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Time-dependent gradients of growing interfaces

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The time evolution of interface gradients for growth on various substrates is investigated. For the Edwards-Wilkinson model we derive an expression that relates the mean-squared gradient to the autocorrelation function of the associated diffusion problem. This expression is corroborated by numerical calculations for growth on Euclidean and fractal substrates. Furthermore, we analyze the mean step heights for a particular growth model that is based on random deposition and relaxation.

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The investigation of interface growth phenomena is a field of current activity [1–3]. An important issue in these investigations is the characterization of the interfaces in terms of roughness, scaling behavior, and corresponding exponents. Many growth models have been introduced and their theoretical descriptions have been based predominantly on continuum equations, for instance, on the Edwards-Wilkinson equation (EW) [4] and on the Kardar-Parisi-Zhang equation (KPZ) [5,6]. Various correlation functions have been studied in order to describe the behavior of the interfaces for regular substrates. Recently also substrates of fractal geometry were proposed [7]. It has been claimed that the mean step height provides a useful quantity for the characterization of surface roughness [8,9]. In this paper we study this quantity in more detail and consider the EW process for the analysis of the local gradient of growing surfaces for both regular and fractal substrates.

We first present the continuum equation for the EW process, which reads [4]

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

where $h(\boldsymbol{x},t)$ is the height of the interface at location $\boldsymbol{x}$ at time t. $\eta(\boldsymbol{x},t)$ denotes the noise term which is assumed to be Gaussian and δ correlated:

$$\langle\eta(\boldsymbol{x},t)\rangle=0,$$

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

Here d is the substrate dimension. For a discrete lattice the continuum equation (1) is equivalent to the form [7]

$$\frac{\partial h(\boldsymbol{x}_j,t)}{\partial t}=\Gamma\sum_{i\in\sigma_j}[h(\boldsymbol{x}_i,t)-h(\boldsymbol{x}_j,t)]+\eta(\boldsymbol{x}_j,t), \tag{2}$$

where $\boldsymbol{x}_j$ are the coordinates of the lattice sites and where σ_j denotes the nearest neighbors of site j. Γ is the hopping rate between nearest neighbor sites. Assuming a uniform coordination number the hopping rate is related to the diffusion constant as $\Gamma=\nu/s^2$, where s is the lattice constant. Initiating the growth process with a flat surface, $h(\boldsymbol{x},0)=0$, the solution of Eq. (2) can be given in terms of the Green's function $P(\boldsymbol{x}_j,t|\boldsymbol{x}_i,t')$, the conditional probability of being at $\boldsymbol{x}_j$ at time t having started at $\boldsymbol{x}_i$ at time t'. One has

$$h(\boldsymbol{x}_j,t)=\int_0^t dt'\sum_i P(\boldsymbol{x}_j,t|\boldsymbol{x}_i,t')\,\eta(\boldsymbol{x}_i,t'). \tag{3}$$

We will use this expression for the calculation of the width $\xi(t)$ of the surface, which is usually defined as

$$\xi^2(t)=\frac{1}{N}\left\langle\sum_j[h(\boldsymbol{x}_j,t)-\bar{h}(t)]^2\right\rangle, \tag{4}$$

where $\bar{h}(t)$ denotes the mean height at time t for a particular surface configuration, $\bar{h}(t)=N^{-1}\Sigma_j h(\boldsymbol{x}_j,t)$, and where N stands for the number of lattice sites in the system. $\bar{h}(t)$ appears in (4) for finite systems; it decreases with the number of sites typically as $\bar{h}(t)\sim N^{-1/2}$. The average in Eq. (4) is taken over all realizations of the noise $\eta(\boldsymbol{x}_j,t)$. The time evolution of the width depends on the system size L; for the description the following scaling law has been introduced [3,4,10]:

$$\xi(t)\sim L^{\alpha}f(t/L^{z}),$$

$$f(x)\sim\begin{cases}x^{\beta}, & x\ll 1\\ \text{const}, & x\gg 1\end{cases} \tag{5}$$

where f is the scaling function indicating two characteristic regimes: the surface width first increases with time as a power law and then crosses over to saturation. The dynamic exponent z is given by the ratio $z=\alpha/\beta$. The scaling law (5) has been shown to hold for the EW and for the KPZ equation [4,10,11]. For the EW process on Euclidean substrates the exponents take the values $\alpha=1/2$ and $\beta=1/4$ for $d=1$. For the marginal case $d=2$, the width increases logarithmically while for $d>2$ the surface remains smooth.

