Multifractal expansions and kinetic surface roughening processes

A. Bershadskii
Post Office Box 39953, Ramat-Aviv 61398, Tel-Aviv, Israel

(Received 12 January 1998; revised manuscript received 27 March 1998)

An analytic continuation method has been developed to improve the multifractal analytic expansions approach to the kinetic surface roughening processes. An analytic result for the dependence of the roughness exponent H_q on the index q of the moments of the pair correlation function is obtained using this method. Application of the method to some geometrical models is discussed, and good agreement established with results of numerical simulations of the molecular beam epitaxy obtained by different authors.
[S1063-651X(98)11308-9]

PACS number(s): 81.15.−z, 68.55.−a, 05.40.+j

I. INTRODUCTION

Kinetic surface roughening has recently been of great interest to scientists owing to its relevance to a number of phenomena of practical importance, such as molecular beam epitaxy, formation of biological patterns, etc. (see, for reviews, Refs. [1–3] and references therein). The surface usually grows from a flat substrate and, due to presence of noisy excitations, becomes rough during its evolution. The generalized roughness exponents H_q are used to describe this multifractal process. They are introduced through the various moments of the height differences (the generalized height-height correlation functions)

$$c_q(r)=\frac{1}{N}\sum_{i=1}^{N}|h(x_i)-h(x_i+r)|^q\sim r^{qHq}, \tag{1}$$

where N is the number of points over which the average is taken, and the limit $r\to 0$ is considered. For a standard partition, $r\sim 1/N$. The authors of Ref. [4] assumed that, when evaluating Eq. (1), r and N may be related in a way different from $r\sim 1/N$. That is, $N\sim r^{-D_{\rm eff}}$ ($D_{\rm eff}$ could be considered here as a fractal dimension of the effective support of the process; for more details, see Sec. V). The choice of a particular partition has no effect on the H_q spectrum. However, $D_{\rm eff}$ enters the relation between H_q and the so-called generalized dimensions D_q. In Ref. [4], a partition of the interval [0,1] into N intervals with the measure

$$p_i(r)=\frac{|h(x_i)-h(x_i+r)|}{\sum_{j=1}^{N}|h(x_j)-h(x_j+r)|} \tag{2}$$

was introduced. This can be viewed as a probability measure, and one can construct the corresponding generating function

$$Z_q(r)=\sum_{i=1}^{N}p_i^q(r),$$

and introduce the corresponding spectrum D_q through the expression $Z_q(r)\sim r^{(q-1)D_q}$ in the limit $r\to 0$. Using this approach, the authors of Ref. [4] obtained the following relationships between D_q and H_q

$$(q-1)D_q=q(H_q-H_1)+(q-1)D_{\rm eff} \tag{3}$$

or

$$H_q=H_1+\frac{(q-1)(D_q-D_{\rm eff})}{q} \tag{4}$$

(generally $D_{\rm eff}$ can be different from D_0; see Sec. V). The simplest way to obtain an analytical representation for D_q [and then, using Eq. (4), for H_q] is to use a Maclaurin power series expansion in a vicinity of $q=0$. It is well known, however, that a linear approximation of the generalized dimension D_q is generally applicable in a narrow vicinity of the point $q=0$ only (see, for instance, Refs. [5–7] and references therein). On the other hand, a quantitative description of multifractals beyond the linear approximation of D_q is now possible due to the possibility of obtaining rather accurate numerical data. In the present paper we shall show that the concept of analytical continuation of standard thermodynamics quantities on a complex (temperature) plane can be adapted in the context of multifractal measures. This adaptation should then provide an improvement of the standard linear approximation of the generalized dimensions D_q. Then we apply this finite-temperature approximation to the kinetic growth processes using relationship (4).

