

## Relaxation of particles in the sloped region in a conserved growth model

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The dynamical scaling properties of conserved growth models, in which the downward (upward) movement of a particle dropped only on the sloped region occurs with a probability  $p$  ( $1-p$ ), are investigated by simulations in the substrate dimension  $d=1$ . By direct analysis of the surface fluctuation  $W$ , the models with  $p > 1/2$  are clearly and cleanly shown to have crossover behavior from Mullins-Herring (MH) universality to Edwards-Wilkinson (EW) universality. In contrast, the models with  $p < 1/2$  are shown to have an instability eventually, even though they initially follow the MH equation. The model with  $p = 1/2$  is shown to belong to the MH universality class and to be the critical model that splits the models with EW behavior from those with the instability. From these results we explain the physical reason for the very slow crossover in models like the Wolf-Villain model.

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Because of its possible relevance to the growth dynamics in molecular beam epitaxy, kinetic interface roughening of growth models [1–12] in which the number of particles dropped on the surface is conserved has been studied extensively. These conserved growth (CG) models are believed to follow the continuum equation

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda \nabla^2 (\nabla h)^2 + \eta(\mathbf{x}, t), \quad (1)$$

$$\langle \eta(x, t) \eta(x', t') \rangle = 2D \delta(x - x') \delta(t - t'). \quad (2)$$

The Family model [3], in which a particle dropped on a chosen column relaxes to a nearest neighbor (NN) column if the height of the NN column is lower than that of the chosen column, is one of the well-known CG models. The growth in the Family model is known to follow the Edwards-Wilkinson (EW) equation, i.e., Eq. (1) with  $\nu_2 \neq 0$  and  $\nu_4 = \lambda = 0$  [13]. The Wolf-Villain (WV) model [4] and the Das Sarma-Tamborenea (DT) model [5] are also well-known CG models. In the WV and DT models, the movement of a dropped particle depends on the lateral coordination numbers of the chosen column and NNs of the chosen column. The lateral coordination number  $k_i$  [2] of a column  $i$  is the number of lateral nearest neighbor bonds that an additional particle would have if it were deposited on the column. In the WV model, a dropped particle moves to a NN column if the movement increases  $k_i$  regardless of the  $k_i$  of the chosen column. In the DT model only a particle dropped on the column with  $k_i = 0$  is allowed, but the movement condition is the same as that of the WV model. Even though there exists a difference between the WV and DT models, they were originally suggested to follow the Mullins-Herring (MH) equation, i.e., Eq. (1) with  $\nu_4 \neq 0$  and  $\nu_2 = \lambda = 0$  [14]. The large curvature model [9] and restricted curvature model [10] were also suggested to follow the MH equation. In these

stochastic growth models for the MH equation the relaxation of a dropped particle to a NN column depends on  $k_i$  or on the local curvature  $\nabla^2 h$ .

However, the WV model was indirectly proved to have a very slow crossover from MH universality to EW universality by various studies such as measurements of the tilt-dependent current  $J$  [2,6] and large-scale simulations [7,8]. In contrast, such a crossover was not found [2] in the DT model [5] and its variant suggested by Krug [2], because negative  $J$  was not found in these models.

In contrast we recently suggested a stochastic growth model [12] following the MH equation in which dropped particles relax to NN columns by comparing the height of the chosen column to those of NNs as in the Family model [3]. The growth algorithm of this modified Family model (MFM) [12] in the substrate dimension  $d=1$  was as follows. Let  $x$  be a randomly chosen column. If  $h(x+1) \geq h(x)$  and  $h(x-1) \geq h(x)$ , then  $h(x) \rightarrow h(x) + 1$ . Otherwise take either the process  $\{h(x+1) \rightarrow h(x+1) + 1\}$  or  $\{h(x-1) \rightarrow h(x-1) + 1\}$  randomly. The condition for a particle to relax to a NN column in the MFM [12] is the same as that in the Family model. However, the directions of movements of particles in the MFM are different from those in the Family model. A particle in the MFM moves to a randomly selected NN column, but one in the Family model moves only to a NN column of lower height.

