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J. Stat. Mech. (2008) P02010

(http://iopscience.iop.org/1742-5468/2008/02/P02010)

Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

Markov analysis and Kramers–Moyal expansion of the ballistic deposition and restricted solid-on-solid models

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Received 29 July 2007
Accepted 6 February 2008
Published 26 February 2008

Online at stacks.iop.org/JSTAT/2008/P02010
doi:10.1088/1742-5468/2008/02/P02010

Abstract. It is well known that the ballistic deposition and the restricted solid-on-solid models belong to the same universality class, having the same roughness and growth exponents. In this paper, we determine some new statistical properties of the two models, such as the Kramers–Moyal coefficients and the Markov length scale, and show them to be distinct for the two models.

Keywords: self-affine roughness (theory), stochastic processes (theory)

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 1742-5468/08/P02010+13$30.00

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1. Introduction

The study of the statistical properties of surfaces growing under the deposition of particles has attracted many researchers over the last two decades [1]–[7]. The theoretical description of the surface growth processes has been accomplished using a number of discrete and continuous models that belong mainly to three groups: the Edwards–Wilkinson model [8], the Kardar–Parisi–Zhang equation (KPZ) [9], and models based on molecular beam epitaxy [10]. The focus of such studies has been the statistical characterization of the growing surface. This is achieved by estimating the roughness exponent of the steady-state surface, the growth exponent [11], and the scaling functions associated with the steady-state evolution of the surface [12]–[16].

The simplest quantitative characteristic of a given surface or interface is its roughness, also called the interface width, defined as the root mean square fluctuation of the height around its average position. The width w is usually averaged over different configurations, and its scaling with the time and length of the substrate is used to characterize the growth process. Consider a sample of size L and define the mean height of the growing film $\overline{h}$ and its roughness w by the following expressions:

$$w(L,t) = (\langle (h-\overline{h})^2 \rangle)^{1/2}, \tag{1}$$

where t is proportional to the deposition time and $\langle \cdots \rangle$ denotes an averaging over different samples. For simplicity, and without loss of generality, we assume that $\overline{h}=0$. Starting from a flat interface (one of the possible initial conditions), it was conjectured by Family and Vicsek that a scaling of space by factor b and of time by factor b^z (z is the dynamical scaling exponent) rescales the roughness w by the factor b^α as [17]

$$w(bL, b^z t) = b^\alpha w(L,t), \tag{2}$$

which implies that

$$w(L,t) = L^\alpha f(t/L^z). \tag{3}$$

If for large t and fixed $L(t/L^z \to \infty)$, w saturates, then $f(x) \longrightarrow g$ as $x \longrightarrow \infty$. However, for fixed and large L and $t \ll L^z$, one expects correlations of the height fluctuations to exist only within a distance $t^{1/z}$ and, thus, they must be independent of L. This implies

doi:10.1088/1742-5468/2008/02/P02010

that for $x \ll 1$, $f(x) \sim x^\beta g'$ with $\beta = \alpha/z$. Thus, for dynamic scaling one postulates that

$$w(L,t) = \begin{cases} t^\beta g \sim t^\beta, & t \ll L^z; \\ L^\alpha g' \sim L^\alpha, & t \gg L^z. \end{cases} \tag{4}$$

The roughness exponent α and the dynamic exponent z characterize the self-affine geometry of the surface and its dynamics, respectively. The dependence of the roughness w on $\overline{h}$ or t indicates that w has a fixed value for a given time.

A main problem in this area of research has been the scaling behavior of the moments of the height difference, $\Delta h = h(x_1) - h(x_2)$, and the evolution of the probability density function (PDF) of Δh, i.e., $P(\Delta h, \Delta x)$, in terms of the length scale Δx. Recently, Friedrich and Peinke were able to derive a Fokker–Planck equation which describes the evolution of the probability distribution function in terms of the length scale, for several stochastic phenomena, such as rough surfaces [18]–[20], turbulent flows [21], financial data [22, 23], heart interbeats [24], etc. They pointed out that the conditional probability density of the field increments (velocity field, etc) satisfies the Chapman–Kolmogorov equation. Mathematically, this is a necessary condition for the fluctuating data to follow a Markov process in the length scales [5].

In this paper we compute the Kramers–Moyal (KM) coefficients for the fluctuating field $\Delta h = h(x + \Delta x) - h(x)$ of the restricted solid-on-solid (RSOS) and the ballistic deposition (BD) models, and show that their first and second KM coefficients have well-defined values, whereas their third- and fourth-order KM coefficients tend to zero. Although the models have the same roughness and dynamical exponents, we show that they have distinct KM coefficients, and are described by distinct stochastic Langevin equations [25]. Hence, our computations make it possible to better distinguish the two models.