II. THERMODYNAMIC INTERPRETATION OF MULTIFRACTALITY

Let us, first of all, recall a thermodynamic interpretation of multifractality (see, for instance, Refs. [8,9] and references therein). Suppose that the total volume of a sample consists of a d-dimensional cube of size L. We divide this volume into N boxes of linear size l [$N\sim(L/l)^d$]. We label each box by the index i, and construct for each box the measure function of a field $\mu(\mathbf{x},t)$,

$$\mu_i(l)=\int_{v_i}\mu(\mathbf{x})dv,$$

where v_i is volume of the ith box. Then the generalized dimension D_q can be introduced by the following scaling relationship (see, for instance, Refs. [8,9] and references therein):

$$D_q = \lim_{(l/L)\to 0} \frac{\ln Z(q)}{(q-1)\ln(l/L)},$$

where the partition function

$$Z(q) = \sum_i \mu_i^q .$$

This follows the scaling

$$Z(q) \sim (l/L)^{\tau(q),}$$

where

$$\tau(q) = D_q(q-1). \tag{5}$$

On the other hand, the partition function can be represented as follows

$$Z(q) \simeq \int \rho(\alpha)(l/L)^{q\alpha - f(\alpha)} d\alpha,$$

where α represents the singularity strength of the measure μ, and the $f(\alpha)$ singularity spectrum describes the statistical distribution of the singularity exponent α. If we cover the support of the measure μ with balls of size l, the number of such balls that scale like $(l/L)^\alpha$, for a given α, behaves like $N_\alpha(l/L) \sim (l/L)^{-f(\alpha)}$. In the limit $(l/L)\to 0$, the sum is dominated by the term $(l/L)^{\min_\alpha[q\alpha - f(\alpha)]}$. Then, from the definition of $\tau(q)$, one obtains

$$\tau(q) = \min_\alpha [q\alpha - f(\alpha)].$$

Thus $\tau(q)$ is obtained by Legendre transforming the $f(\alpha)$. When $f(\alpha)$ and $\tau(q)$ are smooth functions, this relationship can be rewritten in the following way

$$\tau(q) = q\alpha - f(\alpha), \quad \frac{df}{d\alpha} = q. \tag{6}$$

The thermodynamics interpretation of these relationships means that q can be interpreted with an inverse temperature $q = T^{-1}$, and the limit $(l/L)\to 0$ can be seen as the thermodynamic limit of infinite volume $[V = \ln(L/l)\to\infty]$. Then by identifying $\alpha_i = \ln \mu_i / \ln(L/l)$ to the energy E_i (per unit of volume) of a microstate i, one can rewrite the partition function under the familiar form

$$Z(q) = \sum_i \exp(-qE_i). \tag{7}$$

From the definition $f(\alpha) = \ln N_\alpha((l/L))/\ln(L/l)$, the singularity spectrum $f(\alpha)$ plays the role of the entropy (per unit of volume).

III. ANALYTIC CONTINUATION

Expansion of the entropy $f(\alpha(q))$ in a power series (the high-temperature expansion)

$$f(q) = f(0) + q\left(\frac{df}{dq}\right)_{q=0} + q^2 \frac{1}{2}\left(\frac{d^2 f}{dq^2}\right)_{q=0} + \cdots \tag{8}$$

in the first order approximation is

$$f(q) \sim f(0) + q^2 \frac{1}{2}\left(\frac{d^2 f}{dq^2}\right), \tag{9}$$

since generally $(df/dq)_{q=0} = 0$ [see Eq. (6)].

The generalized dimension spectrum corresponding to Eq. (9) is (see, for instance, Ref. [7] and references therein)

$$D_q \sim D_0 + aq, \tag{10}$$

where a is some constant.

It is known that entropy can have singularities in a complex temperature plane (see, for instance, Refs. [10–12] and references therein). If the multifractal entropy $f(q)$ has singularities on the complex q plane, then the radius of convergence of the *real* Maclaurin series expansion (8) is determined by the distance from the point $q=0$ to a nearest singularity of $f(q)$ in the complex plane. One could then use the standard procedure of analytic continuation to obtain a power series expansion beyond the circle of convergence of expansion (8)

$$f(q) = f(q_0) + (q-q_0)\left(\frac{df}{dq}\right)_{q=q_0} + (q-q_0)^2 \frac{1}{2}\left(\frac{d^2 f}{dq^2}\right)_{q=q_0} + \cdots , \tag{11}$$

where q_0 is modulus of the complex-temperature singularity nearest to the point $q=0$.

