Discontinuities in self-affine functions lead to multiaffinity

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Many systems of both theoretical and applied interest display multiaffine scaling at small length or time scales. We demonstrate analytically and numerically that when vertical discontinuities are introduced into a self-affine function, the function becomes multiaffine. The discontinuities may correspond to surface overhangs or some source of discontinuous noise. Two functions are numerically examined with different distributions of discontinuities. The multiaffinity is shown to arise simply from the function of discontinuities, and the analytic scaling form at small scales for the function of discontinuities is derived and compared to numerical results.

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Self-affine and multiaffine functions are used to model a wide range of natural and artificial phenomena, including the structure of rough surfaces of hard [1-3] and soft [4] materials, clouds [5], and such diverse phenomena as financial and stock-market returns [6,7], and geological topography [8]. Recently, an extensive scaling analysis of surfactant templated hydrogel surfaces as measured by atomic force microscopy (AFM) was performed [4]. This analysis indicated that the hydrogel surfaces were self-affine; however, a later numerical study of a frustrated spring-network model of cross-linked hydrogels [9] indicated multiaffine scaling. Reconciliation of these two observed behaviors led to an interesting and universal conclusion: introduction of vertical discontinuities into a self-affine surface leads to multiaffine scaling, or, more generally, discontinuities in an otherwise self-affine function lead to multiaffine scaling. To our knowledge, this has not previously been reported in the literature, most likely because correlations are usually calculated only for the second power of the increments, in which case the function constructed only of discontinuities resembles a random walk on all scales $(\alpha_{q=2} = \frac{1}{2})$. Here, we provide a discussion which explains this source of multiaffine behavior, and we present both numerical and analytic results.

Consider a one-dimensional, real, single-valued function, z(x), where x is a real number on the interval, $x \in [0,1]$. The generalized correlation function [1-3,8-11] for this surface is

$$C_{\alpha}(r) = \langle |z(x+r) - z(x)|^{q} \rangle, \tag{1}$$

where $\langle \cdots \rangle$ denotes an average over all x values, $|r| < \frac{1}{2}$, and q is a positive, nonzero real number. Without loss of generality, we may assume that r is positive, since $C_q(r) = C_q(-r)$ for any real function z(x).

Often, $C_q(r)$ will display power-law behavior for $r \ll r_x$ and will display a constant value for $r \gg r_x$, where r_x is some crossover scale between the two behaviors. Functions displaying power-law correlations, $C_q(r) = A_q r^{q\alpha_q}$, fall into one

of two categories: q-independent scaling, $\alpha_q = \alpha$, called self-affine scaling, and q-dependent scaling, called multiaffine scaling [1–3,8,10,11].

By introducing discontinuities into a self-affine function, we can cause the function to become multiaffine. Consider the function z(x), which is self-affine for all r. For the numerical results, self-affine functions were generated using the method of Ref. [12]. We introduce a finite number N of discontinuities into the function z(x) such that the new function is

$$z'(x) = \left\{ \sum_{i=1}^{N} \delta_i \Theta(x - x_i) \right\} + z(x), \tag{2}$$

where *i* indexes the discontinuities, δ_i is the magnitude of the discontinuity at $x=x_i$, and $\Theta(y)$ is a step function which is zero for y < 0 and 1 for $y \ge 0$. Without loss of generality, we can assume an order to the set $\{x_i\}$ such that $x_{i-1} < x_i$ and $x_0 = 0$.

Physically, z'(x) can be thought of as describing a system with jumps between regions with self-affine scaling, such as for the spring-network model of Ref. [9], the deposition of a very thin self-affine film onto a stepped surface, a surface with overhangs, or any spatial or temporal series containing discontinuities. A typical stochastic realization of z'(x) with equally spaced x_i is shown in Fig. 1(a), and the corresponding generalized correlation function, $C_q(r)$, is shown in Fig. 1(b). Figure 2 shows a similar plot, but the discontinuity positions x_i are chosen randomly and uniformly on the interval (0,1). The number of discontinuities, N, is the same for both Figs. 1 and 2. For length scales $r \ge 1/N$, the stepped function, $z_{\Theta} \equiv z'(x) - z(x)$, is expected to be simply a random walk with α_a =0.5, but this is not obvious in the numerical data because of the relatively small number of discontinuities in the x interval.