2. The Markov nature of the height fluctuations: the drift and diffusion coefficients

The first model analyzed here is the RSOS model [26] in which the incident particle sticks at the top of a growing column only if the differences of heights of all pairs of neighboring columns do not exceed $\Delta H_{\max} = 1$. Otherwise, the attempt for the growth of the surface is rejected. The second model was proposed for etching of a crystalline solid, by Mello *et al* [27]: in each growth attempt a randomly chosen column i, with current height $h(i) = h_0$, has its height increased by one unit $[h(i) \to h_0 + 1]$, and all the neighboring columns whose heights are smaller than h_0 grow to h_0 (this may be called the growth version of the etching model [28]).

In the simplest version of the BD model, particles are released from a randomly chosen position above a d-dimensional substrate, follow trajectories perpendicular to the surface and stick to it upon first contact with a nearest-neighbor occupied site. The resulting aggregate is porous and has a rough surface. Several applications of the BD model or its extensions to real growth processes have already been proposed, which justify the present analysis (see, for example, the recent applications in [29, 30]).

In figures 1 and 2 we show snapshots of the height $h(x)$ and $\Delta h = h(x+1) - h(x)$ for the BD and RSOS models in the stationary state, for samples of size 10^6 (in units of the lattice constant). The complete characterization of the statistical properties of random

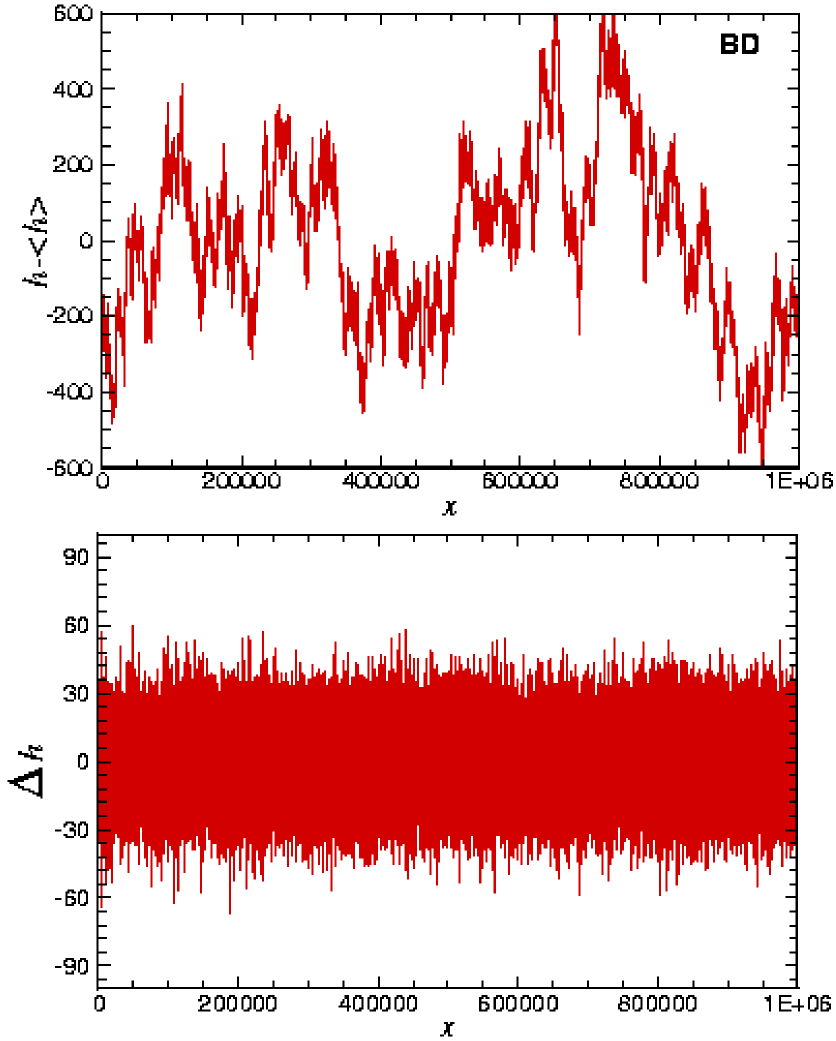

Figure 1. Snapshots of the height fluctuations of $h(x)$ and $\Delta h = h(x+1) - h(x)$ for the BD model, after saturation.

fluctuations of a quantity, such as the height h of the surface in the two models, in terms of a parameter x requires evaluation of the joint PDF, i.e., $P_N(h_1, x_1, \ldots, h_N, x_N)$, for an arbitrary N. If the process is a Markov process, an important simplification arises, since in this case P_N can be generated by a product of the conditional probabilities $P(h_{i+1}, x_{i+1}|h_i, x_i)$, for $i = 1, \ldots, N-1$. As a necessary condition for the fluctuation being a Markov process, the Chapman–Kolmogorov equation [5],

$$P(h_2, x_2|h_1, x_1) = \int \mathrm{d}(h_i)\, P(h_2, x_2|h_i, x_i)\, P(h_i, x_i|h_1, x_1), \tag{5}$$

should hold for any value of x_i, in the interval $x_2 < x_i < x_1$.

