Probe for morphology and hierarchical correlations in scale-invariant structures

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(Received 3 February 1992)

A correlation technique is developed to characterize the distribution of fractal structures. This method generalizes the concept of lacunarity to a scaling function and is naturally suited to distinguish between fractal structures with similar fractal dimensions for already small systems. We therefore propose it as a convenient tool to quantify the vaguely defined concept of morphology. Our lacunarity function is sensitive to logarithmic periodicities and we conjecture that its asymptotic behavior yields information on corrections to scaling in simpler measurements. The formalism we use can be generalized to analyze multifractal structures.

PACS number(s): 64.60.Ak, 61.90.+d

I. INTRODUCTION

Fractal structures appear in an extremely large range of phenomena, touching upon almost every imaginable field of science. These structures were identified by Mandelbrot [1] to exhibit the key property of self-similarity, namely, under scale transformations $r \to r' = Rr$ the structure can be mapped back onto (a subset of) itself. In doing so the "measure" (e.g., the number of points that constitute the structure) must also be rescaled by a factor of R^D to match, and the index D is termed the fractal dimension. Such structures play a significant role in physics in modeling many disordered systems and in studying phase transitions and critical phenomena. The fractal dimension is a crucial characteristic of the structure and without it one cannot make rational comparisons between measurements made on different scales. Self-similarity of the underlying structure leads naturally to the expectation that various properties of the structure will also be governed by power laws. This has been realized for various connective properties (as, for example, in the percolation problem), and in particular for the spectrum of internal excitations. The corresponding lists of exponents have been taken as one way to characterize the structures more completely. This abundance of parameters clearly calls for some organizing principles to exactly characterize the structure of fractals. Also, in dynamically evolving self-similar patterns it is not uncommon to find that structures change dramatically with, or without, the change of some parameter. The identification of such morphological transitions involves usually occular observation, which at best can only be qualitative. Therefore a more quantitative definition of morphology is much in need. Formulations that concentrated on specifying the variance of the spatial distribution of voids in the structure have been attempted [1,2], as well as focusing directly on the spatial distribution of the fractal structure [3].

In this paper we develop and apply a direct method to organize and characterize fractal structures and different morphologies in terms of the correlations between subsets of the structure at different scales, ultimately related to the three-point correlation function (TPCF) of the system. The results reported here show that this method is useful as follows: (i) It enables one to distinguish between structures with similar fractal dimension; (ii) It supplies a criterion to quantify the concept of morphology; (iii) It may be able to identify corrections to scaling from the *large-scale regime,* as we demonstrate for the exactly solvable case of random walks; and (iv) It is sensitive to logarithmic periodicities.

Consider the implications of various continuous symmetries on the measurement of one-, two-, and three-point normalized correlation functions. The one-point function is just the density $\phi_1(\mathbf{r})$, reduced (on average over the volume of the system) to a constant ϕ_1 if the system has, on average, symmetry under translations. The two-point correlation function is derived from the pair density, $\phi_2(\mathbf{r},\mathbf{r}')=\phi_1 C_2(\mathbf{r}-\mathbf{r}')=\phi_1 C_2(|\mathbf{r}-\mathbf{r}'|)$ by translational invariance and rotational symmetry successively. For a statistical fractal, invariance under dilations gives $C_2(r)=Ar^{D-d}$, where only two constants can be determined. For the three-point function translational and rotational invariance lead to

$$\begin{aligned}\phi_3(\mathbf{r},\mathbf{r}',\mathbf{r}'')&=\phi_1 C_3(\mathbf{r}-\mathbf{r}',\mathbf{r}-\mathbf{r}'')\\&=\phi_1 C_3(|\mathbf{r}-\mathbf{r}'|,|\mathbf{r}-\mathbf{r}'|,\theta)\ ,\end{aligned} \tag{1.1}$$

where θ is the angle between the first two vectorial arguments. Applying dilational invariance then gives

$$\phi_3(\mathbf{r},\mathbf{r}',\mathbf{r}'')=\phi_1 C_2(|\mathbf{r}-\mathbf{r}'|)C_2(|\mathbf{r}-\mathbf{r}''|)\mathcal{L}\left[\ln\frac{|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}''|},\theta\right]\ . \tag{1.2}$$

Thus for a fractal which is statistically isotropic and has a continuous dilational symmetry, the three-point correlations reduce to a nontrivial scaling function $\mathcal{L}$ of just two variables.