Let us rewrite Eq. (11) in a form similar to Eq. (8):

$$f(q) = A + Bq + \cdots , \tag{12}$$

where

$$A = f(q_0) - q_0\left(\frac{df}{dq}\right)_{q=q_0}, \quad B = \left(\frac{df}{dq}\right)_{q=q_0}. \tag{13}$$

Using Eq. (6) it is easy to show that $\tau(q)$ corresponding to Eq. (12) has the form

$$\tau_q = -A + (C-B)q + Bq \ln q + \cdots , \tag{14}$$

where C is some constant $(q>0)$. One can see that an additional ''logarithmic'' term appears in the finite-temperature (FT) expansion (14).

Using the condition $\tau(1)=0$ [see Eq. (5)], we obtain, from Eq. (14),

$$A = C - B, \tag{15}$$

and then we can rewrite Eq. (14) as

$$\tau_q = A(q-1) + Bq \ln q + \cdots . \tag{16}$$

It follows from Eqs. (5) and (16) that

$$D_q = A + B\frac{q \ln q}{(q-1)} + \cdots . \tag{17}$$

IV. AN EXAMPLE OF THE MULTIFRACTAL COMPLEX-TEMPERATURE SINGULARITIES

Let us consider the multifractality of a strange attractor of the baker map for which analytical results are available. This transformation is defined as

$$\begin{aligned} [x_{n+1},y_{n+1}] &= [l_1 x_n, y_n/\eta], \quad y_n<\eta, \\ [x_{n+1},y_{n+1}] &= [\tfrac{1}{2}+l_2 x_n, (y_n-\eta)/(1-\eta)], \quad y_n>\eta. \end{aligned} \tag{18}$$

The attractor of this map consists of an infinite number of lines in the y direction which intersect a horizontal line in two interwoven Cantor sets. These sets are characterized by contraction rates l_1 and l_2, and are visited with probabilities η and $1-\eta$, respectively. The dimension spectrum D_q of the cross section follows from

$$\frac{\eta^q}{l_1^{(q-1)D_q}}+\frac{(1-\eta)^q}{l_2^{(q-1)D_q}}=1. \tag{19}$$

If we introduce the definitions $\eta^q=a$, $(1-\eta)^q=b, l_2^{(q-1)D_q}=G$, and $\ln l_1/\ln l_2=k$, then we can rewrite Eq. (19) as

$$G^k-bG^{(k-1)}-a=0. \tag{20}$$

From this equation one obtains

$$\frac{dG}{dq}=\frac{da/dq+(db/dq)G^{(k-1)}}{kG^{(k-1)}-b(k-1)G^{(k-2)}}.$$

dG/dq has a singularity when $G=b(k-1)/k$. Substituting this relationship into Eq. (20) we obtain values of q for which dG/dq is singular:

$$q_0=\frac{\ln c}{\ln[\eta/(1-\eta)^k]}, \tag{21}$$

where

$$c=-\frac{(k-1)^{(k-1)}}{k^k}. \tag{22}$$

Since

$$f(q)=D_q+q(q-1)\frac{dD_q}{dq}, \tag{23}$$

the entropy $f(q)$ of the baker map also has singularities at the same values of $q=q_0$.

The constant c is positive when $(k-1)=-1/n$, where $n=3,5,7,\ldots$. For these specific values of k, corresponding values of q_0 are real numbers, and dG/dq [and, consequently, $f(q)$] has singularities on the real axis. In the general case, however, the values of q_0 are complex.