From examination of the numerical results in Figs. 1 and 2 it is obvious that the multiaffinity is caused by the stepped function, $z_{\Theta}(x)$, and the generalized correlation function of $z_{\Theta}(x)$ can be analytically calculated for $r \ll 1/N$,

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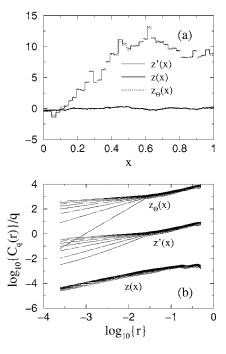


FIG. 1. Multiaffine function generated from Eq. (2) with discontinuities evenly spaced in x. The magnitudes of the discontinuities, δ_i , are drawn independently from a Gaussian distribution with standard deviation 1.0 and mean 0, and N=41. The self-affine function z(x) has α =0.75. (a) The function, z'(x), and related functions. (b) $C_q(r)$ for each function shown in (a) as labeled in the plot. The correlation functions for $z_{\Theta}(x)$ and z(x) have been displaced up by three and down by two units, respectively, for graphical clarity. No graphical distinction is made between curves with different q, but $q \in [0.5, 4.0]$ in steps of 0.5, and for the curves shown here, $C_q(r) > C_p(r)$ when q > p. At r = 1/N, there is a crossover between the self-affine and multiaffine behaviors.

$$C_{q}(r) = \int_{0}^{1} \left| \sum_{i=1}^{N} \delta_{i} \{ \Theta(x + r - x_{i}) - \Theta(x - x_{i}) \} \right|^{q} dx.$$
 (3)

For $r \le 1/N$, $\Theta(x+r-x_i)-\Theta(x-x_i)$, is either 1 $(x_i-r \le x < x_i)$ or 0 (otherwise), and thus, in the integration range $x=x_i-r$ to $x=x_i$, only one of the N discontinuities has a nonzero contribution to the integral, provided that r is sufficiently small. Equation (3) thus reduces to

$$C_q(r) = r \sum_{i=1}^{N} |\delta_i|^q.$$
 (4)

For comparison with Figs. 1 and 2,

$$\frac{1}{q}\log_{10}\{C_q(r)\} = \frac{1}{q}\log_{10}\{r\} + \frac{1}{q}\log_{10}\left\{\sum_{i=1}^{N} |\delta_i|^q\right\}, \quad (5)$$

and thus, $\alpha_q = q^{-1}$ and $\log_{10}\{A_q\} = \log_{10}\{N\langle |\delta_i|^q\rangle\}$ in the small r limit. See Fig. 3. Note that the general form is independent of the x_i distribution and depends on the δ_i distribution only through $\langle |\delta_i|^q\rangle$.

Having derived the small-r scaling behavior for the stepped function, $z_{\Theta}(x)$, it remains to be shown how this multiaffine stepped function influences the multiaffinity of

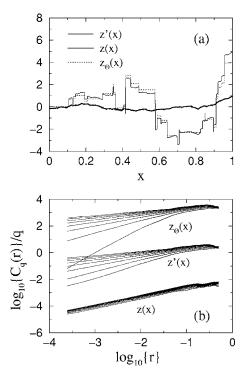


FIG. 2. Multiaffine function generated from Eq. (2) with discontinuities randomly spaced in x. All parameters are the same as in Fig. 1. (a) The function, z'(x), and related functions. (b) $C_q(r)$ for each function shown in (a) as labeled in the plot. The crossover between self-affine and multiaffine behaviors is the same as in Fig. 1, but the crossover region is much broader than in Fig. 1.

