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LETTER TO THE EDITOR

Diffusion in a fractal model with flights

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Abstract. Fractal, walk, and spectral dimensions d_f, d_w and d_s for diffusion on a fractal model with bridges are obtained from an exact renormalisation group transformation of the diffusion time. These results do not support a recent conjecture that $d_w \to 2$ for highly crosslinked systems; nor is d_w simply related (as in the Lévy and Weierstrass models with flights) to exponents representing the distribution of flight lengths. However, an 'Einstein' exponent relationship between diffusion and conductivity is proved.

The importance of fracton and fractal dimensions d_{fr}, d_f of fractal systems [1] with bridges has been recently pointed out in connection with the properties of crosslinked bipolymer models of proteins [2, 3]. In this connection it was speculated [3] that d_{fr} could become equal to d_f when a sufficiently large number of bridges are incorporated. This conjecture, equivalent to having the walk dimension d_w approach 2 in highly crosslinked systems, has since been questioned [4]† on the basis of examples involving bridges of limited length.

At the same time our understanding of the effects of arbitrarily long range hoppings ('flights') on diffusion has been developing, particularly influenced by the discussions of Lévy flights by Mandelbrot [1] and of the Weierstrass random walk by Montroll and Schlesinger [5]. In these cases it is known that non-Gaussian behaviour ($d_w \neq 2$) occurs because the distribution $P(L)$ of flight lengths L has infinite moments, and that d_w is related to an exponent describing the form of $P(L)$. This problem is rather like that referred to in the first paragraph since diffusion on fractals with bridges contains the effects of arbitrarily long range hoppings distributed in a manner to be described subsequently.

In this letter a rather general (two-parameter) fractal model with bridges is introduced and the diffusion problem is exactly solved for it by the use of recursive scaling methods (see for example [6]), in order to see which of the conjectured or possibly special relationships may be generally true. Relevant properties of the distribution $P(L)$ of flight lengths are obtained, and it is shown to have infinite moments. As expected from this, an anomalous relationship between diffusion length R and time t is shown to arise, characterised by walk dimension d_w where

$$R \propto t^{1/d_w}. \tag{1}$$

The walk and fractal dimensions d_w and d_f are both obtained and also the diffusion spectral dimension d_s which is given [7] by $d_s = d_f/d_w = d_{fr}/2$. The walk exponent d_w is not in general 2 and, in contrast to the conjecture, only approaches that value in a

† See also [4a].

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particular limit corresponding to very infrequent bridging. Unlike the Lévy flight and Weierstrass walk models [5] no simple relationship exists between d_w and exponents characterising the distribution $P(L)$ and the reason for this is discussed. One further result concerns the relationship [8, 9], which would result from an Einstein relation [10], between walk dimension and conductance exponent and fractal dimension. The breakdown of this relation in some scale-invariance situations has recently been demonstrated [11]. For the present fractal it is here verified explicitly.

The fractal model is constructed recursively as the limit of a hierarchy of systems, each obtained from the previous one by replacing in it each bond by $(2p+s)$ bonds in series of which an inner portion of s bonds is bridged by a single long bond (a 'flight'), as shown in figure 1. The resulting fractal contains flights of arbitrarily long length. By considering successive members of the hierarchy it can be seen that under a change of length scale by factor $r+s$ (where $r \equiv 2p$) the number of bonds changes by a factor $r+s+1$ so the fractal dimension is

$$d_f = \ln(r+s+1)/\ln(r+s). \tag{2}$$

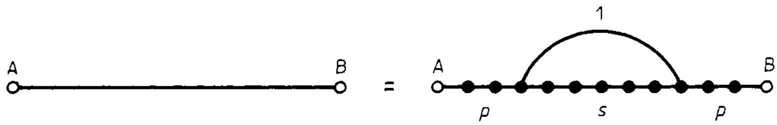

Figure 1. Recursive construction of fractal, by iteratively replacing each single bond by $2p+s$ bonds of which the inner s bonds are bridged by a single long bond.