The construction of this communication is as follows. In Sec. II we reformulate the reduced TPCF in simply measurable terms. Section III shows how two different analyses of the same information are related by a simple differential equation, where the fractal dimension enters with the role of screening rate in logarithmic scale. In Sec. IV we analyze the angular averaged function for selected structures, demonstrating in one example that it shows features related to the way the structure was constructed, and in another that it can distinguish structures of similar fractal dimension. Finally we discuss the results and suggest a way to extend the method to handle multifractal structures.

II. THE LACUANARITY FUNCTION

Given a set of points in d dimensions, equally weighted for simplicity, we choose a point, which we index i, and we construct concentric shells around the coordinates of this point. The shells are chosen to have a uniform width in *logarithm* of the distance $r=|\mathbf{r}|$ from i. For each i, we measure the "mass" $\delta S_i(r)$, which is the number of other points in a spherical shell at radius r from it. The average of this measurement over all choices of i, normalized by the volume of the shell, is the usual pair-correlation function C_2, which gives the mean mass in shell,

$$C_2(r) \equiv \langle \delta S_i(r) \rangle / \delta V(r) \tag{2.1}$$

(in the following averages over i are denoted simply by $\langle\ \rangle$). We can now define the relative fluctuations in the mass distribution about site i in terms of the relative shell masses,

$$\delta\sigma_i(r) = \delta S_i(r) / \langle \delta S(r) \rangle \ . \tag{2.2}$$

For a fractal our expectation would be that $\delta\sigma_i(r)$ has fluctuations of order unity which are correlated over multiplicative ranges of radius, and hence over a simple range in $\rho = \ln r$. We define a correlation matrix,

$$M(\rho,\rho') = \langle \delta\sigma_i(r) \delta\sigma_i(r') \rangle \ , \tag{2.3}$$

and anticipated that M should be overall scale invariant, $M(\rho,\rho') = \mathcal{L}(\rho-\rho')$. Thus defined $\mathcal{L}$ represents an average of the autocorrelation function of the relative shell masses, and we propose to call it a (radial) lacunarity function (LF) because it contains an earlier definition of lacunarity, $M(\rho,\rho)$ [2]. Figure 1 shows a contour plot of the correlation matrix M for several two-dimensional systems: A 4000-monomer-long self-avoiding walk (SAW), and 4096-particle cluster-cluster aggregate (CCA) and a sample of 10^4 particles chosen randomly from a 10^5-particle diffusion-limited aggregate (DLA). Apart from end effects at the largest and smallest separations, contours that are roughly parallel to the diagonal support the idea that the correlations are indeed functions only of the relative logarithmic separation $|\rho-\rho'|$. The corresponding LF's are shown in Fig. 2 and show nontrivial structure. In all three cases $\mathcal{L}$ starts from a value appreciably larger than one at the origin and saturates to unity for $|\rho-\rho'| > \lambda_s$, where λ_s is some finite number. This