In this paper we first want to investigate the critical relation between the original Family model and the MFM [12]. From detailed investigations of various growth processes, we want to show that the growth processes on *the sloped region* can alone decide the scaling behavior. Here the sloped region means the column  $x$  at which the relation  $h(x+1, t) > h(x, t) > h(x-1, t)$  or  $h(x+1, t) < h(x, t) < h(x-1, t)$  is satisfied. (See also the region named ‘‘Growth II’’ in Fig. 1.) Other growth processes that are not on the sloped region, such as those on half-sloped regions (see the region named ‘‘Growth III’’ in Fig. 1) will be shown to be irrelevant for deciding the universality class of the models. If the particles on the sloped region move to a randomly selected NN column, then the growth will be shown to follow the MH equa-

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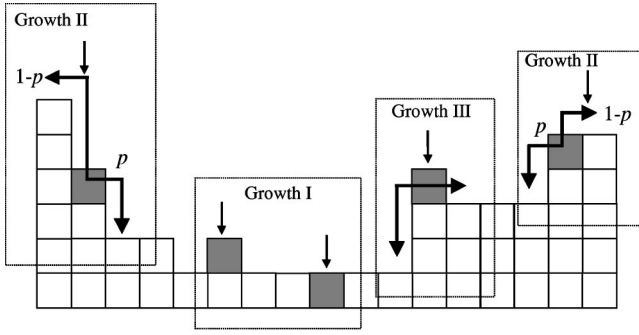


FIG. 1. Schematic diagram for the particle movements in the models defined in this paper. Growth I is the case where the growth occurs at the chosen column as in the original Family model. Growth II is the case for the sloped region.  $p$  is the probability for downward movement and  $1-p$  is the probability for upward movement. Growth III is the case for the half-sloped region, where the probability to move to either of the nearest neighbor columns is  $1/2$ .

tion. In contrast, if the particles on the sloped region move downward more probably than upward, then the growth will be shown to have crossover behavior from the MH to the EW universality class. If the particles on the sloped region are more probably move upward than downward, then the growth will be shown to have a sort of instability. Thus the model with the same probability of a downward movement on the sloped region as that of an upward movement is shown to belong to the MH universality class and to be a critical model which splits the EW universality from a sort of instability.

Another motivation of the present study is to establish a clean model which clearly follows the linear growth equation [15]

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

The physical importance of Eq. (3) is that the equation predicts crossover behavior from EW universality to MH universality with a crossover time  $t_c = \nu_4 / \nu_2^2$  [15]. Until now there has not been a stochastic growth model in which the surface fluctuation  $W$  directly and clearly follows Eq. (3) as far as the crossover behavior is concerned. As discussed previously, the WV model was speculated or indirectly proved to follow Eq. (3) [2,6–8]. In contrast, we shall show that models in which a downward movement of a particle dropped on the sloped region is more probable than an upward movement clearly follow Eq. (3). This will be shown directly from the power-law behavior of  $W$ ,  $W \approx t^\beta$ , where we can estimate the crossover time  $t_c$  accurately. Combining the numerical result for  $\nu_2$  from the measurement of  $J$ , and  $t_c = \nu_4 / \nu_2^2$ , we can also calculate  $\nu_4$ . In this sense models with a more downward probability are those that follow Eq. (3) with the corresponding numerical values of  $\nu_2$  and  $\nu_4$  known.

The third motivation of our study is to explain the physical grounds for such a slow crossover in models like the WV model. The lateral coordination number  $k_i$  [2] of a sloped region is 1. Since movement of a particle dropped on the site

with  $k_i = 1$  in the WV model is allowed, the movement of a particle dropped on the sloped region is very important to understand the crossover behavior of the WV model. From analysis of the models in which the movement of the particle on the sloped region is treated in a careful way, we want to discuss the physical reasons why slow crossover behavior exists in the WV model.

To show the importance of movements of particles dropped on the sloped region, we now introduce a kind of stochastic discrete model in the substrate dimension  $d=1$ . We believe that the extension of our model to those on higher-dimensional substrates can easily be done. The details of our model are as follows. Let  $x$  be a randomly chosen column during a certain growth process. The growth around column  $x$  follows one of three growth processes, Growth I, Growth II, or Growth III.