the complete or mixed function, z'(x). Consider the generalized correlation function for the sum of the two functions,

$$C_{q}(r) = \langle |\Delta_{\Theta}^{r}(x) + \Delta_{z}^{r}(x)|^{q} \rangle, \tag{6}$$

where $\Delta_{\Theta}^{r}(x) = z_{\Theta}(x+r) - z_{\Theta}(x)$ and $\Delta_{z}^{r}(x) = z(x+r) - z(x)$. The two extremes of $\langle |z(x)| \rangle \ll \langle |z_{\Theta}(x)| \rangle$ and $\langle |z_{\Theta}(x)| \rangle \ll \langle |z(x)| \rangle$ should behave as multiaffine and self-affine functions, respectively, but for intermediate mixed functions, the behavior is more complex. For the numerical results shown in Fig. 4, two asymptotic scaling regimes are seen. For large q, the mixed function tends towards multiaffine behavior with $\alpha_{q}=1/q$, and for small q, the mixed function tends towards self-affine behavior with $\alpha_{q}=\alpha$.

We can derive the two asymptotic scaling behaviors for the mixed function by first considering that for $r \le 1/N$,

$$C_{q}(r) = \langle \left| \Delta_{\Theta}^{r}(x) + \Delta_{z}^{r}(x) \right|^{q} \rangle$$

$$= \int_{0}^{1} \left| \Delta_{z}^{r}(x) \right|^{q} \left| \frac{\Delta_{\Theta}^{r}(x)}{\Delta_{z}^{r}(x)} + 1 \right|^{q} dx$$

$$= \sum_{i=1}^{N} \int_{x_{i-1}}^{x_{i-r}} \left| \Delta_{z}^{r}(x) \right|^{q} dx$$

$$+ \sum_{i=1}^{N} \int_{x_{i-r}}^{x_{i}} \left| \Delta_{z}^{r}(x) \right|^{q} \left| \frac{\delta_{i}}{\Delta_{z}^{r}(x)} + 1 \right|^{q} dx, \tag{7}$$

by noticing that $\Delta_{\Theta}^{r}(x)=0$ or δ_{i} in the interval $x \in (x_{i-1},x_{i}]$.

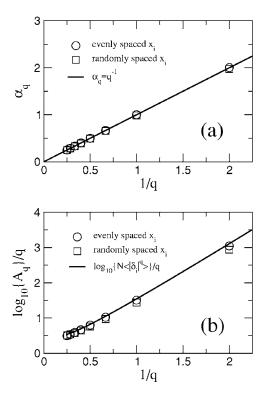


FIG. 3. Small r scaling behavior for stepped functions, $z_{\Theta}(x)$, shown in Fig. 1(b) and Fig. 2(b). (a) The multiaffine scaling exponent. The solid line indicates the analytic solution from Eq. (5). (b) The multiaffine scaling prefactor. The solid line indicates the analytic solution from Eq. (5).

As $q \to 0$, $|[\delta_i/\Delta_z^r(x)]+1|^q \approx 1$, and as $q \gg 1$, $|[\delta_i/\Delta_z^r(x)]+1|^q \approx |[\delta_i/\Delta_z^r(x)]|^q$. Note that this approximation is valid, because $[\delta_i/\Delta_z^r(x)] \gg 1$ when r is small. This gives the following approximations for the two asymptotic regimes, when $r \ll 1/N$:

$$C_q(r) \approx \begin{cases} \langle |\Delta_z^r(x)|^q \rangle = A_q r^{q\alpha} & q \leq 1 \\ A_q r^{q\alpha} + rN\langle |\delta_i|^q \rangle & q \geq 1, \end{cases} \tag{8}$$

where the additional approximation $\int_{x_{i-1}}^{x_i-r} \cdots dx \approx \int_{x_{i-1}}^{x_i} \cdots dx$ is made, which is valid when $r \leq 1$.