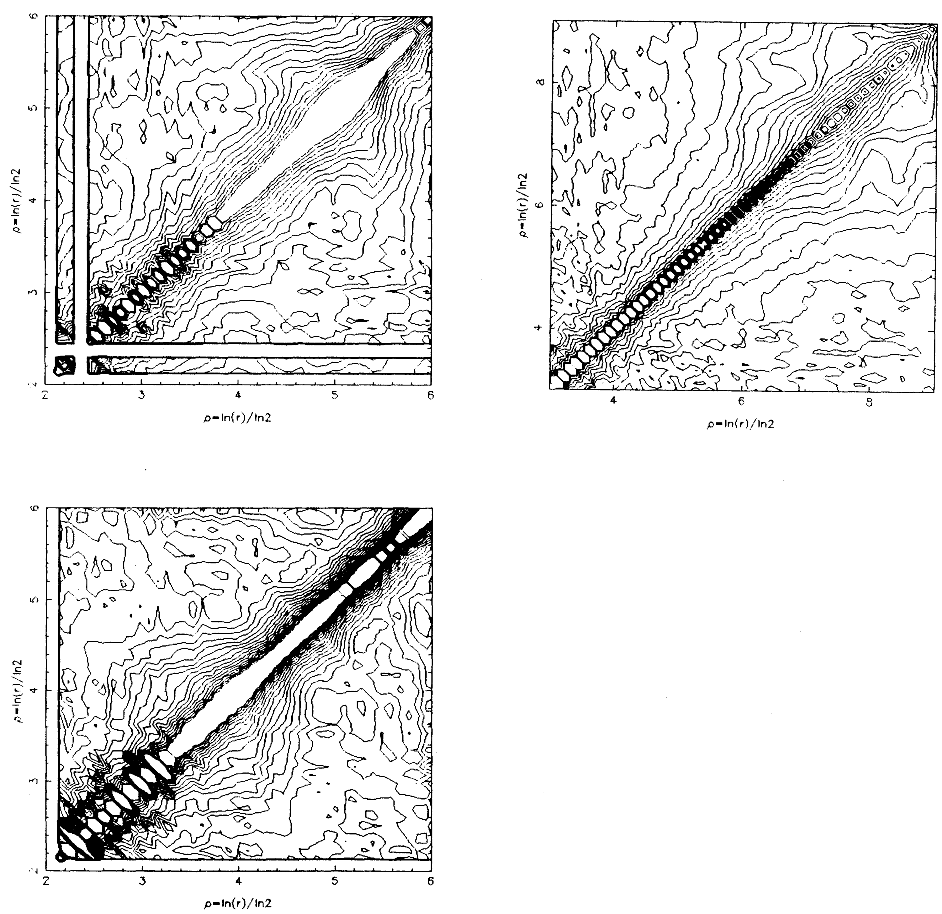

FIG. 1. A contour of the correlation matrix $M(\rho,\rho')$ for three different fractal structures: (a) A 4000-monomer-long SAW, (b) a 4096-particle CCA, and (c) a sample of 10^4 particles chosen randomly from a 10^5-particle DLA.

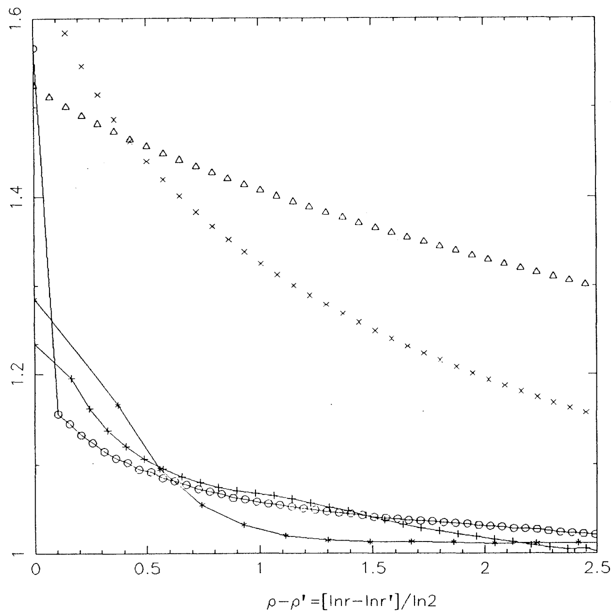

FIG. 2. The lacunarity function $\mathcal{L}$ for ($*$) SAW, (+) CCA, (○) DLA and the approximant function [Eq. (2.8)] with $D=1.33(\times)$ and $D=1.71(\triangle)$.

means that when $r'/r>\exp(\lambda_s)$ the subsets of the structure are uncorrelated.