Let us first check that the height fluctuations represent a Markov process, and determine their corresponding Markov length scales L_{M}. The Markov length scale L_{M} is the minimum length over which the data can be considered as a Markov process. Here,

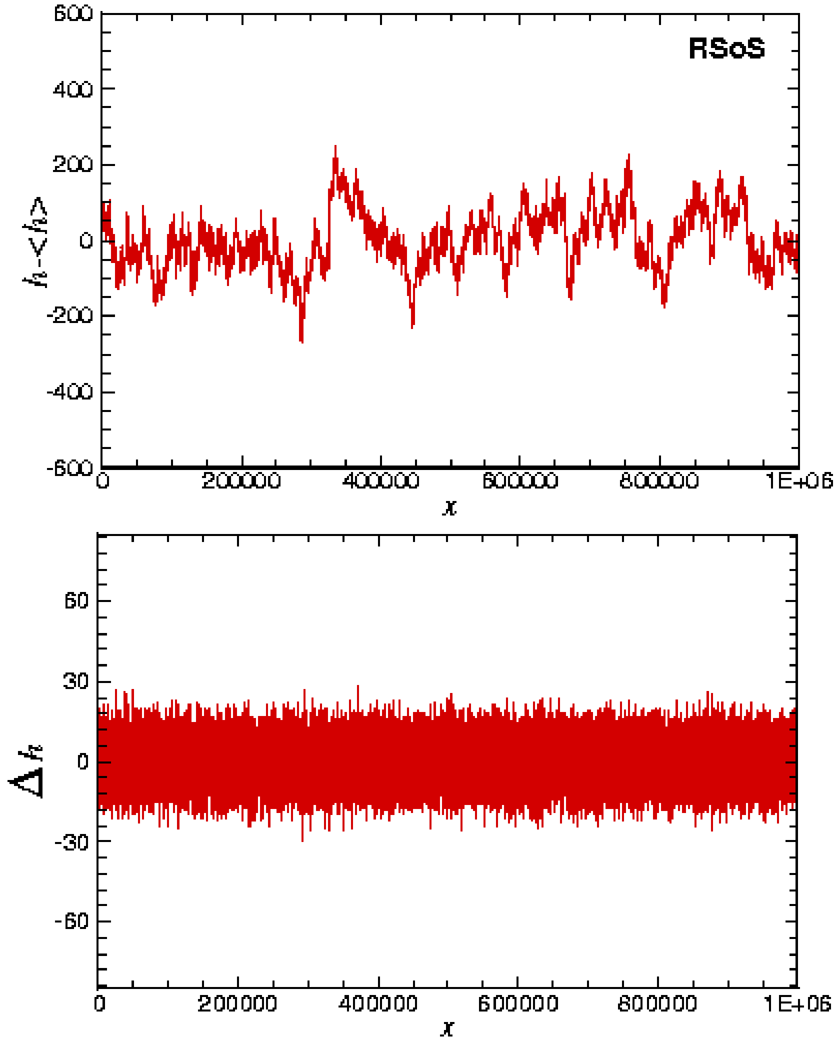

Figure 2. Same as figure 1, but for the RSOS model.

we use the least-squares method to determine the Markov length scale of the height $h(x)$. If $h(x)$ is a Markov process, then, one finds

$$P(h_3, x_3|h_2, x_2; h_1, x_1) = P(h_3, x_3|h_2, x_2). \tag{6}$$

We compare the three-point PDF with that obtained on the basis of the Markov process. The joint three-point PDF, in terms of the conditional probability functions, is given by

$$P(h_3, x_3; h_2, x_2; h_1, x_1) = P(h_3, x_3|h_2, x_2; h_1, x_1)P(h_2, x_2; h_1, x_1). \tag{7}$$

Using the properties of the Markov process and substituting in equation (7), we obtain

$$P_{\mathrm{Mar}}(h_3, x_3; h_2, x_2; h_1, x_1) = P(h_3, x_3|h_2, x_2)P(h_2, x_2; h_1, x_1). \tag{8}$$

In order to check the condition for the data being a Markov process, we must compute the three-point joint PDF through equation (7) and compare the result with equation (8).

