# Spectral dimension of a fractal structure with long-range interactions

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By an exact renormalization method three different dynamical regimes are found for a self-similar structure with long-range interactions. Unlike in translation invariant systems, a transition from nonuniversal to universal anomalous spectral behavior occurs as the range of the forces increases beyond a certain threshold. The model sheds light on possible qualitative mechanisms behind recent experimental results for the density of vibrational states of hemoproteins. Problems of ultradiffusion in hierarchical structures can be solved within similar mathematical frameworks.

Harmonic analysis of structures with a dilation symmetry, or fractals,[1] as well as the related diffusion problems, are of much interest in connection with several issues ranging from electrical conduction in linear polymers[2] to anomalous temperature dependence of ESR spin lattice relaxation times of iron in some proteins.[3]

As a consequence of self-similarity, in a fractal the density of vibrational states $\rho(\omega)$ at small frequency $\omega$ scales like $\omega^{\tilde{d}-1}$. $\tilde{d}$ is the spectral dimensionality, which differs both from $d$, the dimension of the embedding Euclidean space, and from $\bar{d}$, the "geometrical" fractal dimension of the structure.[4,5]

A simple relation, $\tilde{d}=2\bar{d}/d_w$, connects $\tilde{d}$ with $d_w$, the dimension associated with a random walk on the fractal. Moreover, it has been conjectured that $\tilde{d}$ directly determines the scaling behavior of various relevant random-walk properties, like the range, or the probability $P_0$ of return to the original site after time $t$. The latter is expected to behave as $P_0(t)\sim t^{-\tilde{d}/2}$ as $t\to\infty$.[4,5]

Up to now, spectral properties have been studied both on random fractals, such as percolation clusters,[6] and on deterministic fractals, such as Sierpiński gaskets.[5]

In both cases only short-range (harmonic) forces, or hopping probabilities, were considered.

In this article, for the first time, we present and analyze by an exact renormalization method a fractal model allowing for long-range interactions.

Besides filling an obvious gap in the literature on the field, the present investigation was directly motivated by problems which arose recently in connection with experimental determinations of the fracton density of states in hemo and other proteins in solution.[3]

To introduce our model, let us consider a triadic Koch curve in the plane like the one sketched in Fig. 1. Each point on the curve is free to vibrate perpendicular to the plane and is connected by spring forces (elastic constant $K$, continuous bonds) to its nearest neighbors. In addition to these, there are other elastic forces of longer range (dotted bonds, constants $K_1$, $K_2$, ...), acting according to the self-similar scheme indicated in the figure.

Such a structure clearly has $\bar{d}=\ln 4/\ln 3$, since the number of points increases by a factor of 4 whenever the linear size is multiplied by 3.

Putting $\lambda=M\omega^2/K$ and $\alpha_i=K_i/K$, $M$ being the mass of the points, we get the following set of equations:

$$\lambda x_i=\sum_j \beta_{ij}(x_i-x_j) \tag{1}$$

for the displacements $x_i$, at the various sites, appropriate to a vibrational mode $\{xe^{i\omega t}\}$. The sum over $j$ extends to all sites interacting directly with site $i$, and $\beta_{ij}$ is equal to 1 or $\alpha_m$, when the point $j$ is the nearest neighbor of $i$ or is connected to it by a coupling $K_m$, respectively. The low-frequency scaling properties of the above eigenmodes can be studied by a relatively simple renormalization-group procedure. Referring to Fig. 1, we eliminate from the system (1) all variables at the vertices of the elementary triangles having the coupling $K_1$ associated with one of their sides. With this dynamical decimation[5,7] the system is

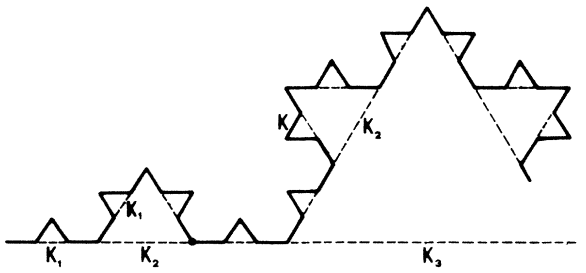


FIG. 1. Sketch of the fractal structure allowing for interactions at all length scales. The continuous curve represents the backbone.

 

spatially rescaled by a factor $l=3$. The displacements at the "surviving" points (which form a structure of the same type as the original one, after a proper rescaling), can be seen to obey a system of the form (1), with new, effective reduced square frequency $\lambda'$ and couplings $\{\alpha'\}$.