One of the main motivations of Mandelbrot [4] and Gefen *et al.* [2] in formulating the concept of lacunarity was to distinguish between different fractal patterns that have the same fractal dimension. Such a discrimination, although easily achieved by the human eye and brain [5], proved very difficult to get by any simple analytic tool. Our LF succeeds in distinguishing between the CCA and SAW whose fractal dimensions are very similar (1.42 and 1.34 in 2D, respectively). Note that we achieve this discrimination already for very moderate sizes of 4000 particles. Namely, the CCA and SAW curves display different structures, indicating different patterns. To distinguish between the structures by measuring the fractal dimensions accurately enough would require systems larger by an order of magnitude. The advantage of our LF is evidenced by the fact that the fractal dimensions we measure for our systems are still indistinguishable at this scale (CCA: 1.45 ± 0.15 and SAW: 1.3 ± 0.2).

Our LF can be readily generalized to take account of direction as well as radius by correlating the masses $\delta S_i(\mathbf{r})$ at fixed vector separation rather than just fixed radius. We then divide each of the above shells around the ith particle into equiangular sections and measure the mass δs_i within such a region at a vector separation $\mathbf{r}$,

$$\delta\sigma_i(\mathbf{r})=\delta s_i(\mathbf{r})/\langle\delta s(\mathbf{r})\rangle .$$

Extending the definition of M in expression (2.3) we then form the correlation operator (which has now 2D indices),

$$M(\mathbf{r},\mathbf{r}')=\langle\delta\sigma_i(\mathbf{r})\delta\sigma_i(\mathbf{r}')\rangle .$$

This form is equivalent to the TPCF of the system, given in terms of M by

$$C_3(\mathbf{r},\mathbf{r}')=M(\mathbf{r},\mathbf{r}')C_2(\mathbf{r})C_2(\mathbf{r}') . \tag{2.4}$$

In two dimensions for a (statistically) scale-invariant and isotropic structure we anticipate that the correlation matrix reduces to

$$M(\mathbf{r},\mathbf{r}')=\mathcal{L}(\ln(r'/r),\theta) . \tag{2.5}$$

This angularly dependent LF contains the full three-point correlation function for a (statistically) scale-invariant and isotropic structure. From it the simpler radial $\mathcal{L}$ function discussed previously may be recovered as its (solid angle weighted) angular average.

Established approximations for the TPCF bear upon the LF which encodes the latter. In particular the approximation

$$C_3(\mathbf{r},\mathbf{r}')=1/2[C_2(\mathbf{r})C_2(\mathbf{r}')+C_2(\mathbf{r}'-\mathbf{r})C_2(\mathbf{r}) + C_2(\mathbf{r}-\mathbf{r}')C_2(\mathbf{r}')] , \tag{2.6}$$

is exact for structures based on Markov sequence, such as (unrestricted) infinite Brownian walks [6] and corresponding linear and randomly branched polymers, and has been claimed to apply to galaxy correlations [7] (albeit with a factor of 1.3 instead of $\frac{1}{2}$). In terms of the full lacunarity function this reduces to

$$\mathcal{L}_a(\ln R,\theta)=[1+(1+R^c)(1+R^2-2R\cos\theta)^{-c/2}]/2 , \tag{2.7}$$

where $R\equiv r/r'=\exp(\rho-\rho')$ and $c\equiv d-D$ is the codimension of the structure. Upon angular average this gives

$$\mathcal{L}_a(\lambda)=1/2+\cosh\frac{c\lambda}{2}[2\sinh\lambda]^{-c/2}\frac{P_\nu^\mu(\coth\lambda)}{P_{-\mu}^\mu(\coth\lambda)} , \tag{2.8}$$

where $\lambda=|\ln R|$, $\mu=1-d/2$, and $\nu=D/2-1$ [12]. This function, for $D=1.33$ and 1.71, is also plotted in Fig. 2 against λ, to compare with the numerical cases. They are clearly different showing that $\mathcal{L}$ is in general nontrivial and cannot be reduced to $C_2(r)$ as for the random-walk case.