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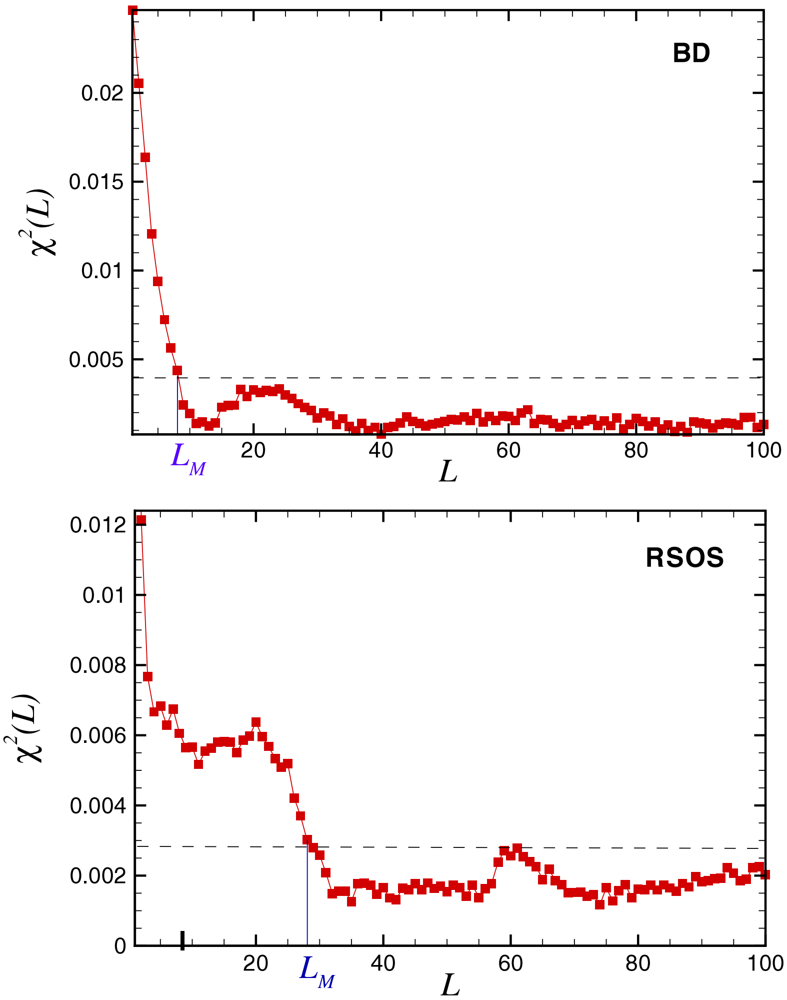

Figure 3. The χ^2 tests for estimating the Markov length scales of the BD and RSOS models, indicating that the Markov length scales are, respectively, 8 and 28 for the BD and RSOS models.

We define χ^2 by [23]

$$\chi^2 = \int \mathrm{d}h_3\, \mathrm{d}h_2\, \mathrm{d}h_1 [P(h_3, x_3; h_2, x_2; h_1, x_1) \\ - P_{\mathrm{Mar}}(h_3, x_3; h_2, x_2; h_1, x_1)]^2 / [\sigma_{3.\mathrm{joint}} + \sigma_{\mathrm{Mar}}], \tag{9}$$

where $\sigma_{3.\mathrm{joint}}$ and σ_{Mar} are the variances of $P(h_3, x_3; h_2, x_2; h_1, x_1)$ and $P_{\mathrm{Mar}}(h_3, x_3; h_2, x_2; h_1, x_1)$, respectively. To compute the Markov length scale, we also used the likelihood statistical analysis. In the absence of a prior constraint, the probability of the set of three-point joint PDFs is given by a product of Gaussian functions:

$$p(x_3 - x_1) = \Pi_{h_3,h_2,h_1} \frac{1}{\sqrt{(\sigma^2_{3.\mathrm{joint}} + \sigma^2_{\mathrm{Mar}})^2}} \\ \times \exp\left[\frac{[P(h_3, x_3; h_2, x_2; h_1, x_1) - P_{\mathrm{Mar}}(h_3, x_3; h_2, x_2; h_1, x_1)]^2}{2(\sigma^2_{3.\mathrm{joint}} + \sigma^2_{\mathrm{Mar}})}\right]. \tag{10}$$