In the $\omega \to 0$ ($\lambda \to 0$) limit these become simply

$$\lambda' = 16 \frac{1+\alpha_1}{1+2\alpha_1} \lambda \ , \tag{2}$$

$$\alpha_n' = 4 \frac{1+\alpha_1}{1+2\alpha_1} \alpha_{n+1} \ . \tag{3}$$

Equations (2) and (3) allow the discussion of the scaling of the eigenfrequencies according to a basic relation[5] which, for our model, becomes

$$\lambda(\{\alpha'\}) = l^{d_w} \lambda(\{\alpha\}) \tag{4}$$

in the limit of an infinite system. Thus $\tilde{d} = 2\bar{d}/d_w$ can be determined by discussing the fixed points $\{\alpha^*\}$ of (3). An interesting feature of (3) is that it shows a whole line of physically acceptable finite fixed points, characterized by the parameter $\alpha_1^*$ in the range $0 \le \alpha_1^* < \infty$. Indeed it turns out that

$$\alpha_n^* = \alpha_1^* \left( \frac{1+2\alpha_1^*}{4(1+\alpha_1^*)} \right)^{n-1} , \quad n = 1,2,3,\ldots \tag{5}$$

is a fixed point of Eq. (3). The corresponding $\tilde{d}$ follows from (2) and (4), and of course depends on $\alpha_1^*$. Taking into account that $l=3$, we get

$$\tilde{d} = \left[ 1 + \frac{1}{4\ln 2} \ln \left( \frac{1+\alpha_1^*}{1+2\alpha_1^*} \right) \right]^{-1} . \tag{6}$$

As $\alpha_1^*$ varies from 0 to $+\infty$, $\tilde{d}$ varies from 1 to $\frac{4}{3}$.

One can easily verify that initial interaction patterns $\{\alpha\}$, such that $\lim_{n\to\infty}(\alpha_{n+1}/\alpha_n) = C$ with $\frac{1}{4} \le C < \frac{1}{2}$, are all attracted by the fixed point (5) with $\alpha_1^* = (1-4C)/(4C-2)$. These $\{\alpha\}$'s, consistent with the fractal geometry, are long-range interactions with power-law decay at large distance $R$, i.e., $\alpha(R) \sim R^{\ln C/\ln 3}$, as $R \to \infty$.

Long-range forces radically change the spectral properties and lead to nonuniversal dynamical critical behavior. Similar effects are also obtained when such forces act on a $d$-dimensional regular structure.[8] However, the effect of long-range interactions cannot be taken into account by simply interchanging the roles of $d$ and $\bar{d}$ in the two cases.[9] As we show below, long-range forces combined with dilation symmetry determine a qualitatively new dynamical regime.

Initial interactions for which $C \ge \frac{1}{2}$, i.e., forces with relatively long range, are attracted by a "line" of fixed points at infinity ($\alpha_{i+1}^*/\alpha_i^* = C$, $\alpha_1^* = \infty$), all having the same $\tilde{d} = \frac{4}{3}$ on the basis of Eq. (6). This line continues the one of finite fixed points given by Eq. (5). By increasing the range of the forces, $\tilde{d}$ has a finite, anomalous saturation value and remains constant, and thus universal, for a wide class of long-range interactions.[9] This new regime is the most remarkable difference with respect to translation-invariant cases, and should always be expected when long-range forces act consistently with a dilation symmetry, as in our model.

A third regime is finally obtained when $C < \frac{1}{4}$, i.e., for finite range or rapidly enough decaying forces. In this case the fixed point is always given by $\alpha_i^* = 0$. We thus learn, in particular, that all situations, in which nearest-neighbor bridges are not extending to all scales (finite range), are finally mapped into the dynamics of a nearest-neighbor model, with the consequent result $\tilde{d} = 1$ (see Fig. 2). Of course, the crossover to this situation will be the slower, the longer the (finite) range of the bridges.

Regarding the problem of continuous-time random-walk diffusion on our structure, we remark that the above renormalization approach actually allows a direct check of the scaling of $P_0(t)$, the quantity associated with renewal theory on the fractal.[5,10] When dealing with diffusion, a system like (1) is satisfied by the Laplace transform $\tilde{P}_i(\omega)$ (replacing $x_i$) of the probability that the walker is at site $i$ at time $t$, after starting at site 0 at $t=0$. The only difference is that the equation for $\tilde{P}_0(\omega)$ has a 1 added on the right-hand side to satisfy the initial condition. In this case $\lambda = \omega$ and the various $\alpha_i$'s are hopping rates. The same renormalization procedure outlined above applies again, and, if site 0 survives decimation, we obtain the following relation for $\omega \to 0$:

$$\tilde{P}_0(l^{d_w'}\omega, \{\alpha'\}) = \frac{2\alpha_1+1}{4(1+\alpha_1)} \tilde{P}_0(\omega, \{\alpha\}) \ , \tag{7}$$

where $d_w' = 2\bar{d}/\tilde{d}'$, with $\tilde{d}'$ given by Eq. (6), with $\alpha_1$ replacing $\alpha_1^*$.