In Ref. [7] an expression was derived for the EW model which relates the behavior of the width to the autocorrelation function of the associated diffusion problem. Fractal substrates were considered and the exponent β was found to depend on the spectral dimension d_s, so that

$$\beta=\begin{cases}1/4 & \text{for } d=1\\ 1/2-d_s/4 & \text{for } 1<d_s<2.\end{cases} \tag{6}$$

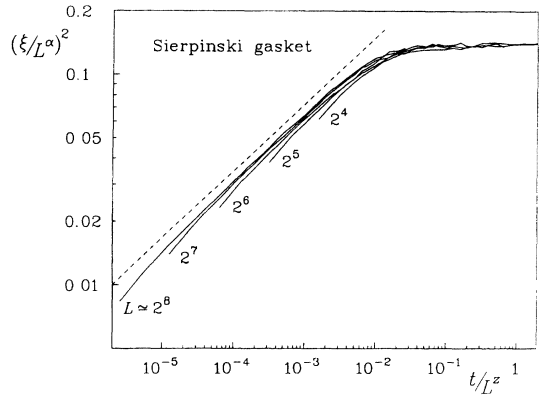

FIG. 1. The surface width as a function of time for the EW process on a Sierpinski gasket embedded in a two-dimensional (2D) space. The width is plotted in the scaling representation as $(\xi/L^{\alpha})^2$ vs the scaling variable t/L^z for various system sizes as indicated. The dashed line gives the theoretical slope according to the exponent $2\beta = 1 - d_s/2$.

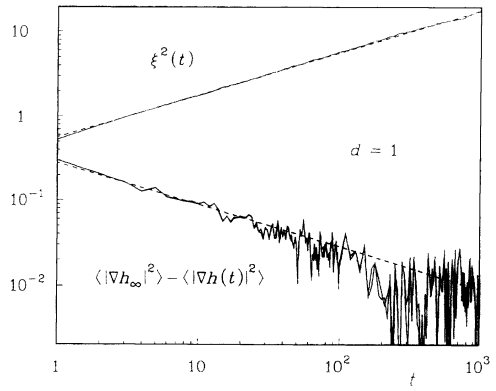

FIG. 2. The width and the mean-squared gradient for the one-dimensional substrate. In the upper part are plotted the numerical results of $\xi^2(t)$ (solid line) and the prediction $(t/\pi)^{1/2}$ (dashed line). In the lower part are given the numerical results $\langle|\nabla h_{\infty}|^2\rangle - \langle|\nabla h|^2\rangle$ and $(\langle|\nabla h_{\infty}|\rangle^2 - \langle|\nabla h|\rangle^2)(\pi/2)$ as full lines. The latter two quantities coincide at short times. The dashed line in the lower part gives the behavior of Eq. (15).

In this paper we present the complementary result for the roughness exponent α. We make use of Eq. (5) and of the following scaling argument: The dynamic scaling behavior characterized by the power-law increase fails when the diffusion front travels over a distance L which indicates the beginning of finite-size effects. The associated crossover time is given by $t_c \sim L^{d_w}$, where d_w is the walk dimension. This dimension is related to the fractal dimension d_f and to the spectral dimension d_s by the ratio $d_w = 2d_f/d_s \geq 2$ [12]. At crossover the power-law behavior of early times has to be met, $\xi(t_c) \sim t_c^{\beta}$; thus the following expression for the roughness exponent is obtained:

$$\alpha = \begin{cases} 1/2 & \text{for } d = 1 \\ d_f\left(\dfrac{1}{d_s} - \dfrac{1}{2}\right) & \text{for } 1 < d_s < 2. \end{cases} \tag{7}$$

In Fig. 1 we present simulation results calculated for the Sierpinski gasket embedded in a $d=2$ Euclidean space with the noise parameter D and the stepping time set equal to unity. For Sierpinski gaskets $d_f = \ln(d+1)/\ln(2)$ and $d_s = 2\ln(d+1)/\ln(d+3)$, thus for $d=2$ one has $\beta \simeq 0.159$ and $\alpha \simeq 0.368$. In the numerical procedure the system of ordinary differential equations, Eq. (2), was solved using the Euler method with a variable step control. The average was taken over typically 10^3 realizations. In the figure the variance ξ^2 is displayed for various system sizes in the scaling representation; as a consequence a data collapse onto a single master curve is obtained which demonstrates that the predicted scaling behavior is obeyed. Furthermore, at early times the time evolution of the width follows reasonably well the theoretical power-law increase.

