to $\alpha = 3/2$, $\beta = 1/4$, and $z = 6$. As shown in Fig. 3, the scaled data collapse to a single curve

Fig. 2 Interface width $W^2(L)$ in the saturated regime versus system size with $N = 3$, for the systems of sizes $L = 8$, 16, 32, and 64

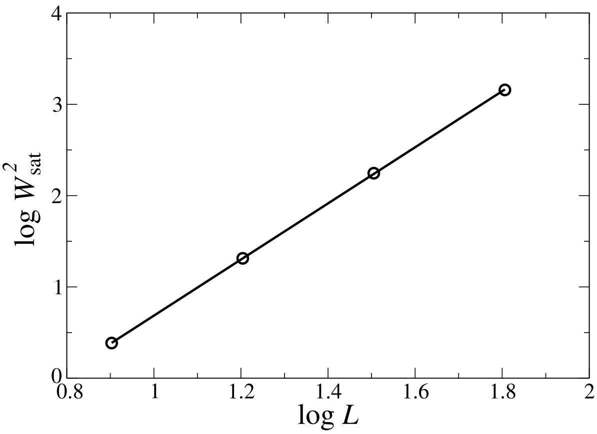
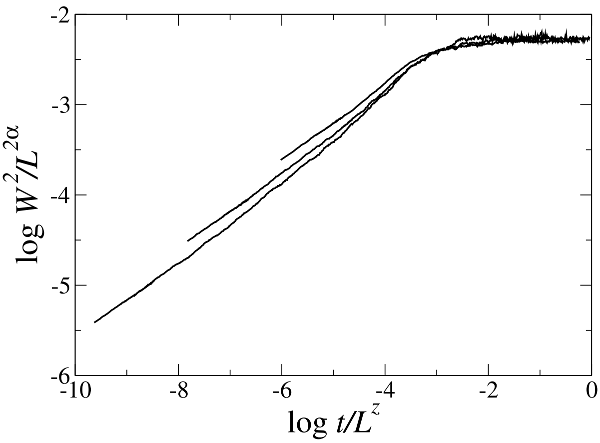


Fig. 3 The scaling plot of $W^2/L^{2\alpha}$ against t/L^z with $\alpha = 1.5$ and $z = 6$



with $\alpha = 1.5$ and $z = 6.0$. Since the β_{eff} increases with time, we could not get a perfect scaling plot in the early time regime. This is probably due to the corrections to the scaling from the small lattice size and early time t.

We also calculate the structure factor [2, 17]

$$S(L,k,t) = \langle h(k,t)h(-k,t)\rangle \tag{6}$$

for a system of lateral size L where $h(k,t)$ is the Fourier transform of the height $h(x,t)$. As expected, Fig. 4 shows that $S(L,k,t\to\infty)$ follows $1/k^\delta$ for small k with $\delta = 4.0 \pm 0.1$ in $d = 2$ being consistent with $\delta = 2\alpha + d - 1 = 4$ with $\alpha = 3/2$.

The CNRC model is analogous to the restricted curvature (RC) model, except that the noise is conserved. Since there is a restriction on the curvature, the continuum Hamiltonian for the CNRC model can be written as

$$H \sim \int d^{d-1}\mathrm{x}|\nabla^2 h|^2. \tag{7}$$

From the conservation law, the model that one can consider is model B of Hohenberg and Halperin [20] such that $\frac{\partial h}{\partial t} = -\nabla^2 \frac{\delta H}{\delta h} + \eta_C$. So the corresponding Langevin dynamic equa-

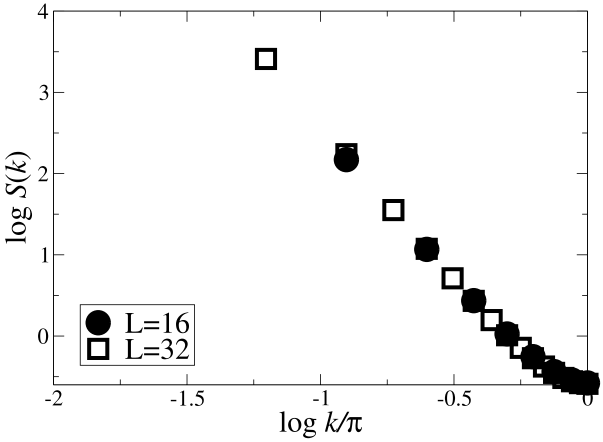


Fig. 4 Structure factor $S(k)$ versus k at saturated regime for $L = 16$ (*circle*) and $L = 32$ (*square*) in $d = 2$

tion becomes

$$\frac{\partial h(\mathrm{x}, t)}{\partial t} = -\nu \nabla^6 h(\mathrm{x}, t) + \eta_C(\mathrm{x}, t), \tag{8}$$

where the ∇^6 term tends to reduce the curvature of the interface with $z = 6$. The conserved noise is given by

$$\langle \eta_C(\mathrm{x}, \mathrm{t}) \eta_C(\mathrm{x}', \mathrm{t}') \rangle = -2D\nabla^2 \delta^{d-1}(\mathrm{x} - \mathrm{x}')\delta(t - t'). \tag{9}$$

This implies that the noise has no correlation in space and time. We solve (8) exactly by Fourier transform [2, 3] of the equation and obtain

$$\alpha = \frac{5-d}{2}, \qquad \beta = \frac{5-d}{12}, \qquad z = 6. \tag{10}$$

One can also check the results easily via the power counting method [2]. It is interesting that z becomes six being larger than four of the ordinary RC model, due to the conservation of the volume. Our numerical simulation of the CNRC model with a periodic boundary condition shows

$$\alpha \approx 1.50, \qquad \beta \approx 0.246, \qquad z \approx 6.09 \tag{11}$$

in $d = 2$. They are consistent with the values of (10). Hence, it is generally believed that the CNRC model can be described by (8) in the continuum limit.

3 Conclusion

In this paper, we have introduced a simple RC model with conservative noise, where the total number of particle is conserved. This model is similar to the restricted solid-on-solid model [12, 13] with noise conservation [17–19] except for the curvature restriction. In our model, the surface width $W(L, t)$ follows the scaling formula with the roughness exponent $\alpha \approx 1.5$, the growth exponent $\beta \approx 0.246$ and the dynamic exponent $z \approx 6.09$ which are in good agreement with $\alpha = 3/2, \beta = 1/4$, and $z = 6$ of (10). This CNRC model can be described by the linear sixth-order equation with conserved noise given by (8). In fact, we think that this correspondence is exact even though we have established it only numerically. The diffusion of adatoms generates a conservative noise where the total number of particles are conserved. Our model would be relevant at a certain experimental configurations such as Pb island on Si(111) surface where the total mass of Pb atoms is conserved [8]. We have shown that the conservation of total number of particles leads to a new universality class which has large value of z. This model can be generalized to any dimensions with the same discrete rules.

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