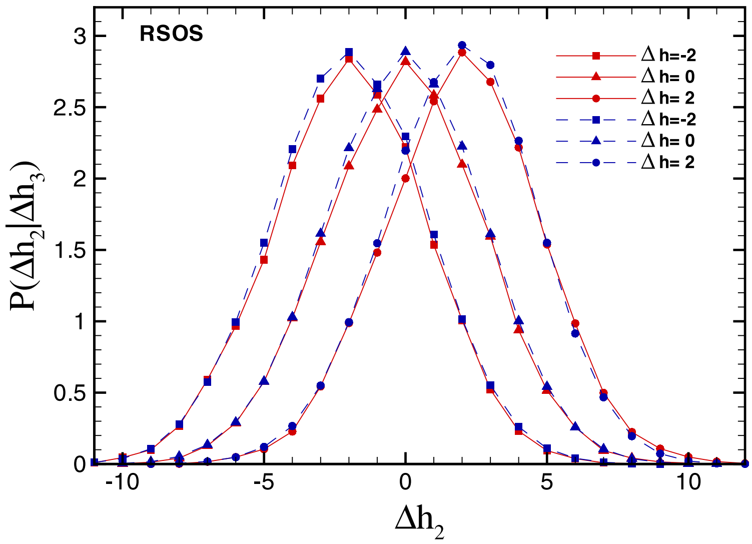

Figure 4. Typical test of the Chapman–Kolmogorov equation for several values, $\Delta h_1 = -2$, $\Delta h_1 = 0$, and $\Delta h_1 = 2$. The bold and dashed lines represent the left and right side of equation (5), respectively. The length scales Δx_1, Δx_2, and Δx_3 are $180, 320$, and 260, respectively. For clarity of presentation the PDFs have been shifted on the Δh-axis.

This probability distribution must be normalized. Evidently, when, for a set of values of the parameters, χ^2_ν attains its minimum, the probability is at its maximum value. Figure 3 shows the normalized χ^2_ν as a function of $L = x_3 - x_1$, where $\chi^2_\nu = \chi^2/N$, with N being the number of degrees of freedom. χ^2_ν has its minimum at $L \approx 40$ and $L \approx 80$ for the BD and RSOS models, respectively, hence yielding the corresponding Markov length scales L_{M}.

The process $\Delta h = h(x+1) - h(x)$ is also Markov. Using the method described above, one can show that Δh has a Markov length scale of 1 and 6 (in units of the lattice constant) for the BD and RSOS models, respectively. At this step we can check also the Markov nature of the height increments in scales, i.e., $\Delta h = h(x+\Delta x) - h(x)$. We checked the validity of the Chapman–Kolmogorov equation for several Δh_1 triplets by comparing the directly evaluated conditional probability distribution $P(\Delta h_2, \Delta x_2|\Delta h_1, \Delta x_1)$ with those calculated according to the right-hand side of equation (5). In figure 4 the directly computed and the integrated PDFs are superimposed, for the purpose of illustration, for the BD and RSOS models. The bold and dashed lines represent, respectively, the left and right sides of equation (5).

It is well known that the Chapman–Kolmogorov equation yields an equation for the evolution of the distribution function $P(\Delta h, \Delta x)$ across the scales Δx. The Chapman–Kolmogorov equation, when formulated in differential form, yields a master equation which takes on the form of a Fokker–Planck equation [5]:

$$\frac{\partial}{\partial x} P(\Delta h, \Delta x) = \left[-\frac{\partial}{\partial \Delta h} D^{(1)}(\Delta h, \Delta x) + \frac{\partial^2}{\partial \Delta h^2} D^{(2)}(\Delta h, \Delta x) \right] P(\Delta h, \Delta x). \tag{11}$$

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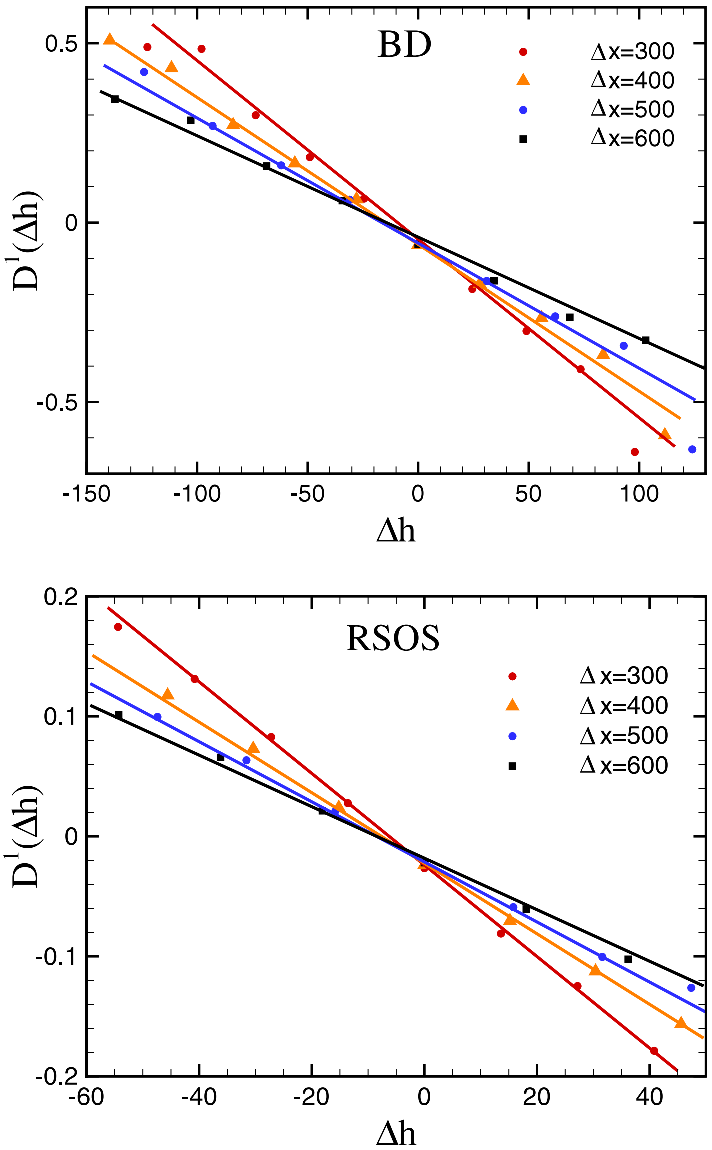