V. APPLICATIONS

To apply the FT approximation to real systems, let us start from simple geometrical examples. In Apollonian packings, for instance, nonoverlapping circles of very different radii are used to tile the region bounded by three touching circles [13]. In Ref. [13], a multifractal analysis of the Apollonian packings was carried out using the scaling behavior of the density distribution of the points where the circles touch each other. The set of these points provides the basis for an appropriate measure. The generalized dimensions D_q associated with the multifractal scaling of the distribution of touching points in an Apollonian packing were calculated in Ref. [13]. Figure 1 (adapted from Ref. [13]) shows a set of D_q is obtained for the Apollonian packing. We chose the axes so that a straight line in this figure corresponds to the representation (17). One can see that in this case $A=D_0$. Another interesting packing analyzed in Ref. [13] is the so-called space-filling bearings [14]. In the space-filling bearings model, cylinders having parallel axes are arranged in space in such a manner that in the limiting case the cylinders to fill the space completely, and, in addition, they can roll on each other without slipping. In Ref. [13], a multifractal analysis of this system was also carried out analogously to the Apollonian packings analysis. The generalized dimensions obtained for a space-filling bearings model are represented in Fig. 2 (adapted from Ref. [13]). Again, we chose the axes so that the representation (17) corresponds to straight lines. One can see that there are two regions of q where a representation like Eq. (17) gives a good approximation of the data. One region (for $q<1$) corresponds to $A=D_0$, while another region corresponds to $A=D_{\text{eff}}<D_0$. One can interpret the last situation as a self-organization process with a new effective capacity dimension $D_{\text{eff}}<D_0$.

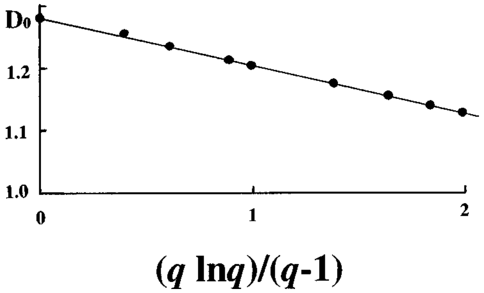

FIG. 1. Spectrum of generalized dimensions D_q (adapted from Ref. [13]) for an Apollonian packing. The straight line is drawn for comparison with the FT approximation (17).

Now we can consider the kinetic surface roughening process, taking into account that $A=D_{\text{eff}}$ in representation (17) can be, generally, different from D_0. Then, if we substitute Eq. (17) into Eq. (4) (with $A=D_{\text{eff}}$), we obtain the finite-

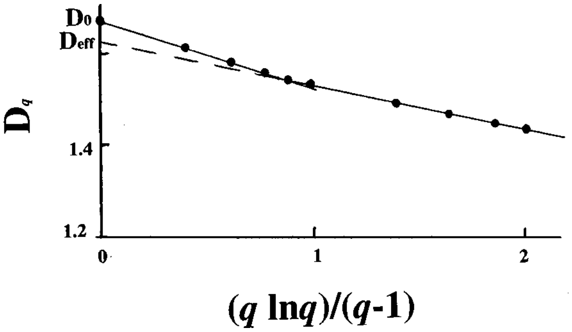

FIG. 2. Spectrum of generalized dimensions D_q (adapted from Ref. [13]) for space-filling bearings. The straight lines are drawn for comparison with the FT approximation (17) for two regions of q.

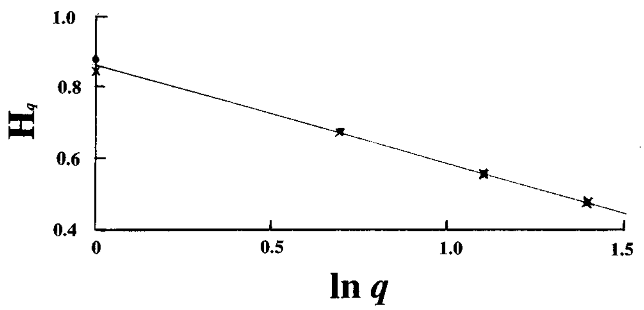

FIG. 3. Generalized roughness exponents H_q against $\ln q$ for molecular beam epitaxy [data taken from Refs. [16] (full circles) and from [17] (crosses)]. The straight line is drawn for comparison with the FT approximation (24).

temperature approximation for the generalized roughness exponents

$$H_q \sim H_1 + B \ln q. \tag{24}$$

The kinetic surface roughening models based on equations of the Langevin type turned out to be very useful to study the molecular beam epitaxy [15–17]. Figure 3 shows the data (H_q) obtained in recent numerical simulations of this process [Refs. [16] (full circles) and [17] (Lai–Das Sarma model, crosses)]. The straight line is drawn for comparison with Eq. (24) (here $B<0$). One can see that the FT approximation (24) is in good agreement with these data.