The diffusion process on the fractal can be exactly treated by a decimation procedure which provides a scaling relationship between the values Δ, Δ' of a diffusion parameter at two successive stages in the recursive construction. Δ is an eigenvalue of the operator shifting time by a unit step (at the stage reached in the hierarchical construction) and occurs as follows in the discrete diffusion equations associated with the three different types of site placing in the fractal, where the numbering of sites is as in figure 2 and u_n is the probability of being at site n:

$$\Delta u_1 = \tfrac{1}{2}(u_0 + u_2) \tag{3}$$

$$\Delta u_2 = \tfrac{1}{2}u_1 + \tfrac{1}{3}u_3 \tag{4}$$

$$\Delta u_3 = \tfrac{1}{2}(u_2 + u_4 + u_5). \tag{5}$$

Such equations can be used to eliminate the sites between A and B in the element on the right of figure 1, so replacing it by a single bond (cf the left of figure 1) with

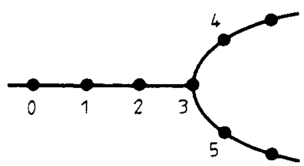

Figure 2. Labelling of sites near a branching vertex of the fractal, for use in specifying the nature of the typical discrete diffusion equations.

renormalised parameter Δ'. The resulting exact scaling relation between Δ' and Δ is

$$\Delta' = \frac{1}{b(c_{1p})^2}[(\Delta - c_{p-1p})(a^2-b^2) - (c_{1p})^2 a] \equiv R(\Delta) \tag{6}$$

where

$$\Delta \equiv \cos\theta \tag{7}$$

$$c_{nm} \equiv \sin n\theta / \sin m\theta \tag{8}$$

$$a \equiv 3\Delta - c_{s-1,s} - c_{p-1,p} \tag{9}$$

$$b \equiv 1 + c_{1s}. \tag{10}$$

The fixed point of (6) is where Δ takes the value

$$\Delta^* = 1. \tag{11}$$

To obtain the walk dimension, we require [6] the eigenvalue λ of equation (6) linearised about the fixed point. The linearised equation takes the form

$$\delta' = \delta\left(\frac{rs+r+s}{s+1}\right)(r+s+1) \equiv \lambda\delta \tag{12}$$

where $\delta \equiv \Delta - 1$, $\delta' \equiv \Delta' - 1$, and only terms linear in δ have been retained; as before, $r \equiv 2p$. λ is the factor by which the diffusion time changes (for long times) when the length changes by $r+s$, hence the exact value of the walk dimension d_w defined by (1) is

$$d_w = \ln\left[\left(\frac{rs+r+s}{s+1}\right)(r+s+l)\right][\ln(r+s)]^{-1}, \tag{13}$$

and hence

$$d_s = \ln(r+s+1)\left\{\ln\left[\left(\frac{rs+r+s}{s+1}\right)(r+s+1)\right]\right\}^{-1}.$$

It can be seen from (13) that, contrary to the conjecture referred to earlier, $d_w = 2$ can only be obtained by taking $r \to \infty$ at fixed s, which is actually the case where crosslinking is rare.

A relationship between d_w, d_f and the exponent $\tilde{t}$ for the length scaling of the conductance has been obtained [8, 9] subject to certain assumptions by combining the Einstein relation [10] between diffusion constant, density and conductance with a crossover argument. Counter examples to this relation can be given [11], but it has been shown to apply exactly for a particular non-random fractal [9] (the Sierpinski gasket) and we now show that it applies also for the fractal with bridges presently being considered. In this case, by combining in series r resistors and an element made from a resistor in parallel with s resistors in series, it can be seen that under a change of length scale by $r+s$ the conductance of the fractal scales by

$$r + \frac{1}{1+1/s} \equiv (r+s)^{\tilde{t}}. \tag{14}$$

This can be identified as the first factor in λ, as given by (12); the other factor $(r+s+1) \equiv (r+s)^{d_f}$ is that associated with the bond number scaling in the expression

(2) for d_f, i.e. with the density scaling in the Einstein relation. Hence we see that in the present case

$$d_w = \tilde{t} + d_f \tag{15}$$

which is an explicit verification of the exponent relation from the Einstein relation/crossover argument for the case of this non-random fractal.