Figure 5. Comparing the drift coefficients of the BD (top) and RSOS models.

The drift and diffusion coefficients, $D^{(1)}(\Delta h, \Delta x)$ and $D^{(2)}(\Delta h, \Delta x)$, are estimated directly from the data and the moments $M^{(k)}$ of the conditional probability distributions:

$$D^{(k)}(\Delta h, \Delta x) = \frac{1}{k!} \lim\nolimits_{r \to 0} M^{(k)},$$
$$M^{(k)} = \frac{1}{r} \int \mathrm{d}h' (\Delta h' - \Delta h)^k P(\Delta h', \Delta x + r | \Delta h, \Delta x). \tag{12}$$

The coefficients $D^{(k)}(\Delta h, \Delta x)$ are known as the KM coefficients. According to the Pawula theorem [5], the KM expansion can be truncated after the second term, provided that the fourth-order coefficient, $D^{(4)}(\Delta h, \Delta x)$, vanishes [5]. The fourth-order coefficients $D^{(4)}$ in our analysis were found to be about $D^{(4)} \simeq 10^{-4} D^{(2)}$, for both models. Thus, in this approximation, we ignore the coefficients $D^{(k)}$ for $k \geq 3$. We note that the

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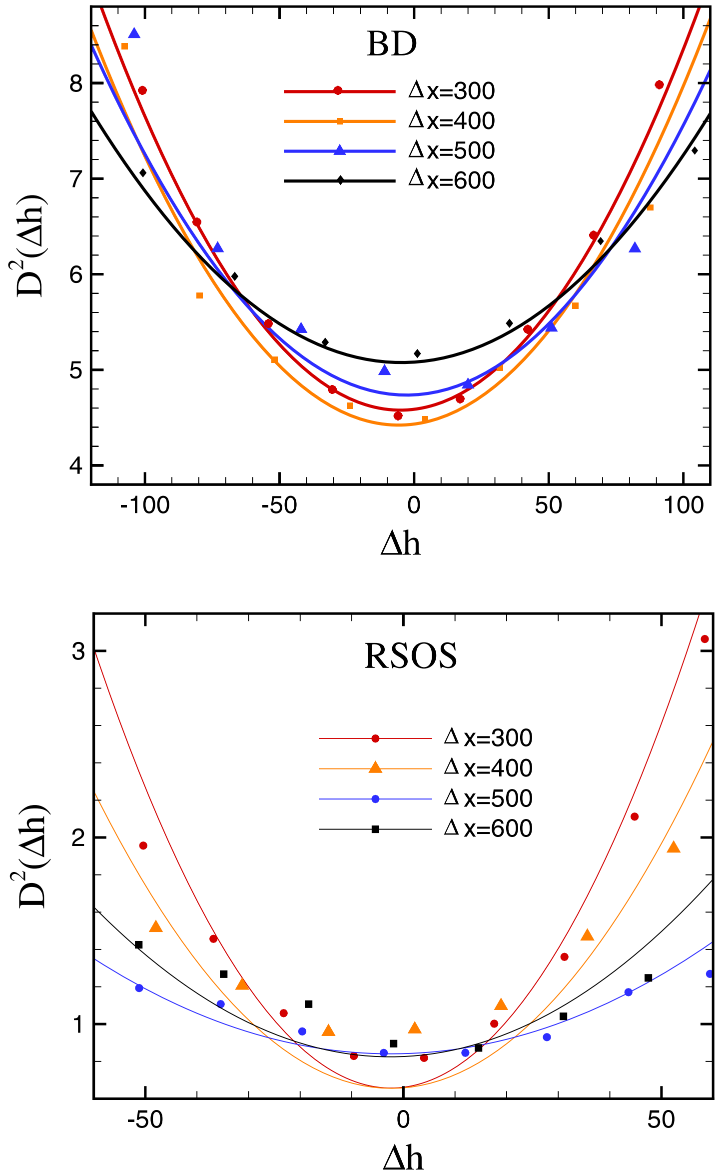

Figure 6. Comparing the diffusion coefficients of the BD (top) and RSOS models.

