Vertical Discontinuities in Self-Affine Surfaces Lead to Multi-affinity

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Many systems of both theoretical and applied interest display multi-affine scaling at small length scales. Recently, an extensive scaling analysis of surfactant templated hydrogel surfaces as measured by atomic force microscopy (AFM) was performed. 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 indicated multi-affine 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 multi-affine scaling. To our knowledge, this has not previously been reported in the literature, most likely because height-height correlations are usually calculated for the second power of the height increments, in which case the surface constructed only of discontinuities resembles a random walk on all length scales. Here, we provide a discussion which explains this source of multi-affine behavior, and we present both numerical and analytic results.

Consider a one-dimensional, real, single-valued surface, z(x), where x is a real number on the interval, x ∈ [0, 1]. The generalized height-height correlation function for this surface is

$$C_q(r) = \langle \left| z(x+r) - z(x) \right|^q \rangle,$$

where \langle \cdots \rangle denotes an average over all x values, \left| r \right| < 1/2, and q is a positive, non-zero real number. Without loss of generality, we may assume that r is positive, since C_q(r) = C_q(-r) for any 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 cross-over length scale between the two behaviors. Surfaces displaying power-law correlations, C_q(r) = A_q r^{\alpha_q}, fall into one of two categories: q-independent scaling, \alpha_q = \alpha, called self-affine scaling, and q-dependent scaling, called multi-affine scaling.

By introducing vertical discontinuities into a self-affine surface, we can cause the surface to become multi-affine. Consider the function z(x), which is self-affine for all r \ll r_x. For the numerical results, self-affine surfaces were generated using the method of Ref. 8. We introduce a finite number, N, of vertical discontinuities into the function z(x) such that the new surface is

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

where \delta_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 \geq 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 overhangs between regions with self-affine scaling, such as for the spring-network model of Ref. 8, or the deposition of a very thin self-affine film onto a stepped surface. A typical stochastic realization of z'(x) with equally spaced x_i is shown in Fig. 1(a), and the corresponding generalized height-height correlation function, C_q(r), is shown in Fig. 1(b). Figure 1 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 Fig. 1 and Fig. 2. For length scales r \gg r_x, the stepped surface, z_\Theta \equiv z'(x) - z(x), is expected to be simply a random walk in height with \alpha_q = 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 multi-affinity is caused by the stepped surface, z_\Theta(x), and the generalized height-height correlation function of z_\Theta(x) can be analytically calculated for r \ll r_x, where r is also much smaller than the smallest x separation between discontinuities for f-
The argument, \( \Theta(x + r - x_i) - \Theta(x - x_i) \), is either 1 \((x_i - r \leq x < x_i)\) 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 non-zero contribution to the integral. Equation (3) thus reduces to

\[
C_q(r) = \frac{1}{q} \log_{10}\left\{ C_q(r) \right\} = \frac{1}{q} \log_{10}\left\{ \sum_{i=1}^{N} \delta_i \sum_{i=1}^{N} \delta_i \right\} = \frac{1}{q} \log_{10} \left\{ \sum_{i=1}^{N} |\delta_i|^q \right\} ,
\]

and thus, \( \alpha_q = q^{-1} \) and \( \log_{10}(A_q) = \log_{10} \left\{ N \log_{10}(\sum_{i=1}^{N} |\delta_i|^q) \right\} \).

For comparison with Figs. 1 and 2,

\[
C_q(r) = \left\langle |\Delta_\Theta(x) + \Delta_\Phi(x)|^q \right\rangle ,
\]

where \( \Delta_\Theta(x) = z_\Theta(x + r) - z_\Theta(x) \) and \( \Delta_\Phi(x) = z(x + r) - z(x) \). The two extremes of \( \left\langle |z(x)| \right\rangle \ll \left\langle \langle z_\Theta(x) \rangle \right\rangle \) and \( \left\langle |z(x)| \right\rangle \ll \left\langle \langle z_\Phi(x) \rangle \right\rangle \) should behave as multi-affine and self-affine surfaces, respectively, but for intermediate mixed surfaces, the behavior is more complex. For the numerical results shown in Fig. 3, two asymptotic scaling regimes are seen. For large \( q \), the mixed surface tends towards multi-affine behavior with \( \alpha_q = 1/q \), and for small
with \( \alpha \) indicates the analytic solution from Eq. (5).

Eq. (5). (b) The multi-affine scaling prefactor. The solid line indicates the analytic solution from Fig. 1(b) and Fig. 2(b). (a) The multi-affine scaling behavior for stepped surfaces, \( z_\delta(x) \), shown in Fig. 3(b) and Fig. 3(b). (a) The multi-affine scaling exponent. The solid line indicates the analytic solution from Eq. (3).

By noticing that \( \Delta r \) the mixed surface 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 \( r \ll r_x \)

\[
C_q(r) = \langle |\Delta_\delta'(x)|^q \rangle = \langle |\Delta_\delta(x)|^q \rangle \frac{\delta}{\Delta_\delta(x)} + 1^q \approx \langle |\Delta_\delta(x)|^q \rangle \frac{\delta}{\Delta_\delta(x)} + 1^q \approx \langle |\Delta_\delta'(x)|^q \rangle \frac{\delta}{\Delta_\delta(x)} + 1^q dx .
\]

By noticing that \( \Delta_\delta(x) = 0 \) or \( \delta_i \) in the interval \( x \in (x_{i-1}, x_i) \),

\[
C_q(r) = \sum_{i=1}^N \int_{x_{i-1}}^{x_i} |\Delta_\delta'(x)|^q \frac{\delta_i}{\Delta_\delta(x)} + 1^q dx 
+ \sum_{i=1}^N \int_{x_{i-1}}^{x_i} |\Delta_\delta'(x)|^q \frac{\delta_i}{\Delta_\delta(x)} + 1^q dx
\]

\[
= \sum_{i=1}^N \int_{x_{i-1}}^{x_i} |\Delta_\delta'(x)|^q dx 
+ \sum_{i=1}^N \int_{x_{i-1}}^{x_i} |\Delta_\delta'(x)|^q \frac{\delta_i}{\Delta_\delta(x)} + 1^q dx .
\]

As \( q \to 0 \), \( \frac{\delta_i}{\Delta_\delta(x)} + 1^q \approx 1 \), and as \( q \to \infty \), \( \frac{\delta_i}{\Delta_\delta(x)} + 1^q \approx \frac{|\delta_i}{\Delta_\delta(x)}|^q \) This gives the following approximations for the two asymptotic regimes,

\[
C_q(r) \approx \begin{cases} 
\langle |\Delta_\delta'(x)|^q \rangle = A_q r^{q\alpha} & q \ll 1 \\
A_q r^{q\alpha} + r N \langle |\delta_i|^q \rangle & q \gg 1 ,
\end{cases}
\]

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

For large \( q \), the scaling may resemble either self-affine scaling or multi-affine 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. 3(b) self-affine scaling is seen for small \( q \) and multi-affine scaling with \( \alpha_q = 1/q \) is seen for large \( q \), but this is not a universal outcome as indicated in Eq. (3).

The scaling behavior of a self-affine surface with vertical discontinuities was investigated numerically and analytically, and it was shown that the surface of discontinuities (the stepped surface) was the source of the multi-affine behavior. It was further shown numerically and analytically, that the general form for the scaling of the stepped surface 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 surface with discontinuities, and for the numerical results shown here, self-affine scaling is seen for small $q$ and multi-affine scaling with $\alpha_q = 1/q$ 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 model and deposition processes onto stepped surfaces. For these processes, the deposition time should have a large effect on the multi-affine scaling behavior.

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