The fixed-point analysis above leads to the conclusion that indeed $\tilde{P}_0(\omega) \sim \omega^{\tilde{d}/2-1}$, with $\tilde{d}$ as obtained above. This is in agreement with a general conjecture by Rammal and Toulouse,[5] which was tested by simulation on Sierpiński gaskets.[11] Using our approach, a formula analogous to (7), and thus a direct analytic test of the scaling behavior of $P_0$, can be obtained in the case treated numerically by the authors of Ref. 11.

On the basis of Eq. (7) and of its analog for the generic site $i$, it is also possible to establish directly the scaling behavior for the average square distance traveled by the particle on the fractal, $R^2 \sim t^{2/d_w}$, as $t \to \infty$.

In a spirit close to that of Ref. 12, one can consider a resistor problem associated with our diffusion model. At

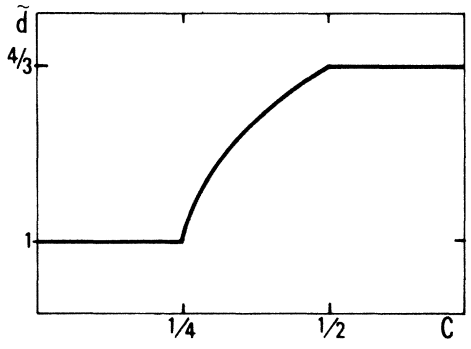


FIG. 2. Qualtitative plot of $\tilde{d}$ vs $C$.

each bond, characterized by a hopping rate $\alpha_i$, we associate a dimensionless resistance $r_i/r_0 = 1/\alpha_i$, $i \geq 1$. The resistance of the structure is expected to scale like $L^{\zeta}$, if $L$ is the spatial distance between the points considered. We could indeed compute $\zeta$, which is also nonuniversal and turns out to satisfy the Einstein relation $\zeta = d_w - \bar{d}$.

The simple model presented here may shed some light on the possible mechanisms leading to the relatively high values of $\tilde{d}$ ($\tilde{d} = 1.3$–$1.7$) measured in some hemoproteins and ferrodoxin.[3] It has been suggested that such values of $\tilde{d}$ should be explained on the basis of crosslinking bonds (e.g., $H$ bridges) between different segments of the fractal folded-chain backbone of the protein.[13] While there is general agreement on the importance of such bonds, there is considerable controversy about the specific mechanism by which they could affect $\tilde{d}$.[14–16] In particular, recent numerical simulations of diffusion on self-avoiding chains clearly indicate that $\tilde{d}$ stays equal to 1, the value without crosslinking bridges, if these are assumed to be short range.[17–19] In our model, the Koch triadic could represent very schematically the backbone of a protein. The elastic couplings $K_i$ could simulate crosslinks between different parts of the backbone. The behavior discussed above suggests that a definite deviation of $\tilde{d}$ from 1, strictly speaking, can be produced only by bridges of infinite range. In proteins, long or infinite range forces can be provided by salt bridges (i.e., weakly screened Coulomb forces) or by effects of elastic distortion of the surrounding frozen solvent. On the other hand, on the scales actually tested by the experiments, the observed $\tilde{d}$'s could be preasymptotic and thus indistinguishable from those which would result from crossovers such as those taking place in our model for long but finite range $\{\alpha\}$'s.

It would be tempting to think of the $\tilde{d}$'s measured for proteins as manifestations of saturation phenomena such as occur in our model for sufficiently long-range forces. Only in this way the $\tilde{d}$ values could show some degree of universality. We just mention, as a curiosity, that appropriate $d = 3$ generalizations of this model (e.g., with tetrahedra replacing the triangles in Fig. 1), with $\bar{d}$ close to the actual protein values,[15] yield saturation $\tilde{d}$'s in the appropriate experimental range.[3,15]

The nonuniversal scaling behaviors found above can also be seen as a consequence of the infinite hierarchy of time scales present in the model. Considering diffusion and assuming a thermal activation mechanism across energy barriers, we can think of $C$ as a function of temperature, e.g., $C \sim \exp(-\text{const}/T)$. The above results thus lead to a temperature dependence of the diffusive exponents in the intermediate region.

Behaviors of the same type have been recently studied with approximate methods by Huberman and Kerszberg[20] on a particular (nonfractal) model of diffusion with a hierarchy of energy barrier scales, and are expected to be relevant for a variety of physical situations, ranging from molecular diffusion on complex macromolecules,[21] to spin-glass systems[22,23] or computing structures.[24] A similar, but more simple problem of ultradiffusion has been considered more recently by Ogielski and Stein[25] and by Paladin, Mezard, and de Dominicis.[26] The main difference between the present model and those mentioned above lies in the fact that in the former the hierarchy of time scales coexists with a nontrivial fractal structure, and long-range forces are allowed. The two types of problems have many similarities also from a formal point of view: This should not surprise us, if we think that also for our model an ultrametric distance can be easily defined.[27]

In this respect, it is worth remarking that the methods of the present article can be properly adapted to solve[28] the model of Ref. 20, providing an exact confirmation of some approximate predictions produced there,[20] but also further results,[28,29] which could not be derived with extensive perturbative and numerical investigation of the same model.[30] In particular, a peculiar dynamical regime, very similar to the one in our model for $C \geq \frac{1}{2}$, could be exactly established and understood.[29]

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[1] B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, 1982).