Fokker–Planck equation is equivalent to the following Langevin equation (using the Ito interpretation [5]):

$$\frac{\partial}{\partial \Delta x}\Delta h(\Delta x) = D^{(1)}(\Delta h, \Delta x) + \sqrt{D^{(2)}(\Delta h, \Delta x)}f(\Delta x), \tag{13}$$

where $f(\Delta x)$ is a random force, with zero mean and Gaussian statistics, δ-correlated in Δx, i.e., $\langle f(\Delta x)f(\Delta x')\rangle = 2\delta(\Delta x - \Delta x')$. Furthermore, given the last expression, it should be clear that we are able to separate the deterministic and the stochastic components of the surface height fluctuations, in terms of the coefficients $D^{(1)}$ and $D^{(2)}$.

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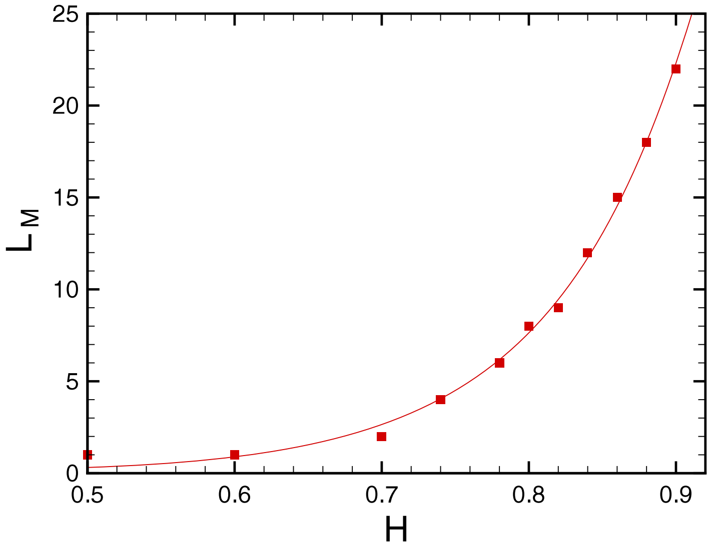

Figure 7. Markov length scale versus roughness or Hurst exponents.

3. The Kramers–Moyal coefficients of the BD and RSOS increments

Using the statistical parameters introduced in the previous sections, it is now possible to obtain some quantitative information about the BD and RSOS models. We computed the drift coefficient, $D^{(1)}(\Delta h)$, and the diffusion coefficient, $D^{(2)}(\Delta h)$; the results are displayed in figures 5 and 6. It turns out that the drift $D^{(1)}$ is a linear function of Δh, whereas the diffusion coefficient $D^{(2)}$ is a quadratic function of Δh. For large values of Δh, our estimates become poor and, thus, the uncertainty increases. From the analysis of the data set we obtain the following approximation for the BD model:

$$\begin{aligned} D^{(1)}(\Delta h, \Delta x) &= [-1.04(\Delta x)^{-1}]\Delta h, \\ D^{(2)}(\Delta h, \Delta x) &= (2.6 \times 10^{-4})(\Delta h)^2 + [(-1.6 \times 10^{-3})(\Delta x)^{0.5} + 0.062]\Delta h, \end{aligned} \tag{14}$$

and for the RSOS model, we find that

$$\begin{aligned} D^{(1)}(\Delta h, \Delta x) &= [-0.84(\Delta x)^{-1}]\Delta h, \\ D^{(2)}(\Delta h, \Delta x) &= (4.1 \times 10^{-4})(\Delta h)^2 + [(-2.4 \times 10^{-4})(\Delta x)^{0.5} + 0.012]\Delta h. \end{aligned} \tag{15}$$

Thus, apart from their Markov length scales being distinct for the BD and RSOS models, we see that the drift and diffusion coefficients of the two models are also distinct. The diffusion coefficient of the BD model is greater than that of the RSOS model. According to the Langevin equation, it is multiplied by the random white noise f, which means that the random part of the corresponding Langevin equation for BD model is stronger. This is related to the existence of jumps in the surface generated by the BD model.

4. Markov length scale and roughness exponent of the surface

In this section we wish to determine the relation between the roughness exponent of a rough surface and the Markov length scale L_{M}, and the consequence of the relation for