*Growth I.* If  $h(x+1) \geq h(x)$  and  $h(x-1) \geq h(x)$ , then  $h(x) \rightarrow h(x) + 1$ .

*Growth II.* If  $h(x-1) < h(x) < h(x+1)$ , take the growth process  $h(x-1) \rightarrow h(x-1) + 1$  with probability  $p$  or the growth process  $h(x+1) \rightarrow h(x+1) + 1$  with probability  $1-p$ . If  $h(x+1) < h(x) < h(x-1)$ , take the growth process  $h(x+1) \rightarrow h(x+1) + 1$  with probability  $p$  or the growth process  $h(x-1) \rightarrow h(x-1) + 1$  with probability  $1-p$ .

*Growth III.* Otherwise take either the process  $h(x+1) \rightarrow h(x+1) + 1$  or the process  $h(x-1) \rightarrow h(x-1) + 1$  randomly (or with the same probability).

In Fig. 1 the possible movements of the dropped particles in our models are shown. Growth I is the growth process at the chosen column. Growth II is the growth process on the sloped region. The downward movement of a dropped particle on the sloped region occurs with probability  $p$ . If  $p = 1$ , then the growth process on the sloped region is the same as that of the Family model. If  $p > 1/2$ , then a downward movement is more probable than an upward movement. If  $p = 1/2$ , a dropped particle on the sloped region makes a downward or upward movement randomly and thus the growth process on the sloped region is the same as that of the MFM model [12]. If  $p < 1/2$ , then upward movement on the sloped region is more probable. Growth III is the growth process on the half-sloped region. Here the half-sloped region means the case  $\{h(x-1, t) < h(x, t) = h(x+1, t)\}$  or  $\{h(x-1, t) = h(x, t) > h(x+1, t)\}$ . In Growth III, the relaxation of a dropped particle to either of the NN columns occurs completely randomly, or the probability of relaxation to either of the NN columns is assigned to be  $1/2$ . In the Family model a particle dropped on the half-sloped region moves to the NN column of lower height. In contrast, a particle on the half-sloped region moves to one of the NN columns randomly in the present model.

To find the scaling behaviors of the growth models defined above, the fluctuations of growing surfaces were studied by simulations. The simulations were performed with a periodic boundary condition on a flat substrate in the substrate dimension  $d=1$ . To see the early-time behavior of the surface fluctuation  $W(L, t)$  for various  $p$ 's, we measured  $W(t \ll L^z)$  as a function of  $t$  on a substrate of size  $L=1024$  and the results are shown in Fig. 2. The data for each  $p$  in Fig. 2 were taken by averaging over more than 50 indepen-