For large q, the scaling may resemble either self-affine scaling or multiaffine scaling, depending on the exact behavior of A_q for z(x) and the behavior of $\langle |\delta_i|^q \rangle$; however, for small q, the behavior will always resemble self-affine scaling, provided, of course, that the signal strength of z(x) is sufficiently large compared to the stepped function signal strength to be numerically noticeable. For the mixed functions examined in Fig. 4, self-affine scaling is seen for small q and multiaffine scaling with $\alpha_q = 1/q$ is seen for large q, but this is not a universal outcome as indicated in Eq. (8).

The scaling behavior of a self-affine function with vertical

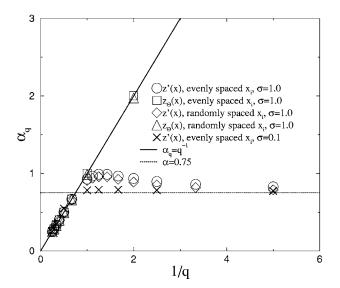


FIG. 4. Dependence of α_q on q and the relative magnitude of the stepped function. The distribution of the discontinuities, δ_i , is Gaussian with mean zero and standard deviation σ , and all parameters are the same as in Figs. 1 and 2 unless otherwise indicated. The lines indicate the two asymptotic behaviors, $\alpha_q = 1/q$ when z(x) = 0 and $\alpha_q = 0.75$ when $z_{\Theta}(x) = 0$. The data indicated by the symbols are each taken from a single realization of the function, and one can see that the distribution of the discontinuities, x_i , has no effect on α_q .

discontinuities was investigated numerically and analytically, and it was shown that the function of discontinuities (the stepped function) was the source of the multiaffine behavior. It was further shown numerically and analytically, that the general form for the scaling of the stepped function at small length scales depends on the distribution of discontinuities only through $\langle |\delta_i|^q \rangle$. Two asymptotic scaling behaviors were derived for the self-affine function with discontinuities, and for the numerical results shown here, self-affine scaling is seen for small q and multiaffine scaling with α_q =1/q is seen for large q. The large-q asymptotic behavior is not universal and depends on the detailed q dependence of the mixed function.

These results suggest the need to further study scaling and universality for a variety of systems where vertical discontinuities are known or are expected to exist. Such systems include many thin film deposition models and deposition processes onto stepped surfaces. For these processes, the deposition time should have a large effect on the multiaffine scaling behavior.

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- [1] A. L. Barabási, R. Bourbonnais, M. Jensen, J. Kertész, T. Vicsek, and Y. C. Zhang, Phys. Rev. A 45, R6951 (1992).
- [2] S. Das Sarma, C. J. Lanczycki, R. Kotlyar, and S. V. Ghaisas, Phys. Rev. E 53, 359 (1996).
- [3] C. V. Dharmadhikari, R. B. Kshirsagar, and S. V. Ghaisas, Europhys. Lett. 45, 215 (1999).
- [4] M. Chakrapani, S. J. Mitchell, D. H. Van Winkle, and P. A. Rikvold, J. Colloid Interface Sci. 258, 186 (2003).
- [5] K. Ivanova, M. Ausloos, E. E. Clothiaux, and T. P. Ackerman, Europhys. Lett. 52, 40 (2000).

- [6] N. Vandewalle and M. Ausloos, Eur. Phys. J. B 4, 257 (1998).
- [7] K. Ivanova and M. Ausloos, Eur. Phys. J. B 8, 665 (1999).
- [8] K. Kim and Y. S. Kong, J. Korean Phys. Soc. 36, 245 (2000).
- [9] G. M. Buendia, S. J. Mitchell, and P. A. Rikvold, Phys. Rev. E 66, 046119 (2002).
- [10] A. L. Barabási, P. Szépfalusy, and T. Vicsek, Physica A 178, 17 (1991).
- [11] A. L. Barabási and T. Vicsek, Phys. Rev. A 44, 2730 (1991).
- [12] R. Voss, in *Fundamental Algorithms in Computer Graphics*, edited by R. Earnshaw (Springer-Verlag, Berlin, 1985).