III. SHELL CORRELATIONS VERSUS SPHERE CORRELATIONS

An alternative way to analyze the correlations within the structure is by considering the total mass within a sphere of radius r, $\mathcal{M}(r)$, and correlate it with the mass within a sphere of radius r'. This method is better behaved statistically than correlating shells, but they are closely related as we now demonstrate. Consider the total mass within distance r from the point i, $\mathcal{M}_i(r)$. Averaging over i gives the usual fractal behavior,

$$\mathcal{M}(r)\equiv\langle\mathcal{M}_i(r)\rangle=Br^D , \tag{3.1}$$

which relates to the two-point correlation function $C_2(r)\approx r^{1-d}\partial_r\mathcal{M}(r)$. It is the fluctuations of $\mathcal{M}_i(r)$ around $\mathcal{M}(r)$ which we now investigate by considering

$$\langle \mathcal{M}_i(r)\mathcal{M}_i(r')\rangle = \mathcal{K}(\ln(r'/r))\mathcal{M}(r)\mathcal{M}(r') , \tag{3.2}$$

where we expect $\mathcal{K}(\ln(r'/r'))$ to be a (scale-independent) measure of the correlations. The formulation we used in the previous section amounts to

$$\langle \partial_r\mathcal{M}_i(r)\partial_{r'}\mathcal{M}_i(r')\rangle = \mathcal{L}(\ln(r'/r))\partial_r\mathcal{M}(r)\partial_{r'}\mathcal{M}(r') . \tag{3.3}$$

The function $\mathcal{L}$ can now be related to $\mathcal{K}$ as follows:

$$\begin{aligned}\mathcal{L}(\ln(r'/r))\partial_r\mathcal{M}(r)\partial_{r'}\mathcal{M}(r') &= \partial_{rr'}\langle \mathcal{M}_i(r)\mathcal{M}_i(r')\rangle \\ &= \partial_{rr'}[\mathcal{K}(\ln(r'/r))\mathcal{M}(r)\mathcal{M}(r')] . \end{aligned}\tag{3.4}$$

Carrying out the differentiation explicitly and identifying the fractal dimension as $D = r\partial_r[\ln\mathcal{M}(r)] = r'\partial_{r'}[\ln\mathcal{M}(r')]$, we find

$$\mathcal{L}(\lambda) = \mathcal{K}(\lambda) - \partial_{\lambda\lambda}\mathcal{K}(\lambda)/D^2 , \tag{3.5}$$

where $\lambda = \ln(r'/r)$. It is important to note that both $\mathcal{L}$ and $\mathcal{K}$ are even functions of their argument. Equation (3.5) and its inverse $\mathcal{K}(\lambda) = (D/2)\int_{-\infty}^{\infty} e^{-D|\lambda'-\lambda|}\mathcal{L}(\lambda')d\lambda'$ show that $\mathcal{L}$ is more sensitive to some details than $\mathcal{K}$. For example at small $|\lambda|$ the expansion of $\mathcal{L}_a$ yields [8] $\mathcal{L}_a(\lambda) \approx A - B|\lambda|^{D-1}$, corresponding to $\mathcal{K}_a(\lambda) \approx A + BD/(D+1)|\lambda|^{D+1}$, where A and B are positive constants.

IV. LOGARITHMIC PERIODICITIES AND CORRECTIONS TO SCALING

It has been suggested that self-similar patterns formed by processes of stochastic growth entertain periodicities in ρ space that manifest through geometrically increasing spacing between major sidebranches [9]. Examples include cracking and noise-reduced DLA. Understanding the origins of the particular spacing patterns plays a significant role in understanding the basic mechanisms that select the resultant macroscopic structures. Our function $\mathcal{L}$ should detect such periodicities in logarithmic space coordinates. If one measures $\mathcal{L}$ for a given distribution of data points and finds a distinct peak, one can conclude that at the corresponding ratio of length scales there is some repetition in the structure *regardless of absolute scale.*