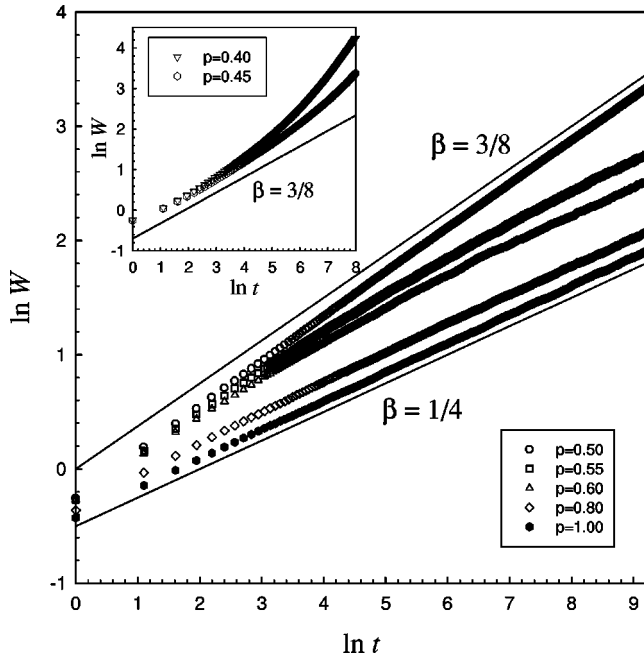


FIG. 2. Plots of  $\ln W(L,t)$  against  $\ln t$  for  $p \geq 1/2$ .  $p > 1/2$  means that a downward movement in the sloped region is more probable than an upward movement. The size of the substrate used is  $L = 1024$ . The solid line with index  $\beta = 3/8$  describes the line that satisfies the relation  $W \approx t^{3/8}$  and the line with index  $\beta = 1/4$  corresponds to the relation  $W \approx t^{1/4}$ . Inset shows the plots of  $\ln W(L,t)$  against  $\ln t$  for  $p < 1/2$ , i.e., for cases in which an upward movement is more probable than a downward movement.

dent runs.  $W(L,t)$  for  $p=0.5$  in the early-time regime or the regime for  $t \ll L^z$  satisfies the relation  $W(L,t) \approx t^\beta$  quite well. From the fit of the data for  $p=0.5$  to the relation  $W(L,t) \approx t^\beta$ , we obtained  $\beta = 0.37(2)$ . As far as the early-time behavior is concerned, the model with  $p=1/2$  is sure to belong to the MH universality class [12], since the exact  $\beta$  for the MH equation is  $\beta = 3/8$  [1,2,4,5]. The data for  $p=1$  in the regime for  $t \ll L^z$  satisfy  $W(t \ll L^z) \approx t^\beta$  with  $\beta = 0.25(1)$  well and this model is the same as the Family model in its critical behavior. In contrast, the data for  $p > 1/2$  in Fig. 2 show rather complex behaviors. For detailed analyses of the data with  $p > 1/2$ , the data for  $p=0.55$  and  $p=0.60$  are redrawn in Fig. 3. As can be seen from the fitted lines in Fig. 3,  $W(t \ll L^z)$  for  $p > 1/2$  initially follows  $W(L,t) \approx t^{\beta_i}$  with  $\beta_i = 0.37(2)$  well. Then, after a crossover time  $t_c$ ,  $W(L,t)$  follows  $W(L,t) \approx t^{\beta_f}$  with some other exponent  $\beta_f$ . For  $p=0.55$  the best estimates for  $t_c$  and  $\beta_f$  are  $t_c \approx 110.0$  ( $\ln t_c \approx 4.7$ ) and  $\beta_f = 0.27(1)$ . (See the inset of Fig. 3.) For  $p=0.60$  the estimated  $t_c$  and  $\beta_f$  are  $t_c \approx 59.2$  ( $\ln t_c \approx 4.1$ ) and  $\beta_f = 0.25(1)$ . Even though the exponent  $\beta_f$  ( $\approx 0.27$ ) for  $p=0.55$  is slightly larger than  $\beta = 1/4$  for the EW equation, it can be concluded that the early-time behavior of the models for  $p > 1/2$  shows crossover behavior from the initial MH behavior to the eventual EW behavior. Furthermore, we confirmed that the crossover time  $t_c$  becomes smaller as the downward probability  $p$  increases from  $1/2$ .

As we discussed when explaining the motivations of this paper, this kind of crossover behavior is a typical one which