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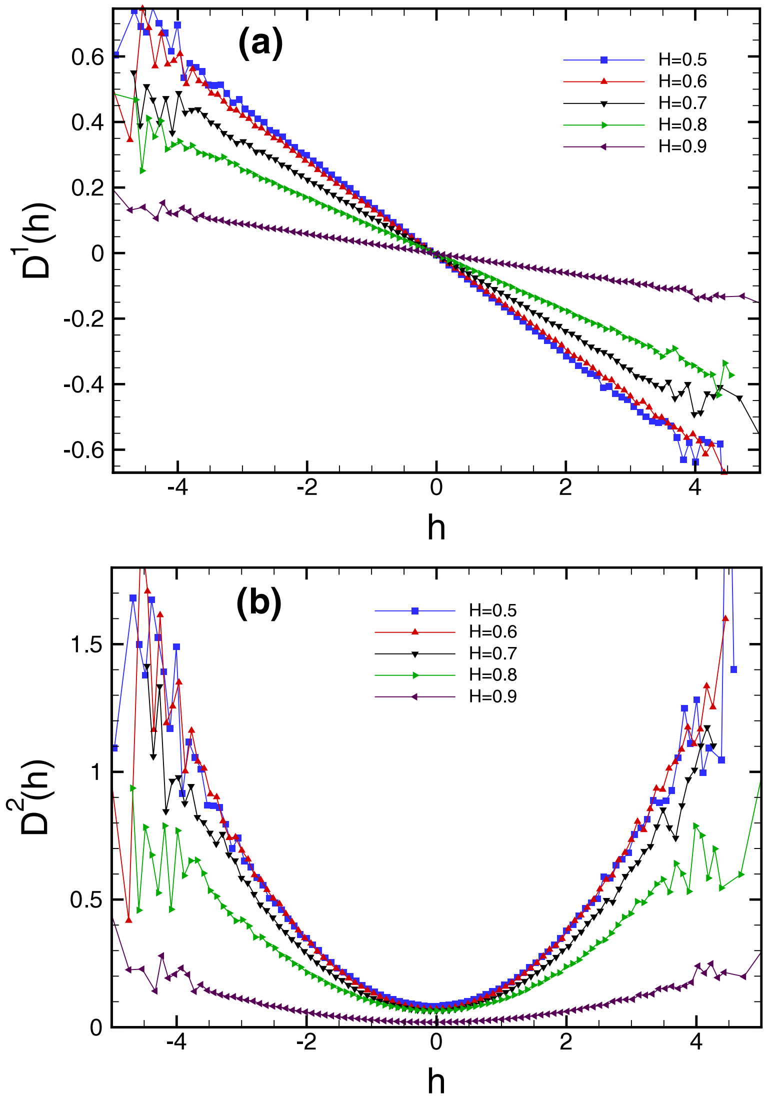

Figure 8. Comparing the drift and diffused coefficients for surfaces with different roughness or Hurst exponents.

the drift and diffusion coefficients. We generated a rough surface by using the Fourier filtering algorithm with various Hurst exponents H and unit roughness [31]. For $H < 1$ the roughness and Hurst exponents are equal. First, we calculate the dependence of the Markov length scale L_{M} on the Hurst exponent of the surface. The results are shown in figure 7. It is evident that L_{M} is an increasing function of roughness exponent H. In correlated data series, the height differences between the neighbors are small, which is due to the fact that such series have persistent nature. As the correlation or Hurst exponent increases, the height difference decreases. This means that data series have long memory. One can translate the memory to the physical meaning of the Markov length scale: the data with larger H also have long Markov length scale L_{M}. We note, however, that for a process with a given Hurst exponent one finds a unique L_{M}, whereas, in general, the opposite is not true. One may fit the functional dependence of L_{M} on H using different functions. The simplest functions are exponential and power-law functions. We obtain $L_{\mathrm{M}} = 0.01\exp(10.48H)$ and $L_{\mathrm{M}} = 56.58H^{8.94}$ as the candidates.

Moreover, the same effect can also be analyzed for the drift and diffusion coefficients. Figure 8(a) presents the calculated drift coefficient for the generated surfaces using several Hurst exponents. It is seen that the drift coefficient exhibits a linear dependence on H. Increasing the Hurst exponent results in a decreasing drift coefficient. We find that the drift coefficient behaves as $D^{(1)}(h,H) = -f_1(H)h$, where $f_1(H)$ is given by $f_1(H) = 0.255 + 1.810H - 1.643H^2$. The dependence of the diffusion coefficient of the generated rough surface on the Hurst exponents is shown in figure 8(b). A decreasing diffusion coefficient with increasing Hurst exponent is seen. The diffusion coefficients exhibit quadratic dependence on the height h given by $D^{(2)}(h,H) = f_2(H)h^2$, where $f_2(H)$ is fitted by $0.02 + 0.54H + 0.57H^2$.

In summary, we showed that the probability densities of the height increments in the BD and RSOS models satisfy a Fokker–Planck equation, which encodes the Markov property of these fluctuations in a necessary way. We computed the Kramers–Moyal coefficients for the field $\Delta h = h(x+\Delta x) - h(x)$, and determined their corresponding Langevin equations. We showed that the Markov length scales of the two models are different, and that they also have distinct KM coefficients. In addition, we investigated the dependence of the Markov Length scale on the roughness exponents of a rough surface.

Acknowledgment

We would like to thank M Sahimi for useful discussions and comments.

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