To illustrate this we have examined disordered cantor sets. The structures are constructed by deleting at the nth stage a third section of each line that survived the deletion at the $(n-1)$th stage, but letting the location of the deleted section fluctuate about the center. As the fluctuations increase the resulting structures would have, on statistical averages, no preferred absolute length scales only relative ones. Indeed to the eye the resulting structures seem very disordered. Nevertheless, as shown in Fig. 3, the LF can easily detect the underlying length scale factor of the recurrence procedure, which shows up as a periodicity in $\mathcal{L}$, damped by the disorder.

We have considered whether the results for physical structures can be interpreted similarly. The CCA clusters are constructed by successive dimerization of (hitherto unrelated) clusters of equal mass, so it is expected that the range of correlation shown by $\mathcal{L}$ should be short. Doubling the mass of a structure with a fractal dimension D by dimerization increases the cluster size by a factor $r'/r = 2^{1/D}$. Hence one could argue that the LF should show some features at this scaling factor. The SAW, on the other hand, is not expected to show any such feature. We have plotted the function $\mathcal{L}-1$ vs $\rho-\rho'$ for the SAW and CCA, on a semilog scale in Fig. 4, to compare detail at small λ. Indeed an irregularity (which we have checked is reproducible) appears for the CCA around $\lambda = \ln 2/D$, before and after which there is a smooth decay of λ. The corresponding plots for DLA and for $\mathcal{L}_a$ for $D = 1.33$ and 1.17 are also shown for comparison.

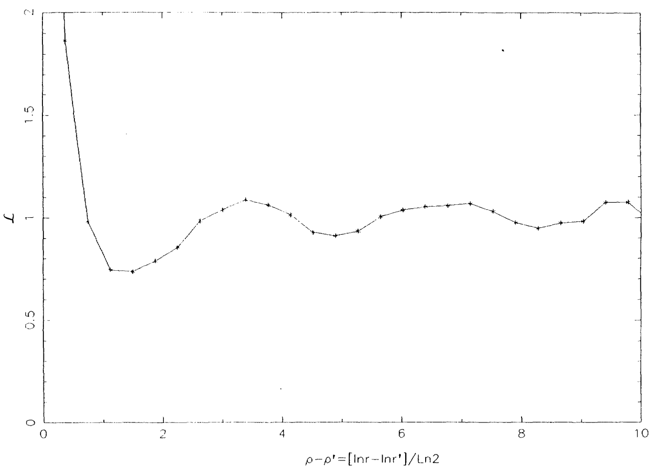

FIG. 3. The LF of a disordered cantor set displaying the characteristic oscillations.

However, the most distinct difference between the CCA and the SAW structures is in the different rate of decay to unity. Thus Fig. 4 also suggests another interpretation of the data. Straight-line segments for $\lambda > 1$ would indicate that a good fit would be obtained to a sum of powers,

$$\mathcal{L} = 1 + A_p(r'/r)^{-p} + O((r'/r)^{-q}), \quad q > p > 0 . \tag{4.1}$$

We conjecture that *the power p, and other corrections, should match ordinary corrections to scaling.* This conjecture is motivated by analogy with conventional relations between correlations and response functions in thermal and quantum physics. For random walks we have confirmed this conjecture analytically with $p = c$ and $q = 2$ corresponding to corrections to scaling in $C_2(r)$ from finite length and discrete steps, respectively. To pursue this quantitatively by simulations requires data of higher quality than presently available. Such an analysis is also strongly sensitive to whether the leading constant term (expected unity) should be adjusted to the data or not [7]. We expect logarithmic corrections to scaling to generate terms in this regime that decay as powers of λ. The important overall point is that the structure of the LF in the *pure scaling regime* may dictate the forms of the *corrections to scaling* in simpler measurements.