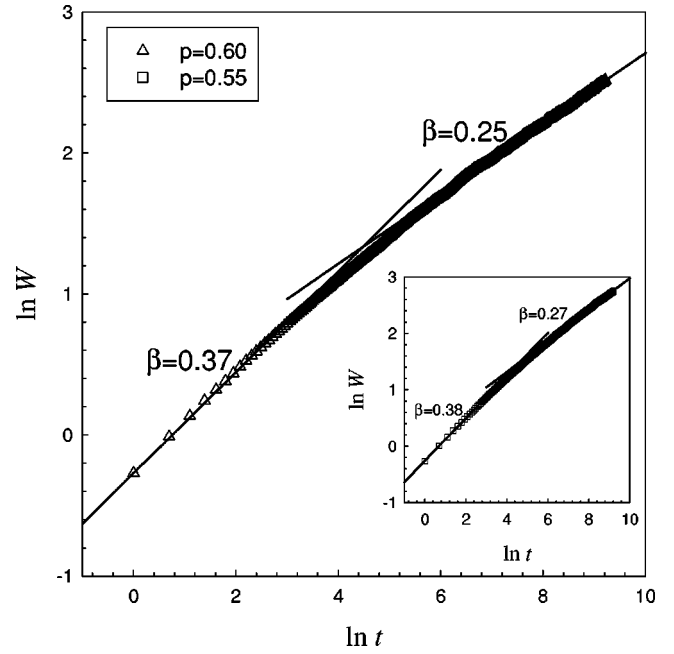


FIG. 3. Detailed plots of the data in Fig. 2 for  $p=0.55$  (inset) and  $0.60$ . The solid lines denoted by  $\beta=0.37$  are from the fitting of the initial data to the relation  $W \approx t^\beta$  to obtain  $\beta=0.37$ . The lines denoted by  $\beta=0.27$  and  $\beta=0.25$  are also from the fitting of data for  $t > t_c$  to  $W \approx t^\beta$  to obtain  $\beta=0.27$  or  $\beta=0.25$ , respectively.

can be described by Eq. (3). So our model with  $p > 1/2$  is a stochastic growth model that follows Eq. (3). The crossover time  $t_c$  from the regime with  $W(L,t) \approx t^{3/8}$  (MH regime) to the regime with  $W(L,t) \approx t^{1/4}$  (EW regime) for the growth described by Eq. (3) is known to satisfy  $t_c = \nu_4 / \nu_2^2$  [15] and thus  $t_c$  should be a function of the probability  $p$  in our model. As is well known, the coefficient  $\nu_2$  in Eq. (3) can be obtained by measuring the tilt-dependent surface current  $J(m)$  as a function of  $m$ , where  $m$  is the average slope of the tilted substrate [6].  $J(m)$  is measured by counting the difference between the number of jumps in the uphill and downhill directions. If the net current is in the uphill direction,  $J(m)$  is positive.  $\nu_2$  can be determined by the relation  $\nu_2 = -(\partial J / \partial m)|_{m=0}$ . The measurement of  $J(m)$  is important, because  $J(m) < 0$  means  $\nu_2 > 0$  and guarantees the EW term ( $\nu_2 \nabla^2 h$ ). We measured  $J(m)$  for the model with  $p \geq 1/2$  by dropping more than  $10^8$  particles in the steady-state regime (or  $t \gg L^z$ ) using a system with size  $L = 1024$ . The data for  $J(m)$  are shown in Fig. 4. The magnitude of  $J(m)$  for  $p=1/2$  in Fig. 4 is very small (or less than  $0.0001$ ) and  $J(m)$  for  $p=1/2$  does not have any special trend when  $m$  is varied. So we believe that  $\nu_2(p=1/2) = 0$ . For the model with  $p > 1/2$ , negative  $J(m)$ 's were found. From the data in Fig. 2 and the relation  $\nu_2 = -(\partial J / \partial m)|_{m=0}$ , we can calculate the values for  $\nu_2$  for  $p > 1/2$ . The calculated values of  $\nu_2$  for  $p=0.55$  and  $p=0.60$  are displayed in Table I. One can also estimate the dependence of  $\nu_4$  on  $p$  [ $\nu_4(p)$ ] from the obtained values of  $\nu_2(p)$  and  $t_c(p)$  and the relation  $t_c = \nu_4 / \nu_2^2$ . The estimations of  $\nu_4$  for  $p=0.55$  and  $p=0.60$  are also displayed in Table I. As was emphasized when explaining the motivations of this paper, our model with  $p > 1/2$  is