[2] S. Estemad, A. J. Heeger, and A. G. MacDiarmid, Ann. Phys. Chem. **33**, 443 (1982).

[3] H. J. Stapleton, J. P. Allen, C. P. Flynn, D. G. Stinson, and S. R. Kuntz, Phys. Rev. Lett. **45**, 1456 (1980).

[4] S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).

[5] R. Rammal and G. Toulouse, J. Phys. (Paris) Lett. **44**, L13 (1983).

[6] D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1986).

[7] For a review of similar methods, see, e.g., R. B. Stinchcombe, in *Static Critical Phenomena in Inhomogeneous Systems*, edited by A. Pekalski and J. Sznajd, Lecture Notes in Physics, Vol. 206 (Springer, Berlin, 1984).

[8] B. R. Hughes and M. F. Shlesinger, J. Math. Phys. 23, 1688 (1982).

[9] For harmonic forces decaying as $R^{-p}(d < p < d+2)$ one finds on a regular lattice $\tilde{d} = 2d/(p-d)$ (Ref. 8). We instead obtain $\tilde{d} = 2\bar{d}/(p+\bar{d})$, with $\bar{d}/2 \leq p = -\ln C/\ln 3 \leq \bar{d}$. Thus, for slowly enough decaying forces, $\tilde{d}$ becomes infinite in the translation invariant case ($p \leq d$), but, as we show below, remains finite in our model ($p < \bar{d}/2$).

[10] R. Rammal, Phys. Rep. **103**, 151 (1984).

[11] J. C. Angles d'Auriac, A. Benoit, and R. Rammal, J. Phys. A **16**, 4039 (1983).

[12] Y. Gefen, A. Aharony, and S. Alexander, Phys. Rev. Lett. **50**, 77 (1983).

[13] J. S. Helman, A. Coniglio, and G. Tsallis, Phys. Rev. Lett. **53**, 1195 (1984).

[14] M. E. Cates, Phys. Rev. Lett. **54**, 1733 (1985).

[15]H. J. Stapleton, Phys. Rev. Lett. **54**, 1734 (1985).
[16]J. S. Helman, A. Coniglio, and C. Tsallis, Phys. Rev. Lett. **54**, 1735 (1985).
[17]Y. S. Yang, Y. Lin, and P. M. Lam, Z. Phys. (to be published).
[18]A. L. Stella, R. Dekeyser, and A. Maritan, in *Sixth Trieste International Symposium: Fractals in Physics,* edited by L. Pietronero and E. Tosatti (North-Holland, Amsterdam, 1986).
[19]D. Chowdhury and B. K. Chakrabarty, J. Phys. A **18**, L377 (1985), reported recently a slight deviation from unity. However, their Monte Carlo results are most probably affected by strong boundary effects. For more systematic and reliable numerical work on this and related issues, like diffusion on a random walk (for which $\tilde{d}$ is found equal to $\frac{4}{3}$ for $d=2$, as in the saturation regime of our model), see Ref. 18.
[20]B. A. Huberman and M. Kerszberg, J. Phys. A **18**, L331 (1985).
[21]R. H. Austin, K. W. Berson, L. Eisenstein, L. H. Frauenfelder, and I. C. Gunsalus, Biochem. **14**, 5355 (1975).
[22]H. Sompolinsky, Phys. Rev. Lett. **47**, 935 (1981).
[23]R. G. Palmer, D. L. Stein, E. Abrahams, and P. W. Anderson, Phys. Rev. Lett. **53**, 958 (1984).
[24]B. A. Huberman and T. Hogg, Phys. Rev. Lett. **52**, 1048 (1984).
[25]A. T. Ogielski and D. L. Stein, Phys. Rev. Lett. **55**, 634 (1985).
[26]G. Paladin, M. Mezard, and C. de Dominicis, J. Phys. (Paris) Lett. **46**, L985 (1985).
[27]In the present model two points can be said to have an ultrametric distance $n$, if $K_n$ is the highest-order coupling acting on the portion of backbone between the two points.
[28]A. Maritan and A. L. Stella, J. Phys. A **19**, L269 (1986).
[29]A. Maritan and A. L. Stella, Phys. Rev. Lett. (to be published).
[30]S. Teitel and E. Domany, Phys. Rev. Lett. **55**, 2176 (1985).