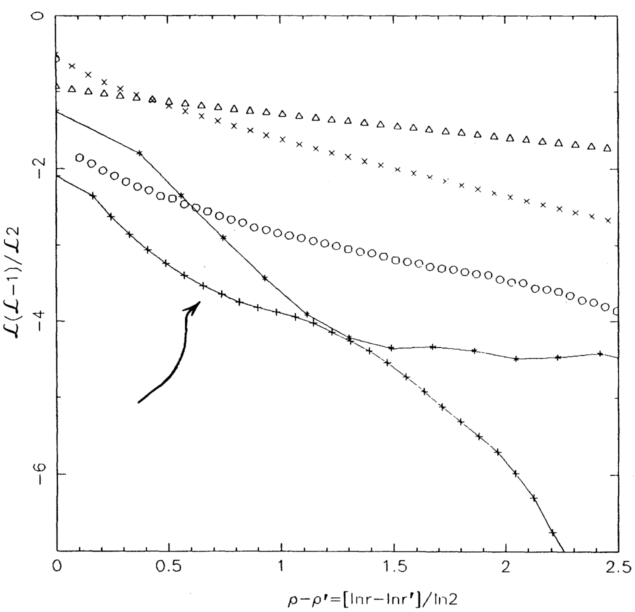

FIG. 4. The function $\log_2[\mathcal{L}-1]$ for (*) SAW, (+) CCA, (○) DLA and the approximant function with $D=1.33$(×) and $D=1.71$ (△). Note the deviation from smooth decay, and the shift of the curve to the right, starting around $0.7 \approx 1/D$.

V. APPLICATION TO MULTIFRACTALS AND DISCUSSIONS

It appears that the LF can also be defined for multifractal measures, although it requires more care with normalization. Simple box counting arguments suggest that the correlation matrix as defined in (2.2) and (2.3) takes the more general form [10],

$$M(\rho,\rho') \approx (r/R_0)^{2\tau(2)-\tau(3)} \mathcal{L}(\rho-\rho') ,$$

where r is the larger of the two radii, R_0 is the radius of the sample, and $\tau(q)$ are the conventional moment scaling exponents of the measure [11]. Thus the correlation matrix in general contains two different sorts of information: on the diagonal $M(\rho,\rho)$ reveals $2\tau(2)-\tau(3)=2(D_2-D_3)$ for a multifractal, but is constant for a simple fractal. The off-diagonal behavior reveals the lacunarity through

$$\mathcal{L}(\rho-\rho')/\mathcal{L}(0)=M(\rho,\rho')/M(\rho,\rho), \quad \rho>\rho' .$$

This result leads us to expect that the LF of multifractal measures reflects basically the spatial distribution of the support of the second moment of the measure. In principle, by correlating higher powers of the measure, the lacunarity of the support for higher moments can also be probed.

To conclude we have proposed a method to analyze fractal structures through the three-point correlation function in logarithmic coordinates. We have introduced a lacunarity function that distinguishes morphologies with very similar fractal dimensions but different spatial distributions, as demonstrated for the case of cluster-cluster aggregation and self-avoiding walks. This distinction can be achieved already for small sizes, where the usual measurements of fractal dimensions are still too noisy for separation. The method proposed here is also well suited to probe scale-invariant periodicities in the pattern formed by stochastic processes, as we demonstrated in the case of disordered Cantor sets. Finally, we propose that it may also retrieve corrections to scaling from the *large-scale behavior.* It is hoped that this technique can assist in a better understanding of growth processes such as noise-reduced diffusion-limited aggregation, dendritic solidification, etc. Generalizations of the formalism have been proposed for the angle-dependent LF, and we have briefly outlined a generalization for multifractal distributions.

ACKNOWLEDGMENTS

We are grateful to Dr. P. B. Warren for providing the data on CCA and to Professor P. Meakin for providing the data on DLA. We thank Professor B. B. Mandelbrot for useful comments. This research is supported by Science and Engineering Research Council, UK.

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[12] Note that (2.8) requires the complex convention of a $[-1,1]$ branch cut in $P_\nu^\mu(Z)$.