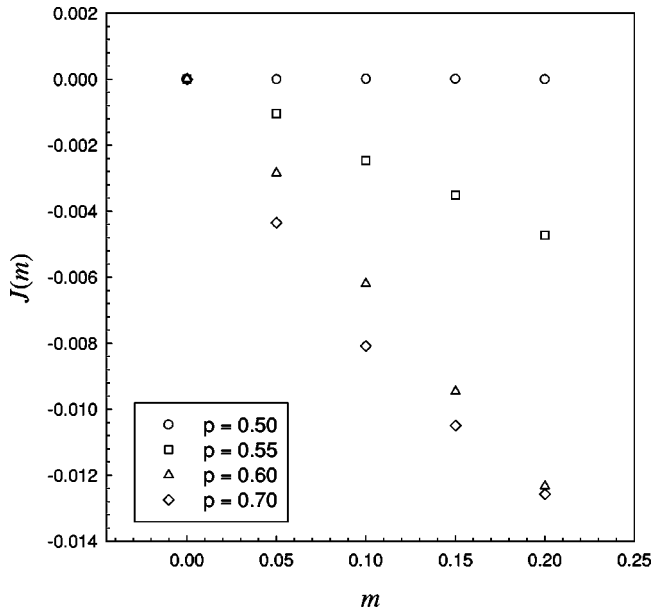


FIG. 4. The dependence of current  $J(m)$  for model with  $p \geq 1/2$  on the slope  $m$  of the tilted substrate.

one of very rare models in which corresponding values of  $\nu_2$  and  $\nu_4$  are calculable.

In Fig. 5, we display the data for the model with  $p \geq 1/2$  for surface width  $W$  in the saturated regime ( $t \gg L^z$ ). The substrate sizes used are  $L = 32, 64, 128, 256, 512$ . From the formula  $W(t \gg L^z) \approx L^\alpha$ , the estimated roughness exponents  $\alpha$  for various  $p$ 's are as follows:  $\alpha = 1.42(2)$  for  $p = 1/2$ ,  $\alpha = 0.54(2)$  for  $p = 0.55$ , and  $\alpha = 0.52(1)$  for  $p = 0.60$ . The estimated  $\alpha$  for  $p = 1/2$  is close to  $3/2$ , which is the exact value of  $\alpha$  for the MH equation. For  $p = 0.55$  and  $p = 0.60$ , the estimated  $\alpha$ 's are close to  $1/2$ , where  $\alpha = 1/2$  is the exact value for the EW equation. These data in Fig. 5 support the conclusion that the critical property of the saturation regime of the model with  $p = 1/2$  is the same as that of the MH equation, whereas the critical property of the saturation regime of the model with  $p > 1/2$  is very close to that of the EW equation. From the results in Figs. 2–5, we can conclude that the model with  $p = 1/2$  follows the MH equation. In contrast, the model with  $p > 1/2$  follows the linear growth equation (3). In other words, the models with  $p > 1/2$  show crossover behavior from MH behavior to EW behavior clearly and cleanly.

We now want to discuss the simulation results for the model with  $p < 1/2$ , in which an upward movement of the dropped particles on the sloped region is more probable than a downward movement. The data of  $W(t \ll L^z)$  for  $p < 1/2$  are displayed in the inset of Fig. 2. Initially  $W(t \ll L^z)$  for  $p > 1/2$  seems to follow  $W \approx t^{3/8}$ . But after some time  $W(t)$

TABLE I. Estimates of the coefficients  $\nu_2$  and  $\nu_4$  of Eq. (3) for models with different  $p$ .