We continue by analyzing the local gradient $\nabla h(\boldsymbol{x},t)$. For the lattice model we consider the discretized derivative

$$\nabla h(\boldsymbol{x},t) = s^{-1}[h(\boldsymbol{x}+\boldsymbol{s},t) - h(\boldsymbol{x},t)], \tag{8}$$

where $\boldsymbol{s}$ is a vector of length s denoting the displacement between nearest neighbors. The gradient is specified along the direction of $\boldsymbol{s}$; apart from s^{-1}, the right-hand side of Eq. (8) also denotes the step height. Aiming at the behavior of the mean-squared step height, the average has to be taken over pairs of nearest neighbors, i.e., over sites and directions. We therefore disregard the proper vector notation for the gradient and with this simplification we also avoid the difficulty concerning the definition of the gradient for fractal substrates. Inserting Eq. (3) into Eq. (8) we find

$$\nabla h(\boldsymbol{x}_j,t) = s^{-1}\int_0^t dt' \sum_i [P(\boldsymbol{x}_j+\boldsymbol{s},t|\boldsymbol{x}_i,t') - P(\boldsymbol{x}_j,t|\boldsymbol{x}_i,t')]\eta(\boldsymbol{x}_i,t'). \tag{9}$$

The mean-squared gradient results from the averaging over sites and directions which yields

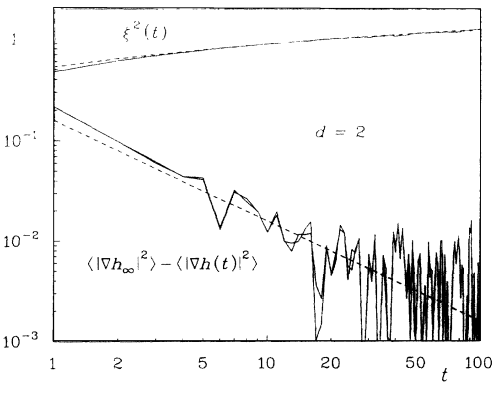

FIG. 3. Same as Fig. 2 but for the two-dimensional substrate. The dashed line in the upper part follows the logarithmic increase $\ln(t)/(2\pi) + 0.5577$ [7].

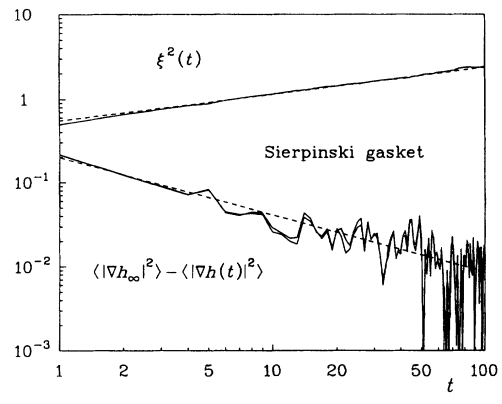

FIG. 4. Same as Fig. 2 but for the 2D Sierpinski gasket. The dashed lines in the upper and lower part give the theoretical slopes of $1-d_s/2$ and $-d_s/2$ according to Eqs. (6) and (15), respectively.

$$\langle|\nabla h(t)|^2\rangle=\frac{1}{N}\left(\frac{D}{s^2\tilde{z}^2}\right)\int_0^t dt'\sum_{i,j,s}\{[P(\boldsymbol{x}_j+\boldsymbol{s},t|\boldsymbol{x}_i,t')]^2 +[P(\boldsymbol{x}_j,t|\boldsymbol{x}_i,t')]^2 -2P(\boldsymbol{x}_j+\boldsymbol{s},t|\boldsymbol{x}_i,t')P(\boldsymbol{x}_j,t|\boldsymbol{x}_i,t')\}. \quad (10)$$

$\tilde{z}$ is the coordination number which for Euclidean lattices and for Sierpinski gaskets takes the value $\tilde{z}=2d$. Expression (10) is exact for Euclidean lattices and a vectorial notation in Eq. (8). Making use of the Chapman-Kolmogorov relation [7] and introducing the spatially averaged Green's function [15]:

$$P(\boldsymbol{r},t)=N^{-1}\sum_j P(\boldsymbol{x}_j+\boldsymbol{r},t|\boldsymbol{x}_j,0) \quad (11)$$

we find

$$\langle|\nabla h(t)|^2\rangle=2\left(\frac{D}{s^2\tilde{z}^2}\right)\int_0^t dt'\sum_s[P(0,2t')-P(\boldsymbol{s},2t')]. \quad (12)$$

Our next step of derivation is based on the continuous-time random walk theory [13,14]. We assume an exponential distribution $\tau^{-1}\exp(-t/\tau)$ for the probability of a jump to occur at time t, where τ is the stepping time, $\tau=\tilde{z}\Gamma$. We derive the following recursion relation:

$$P(\boldsymbol{x},t|\boldsymbol{x},0)=\frac{1}{\tau\tilde{z}}\sum_s\int_0^t P(\boldsymbol{x},t|\boldsymbol{x}+\boldsymbol{s},t')e^{-t'/\tau}dt'+e^{-t/\tau}, \quad (13)$$

where the sum runs over the nearest neighbors of $\boldsymbol{x}$. The first term in Eq. (13) denotes the probability to have reached a nearest neighbor site in the first step at time t' multiplied by the probability to return to the initial location in the remaining time, while the second term is the probability for not having moved at all. We note that for translational symmetric lattices all nearest neighbors are equivalent in Eq. (13) while for fractal lattices we assume that they are equivalent. Inserting Eq. (13) into Eq. (12) we obtain after some formal steps