The question of location the nearest (to point $q=0$) singularities in the complex-q plane for these processes is open. Therefore we cannot give *a priori* estimates of the radii of convergence of the FT approximation for these processes. On the other hand, to understand reasons for the ''logarithmic'' approximation (24), it is useful to recall the recently suggested (and argued) connection between height fluctuations in epitaxial growth models and intermittent fluctuations in fluid turbulence [16] (see also Ref. [18]). Indeed, it was shown in a recent paper [19] that a *stretched exponential* distribution of the local velocity gradient [20] is a reason for the appearance of the logarithmic term in the generalized scaling laws. On the other hand, the numerical simulations performed in Refs. [16,17] give evidence that the distribution of step sizes at the epitaxial growth has the form of a stretched exponential as well.

Moreover, the logarithmic corrections behind the linear (''parabolic'') approximation [7] can also appear in thermodynamics approaches considering the real temperatures only (see, for instance, a constant-specific-heat approach to the multifractality of mesoscopic systems [21]). In the last case, however, the analytic character of the logarithmic correction is not so clear as for the approach considered in the present paper. To obtain *a priori* criteria for the applicability of the different thermodynamic approaches to concrete physical systems one should stay a step behind the framework of the thermodynamic interpretation. This seems to be an interesting problem for future investigations.

---

[1] T. Vicsek, *Fractal Growth Phenomena* (World Scientific, Singapore, 1988).
[2] A.-L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, Cambridge, 1995).
[3] J. Krug, Adv. Phys. **46**, 139 (1997).
[4] A.-L. Barabasi, P. Szepfalusy, and T. Vicsek, Physica A **178**, 17 (1991).
[5] T. C. Halsey *et al.*, Phys. Rev. A **33**, 1141 (1986).
[6] G. Paladin and A. Vulpiani, Phys. Rep. **156**, 147 (1987).
[7] M. Janssen, Int. J. Mod. Phys. B **8**, 943 (1994).
[8] H. E. Stanley and P. Meakin, Nature (London) **335**, 405 (1988).
[9] A. Arneodo, E. Bacry, and J. F. Muzy, Physica A **213**, 232 (1995).
[10] M. Fisher, *The Nature of Critical Points*, Lectures in Theoretical Physics Vol. 12C (University of Colorado Press, Boulder, 1965), p. 1.
[11] V. Matveev and R. Shrock, J. Phys. A **28**, 1557 (1995).
[12] C. Itzykson, R. B. Pearson, and J. B. Zuber, Nucl. Phys. B **220**, 415 (1983).
[13] S. S. Manna and T. Vicsek, J. Stat. Phys. **64**, 525 (1991).
[14] H. J. Herrmann, in *Correlations and Connectivity*, edited by H. E. Stanley and N. Ostrowski (Kluwer, Dordrecht, 1990).
[15] D. E. Wolf and J. Villain, Europhys. Lett. **13**, 389 (1990).
[16] J. Krug, Phys. Rev. Lett. **72**, 2907 (1994).
[17] S. Das Sarma, C. J. Lanczyski, R. Kotlyar, and S. V. Ghaisas, Phys. Rev. E **53**, 359 (1996).
[18] A. Kundagrami, C. Dasgupta, P. Punyindu, and S. Das Sarma, Phys. Rev. E **57**, R3703 (1998).
[19] A. Bershadskii, Europhys. Lett. **39**, 587 (1997).
[20] P. Kailasnath and K. R. Sreenivasan, Phys. Rev. Lett. **68**, 2766 (1992).
[21] A. Bershadskii, Mod. Phys. Lett. B **12**, 11 (1998).