$p$	0.55	0.60
$\nu_2$	0.025	0.062
$\nu_4$	0.69	0.23

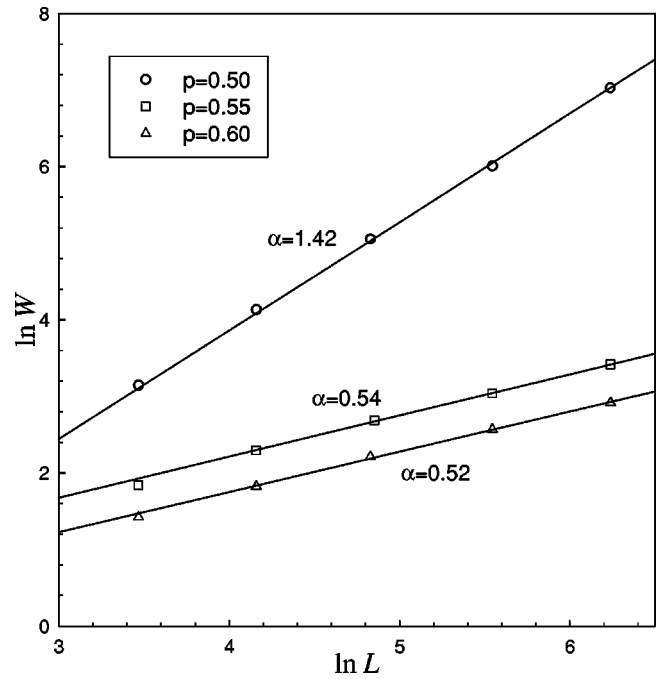


FIG. 5. Plots of  $\ln W(t \gg L^z)$  against  $\ln L$  for model with  $p \geq 1/2$ . The solid lines denoted by the corresponding values  $\alpha$  are obtained by fitting the data to the relation  $W(t \gg L^z) \approx L^\alpha$ .

rapidly grows. We did not find saturation of  $W$  for the model with  $p < 1/2$  in any simulation. This result means that the model with  $p < 1/2$  shows unlimited growth of  $W$  as in random deposition, and a sort of instability in  $W$ .

In summary we have shown by simulations that the model with  $p > 1/2$  can be described by the linear growth equation (3), where the corresponding values of  $\nu_2$  and  $\nu_4$  are calculable. The model with  $p > 1/2$  has been shown to have crossover behavior from MH behavior to EW behavior clearly and cleanly. In contrast, the model with  $p < 1/2$  has been shown to have some kind of instability, even though initially the model follows the MH equation. The model with  $p = 1/2$  has been shown to belong to the MH universality class, and to be the critical model which splits the eventual EW behavior from the instability.

Now we want to discuss the physical grounds for such a slow crossover in models like the WV model. For this, we monitored the details of the growth process for the model with  $p = 1/2$  in the saturation regime. The monitoring was done by watching the growth process for  $10^8$  dropped particles on the substrate with  $L = 1024$  in the saturation regime (or  $t \gg L^z$ ). About 71% of the particles were dropped on the sloped region, where 50% of particles dropped on the sloped region of course moved upward and 50% of them moved downward. Among the downward movements only 2.5% increased the lateral coordination number and 97.5% did not change the lateral coordination number. 27% of the upward movements decreased the lateral coordination number and 73% of them did not change the lateral coordination number. From these results of the monitoring the following conclusions are drawn. First, the main growth processes in the saturation regime of the model with  $p = 1/2$  are those on the sloped region. Second, only a small portion of the downward

movement on the sloped region increases the lateral coordination number. We can expect that the morphology of models like the WV model at very large  $t$  is structurally and critically the same as that of the model with  $p = 1/2$ , because both models follow  $W \approx t^{3/8}$  in the initial regime. Then in both models the main growth processes at very large  $t$  are expected to occur on the sloped region. A particle dropped on the sloped region or on a site with lateral coordination number  $k_i = 1$  in the WV model [2,4] can relax to a NN column provided that the relaxation increases  $k_i$ . Since the movements on the sloped region that increase  $k_i$  are downward movements and only a small amount (or about 2.5%) of the downward movements increase  $k_i$  in models like the one with  $p = 1/2$  or the WV model, a small negative current  $J$  in the WV model is expected due to the particles on the sloped region. Since negative  $J$  has not been found [2] in the DT model [5] and its variant [2] in which movements on the sloped region or on the site with  $k_i = 1$  are not allowed, we believe that growth processes not on the sloped region are

not critical for the explaining the slow crossover phenomenon from MH universality to EW universality. So we can understand the slow crossover in models like the WV model in terms of the small negative  $J$ , which comes from the downward movement of particles on the sloped regions or on sites with  $k_i = 1$ .

Our final discussion is about the upward movements we considered. Similar upward movements on the sloped regions were also considered in other models [7,16]. However, such upward movements [7,16] were considered only when the number of connected bonds at the chosen column is tied to that of the NN column, and the resulting interfaces were either unstable ( $\beta = 1$ ) [7] or grooved [16]. In contrast, upward movements in our model are based on comparison of the heights of NN columns to that of the chosen column.

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