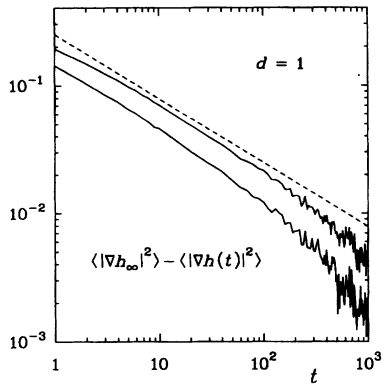

FIG. 5. The mean step height for the growth model based on deposition and lateral relaxation on a one-dimensional substrate. The two solid lines represent $\langle|\nabla h_\infty|\rangle^2-\langle|\nabla h|\rangle^2$ (lower line) and $\langle|\nabla h_\infty|^2\rangle-\langle|\nabla h|^2\rangle$ (upper line). The dashed line indicates the slope of $-1/2$.

$$\langle|\nabla h(t)|^2\rangle\simeq\frac{D\tau}{s^2}[1-P(0,2t)]. \quad (14)$$

This expression relates the mean-squared gradient to the autocorrelation function which for longer times follows the behavior $P(0,t)\sim(d\tau/2\pi t)^{d/2}$ for Euclidean lattices, and $P(0,t)\sim t^{-d_s/2}$ for fractals [12]. We are interested in how fast the asymptotic value is reached; accordingly we write

$$\langle|\nabla h_\infty|^2\rangle-\langle|\nabla h|^2\rangle \sim\begin{cases}t^{-d/2} & \text{for Euclidean lattices}\\ t^{-d_s/2} & \text{for fractals,}\end{cases} \quad (15)$$

where $\langle|\nabla h_\infty|^2\rangle$ denotes the gradient at $t=\infty$.

Expression (15) is the main result of this paper. In Figs. 2–4 we present simulation results of the mean-squared gradient for Euclidean lattices and for the Sierpinski gasket with the noise parameter D and the stepping time τ set equal to unity. The same numerical procedure was applied as for the

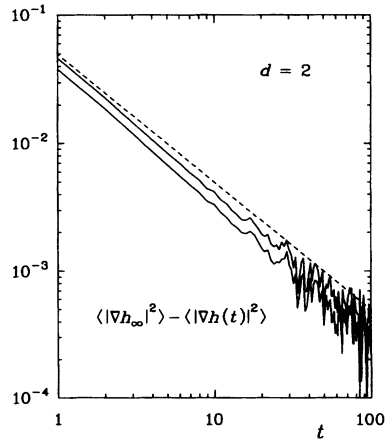

FIG. 6. Same as Fig. 5 but for the two-dimensional substrate. The dashed line indicates the slope of -1.

results of Fig. 1. Typically 10^4–10^5 sites were considered for a realization. In all cases $\langle|\nabla h|^2\rangle$ and $(\pi/2)\langle|\nabla h|\rangle^2$ are displayed. The close agreement between the two quantities indicates that the gradients ∇h are Gaussian distributed. Moreover, the numerical results follow reasonably well the predicted power law and corroborate the theoretical behavior of expression (15). For comparison reasons the numerically calculated $\xi^2(t)$ are also presented.

Finally we report on the application of this study to growth models. While in the above we studied differential equations with a continuous noise source, here we consider a discrete particle model. As a candidate we chose the model of random deposition with lateral relaxation to the nearest minimum, a model which has been shown to belong to the universality class of the EW process; this conclusion was achieved on the basis of the surface width [16]. We extended these studies by calculating the mean step height for growth on one-dimensional (1D) and two-dimensional (2D) substrates. The asymptotic value $\langle|\nabla h_\infty|^2\rangle$ was computed independently for various sizes L; we found that $\langle|\nabla h_\infty|^2\rangle$ takes the values 0.692 and 0.462 for the 1D and 2D substrates, respectively. The time evolution of the mean step height is shown in Fig. 5 for the 1D substrate of size $L=20\,000$ and in Fig. 6 for for the 2D substrate of size $L\times L=400\times 400$. The average was taken over 100 samples. Also in these figures we present the results of $\langle|\nabla(t)|\rangle$. We observe that for both quantities the numerical results follow reasonably well the power law of Eq. (15).

In conclusion we have studied the mean-squared gradient for the Edwards-Wilkinson process and we have derived an expression which relates the mean-squared gradient to the autocorrelation function of the associated diffusion process. The simulation results for the Edwards-Wilkinson process and for a growth model agree well with the theoretical predictions.

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