The last point to be investigated is a possible relationship of d_w to an exponent characterising the distribution $P(L)$ of flight lengths on the fractal. $P(L)$ can be obtained as the limit for large n of the distribution $P_n(L)$ of flight lengths on the nth member of the hierarchy used in the recursive construction of the fractal. The relationship between the distributions P_n, P_{n+1} of two successive members is easily shown to be

$$(r+s+1)P_{n+1}(L) = (r+s)P_n(L) + (1/s)P_n(L/s). \tag{16}$$

So $P(L)$ satisfies

$$P(L) = (1/s)P(L/s). \tag{17}$$

Defining the αth moment by

$$\langle L^\alpha \rangle \equiv \int \mathrm{d}L L^\alpha P_n(L) \tag{18}$$

it follows from (16) that

$$\langle L^\alpha \rangle_n \propto \left(\frac{r+s+s^\alpha}{r+s+1} \right)^\alpha \tag{19}$$

so

$$\begin{aligned} \langle L^\alpha \rangle \equiv \int \mathrm{d}L L^\alpha P(L) \equiv \lim_{n\to\infty} \langle L^\alpha \rangle_n &= 0 \qquad \alpha < 0 \\ &= 1 \qquad \alpha = 0 \\ &= \infty \qquad \alpha > 0. \end{aligned} \tag{20}$$

The divergence of the moments (for $\alpha > 0$) is the reason for the non-Gaussian character of the diffusion process [5].

From (17) it can be seen that $P(L)$ can be written in the form $L^{-(F+1)}Q(L)$ where Q is periodic in $\ln L$ with period $\ln s$ and $F = 0$. A similar form applies for the Weierstrass walk and there the (non-zero) exponent F is related to the dimension d_w of the walk [5]. A similar result holds for Lévy flights [1]. In the present case however, d_w is not determined by F and this breakdown of the result which applies for the Lévy flights and Weierstrass walk is due to the complicated recursion equation for $P_n(L)$ which applies in the present case: (16) has two terms on the right-hand side (from the superposition of two 'dilatations', by s and by unity) while the corresponding equation for the Weierstrass walk has only one term and the resulting $P(L)$ can be characterised adequately by F. In the present case detailed expressions for $P(L)$ can be obtained by iterating (16) from the distribution $P_0(L) = \delta(L-1)$ for a single bond, or by combinatoric methods. One asymptotic result, which shows clearly the appearance of arbitrarily long flights, is

$$P(L) = \lim_{n\to\infty} A(n, r, s)\frac{1}{L}\sum_{N=0}^{\infty}\delta(\ln L - N\ln s) \times \exp\left[-\frac{(r+s+1)^2}{2n(r+1)}\left(\frac{\ln L}{\ln s} - \frac{n}{r+s+1}\right)^2\right] \tag{21}$$

(where $A(n, r, s)$ is a normalisation constant).

The conclusions of this work are that in the rather general fractal models with bridges of unlimited length here considered, or the associated problems of diffusion with flights, the walk dimension d_w is not in general related to the exponent F characterising the flight distribution, nor can it be made equal to 2 except in the limit of rare crosslinking. In addition it was shown that the Einstein/crossover relationship between d_w, d_f and the conductance exponent $\tilde{t}$ does apply.

References

[1] Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
[2] Stapleton H J, Allen J P, Flynn C P, Stinson D G and Kurtz S R 1980 *Phys. Rev. Lett.* **45** 1456
[3] Helman J S, Coniglio A and Tsallis C 1984 *Phys. Rev. Lett.* **53** 1195
[4] Cates M E 1985 *Phys. Rev. Lett.* **54** 1733
[4a] Stapleton H J 1985 *Phys. Rev. Lett.* **54** 1734
Helman J S, Coniglio A and Tsallis C 1985 *Phys. Rev. Lett.* **54** 1735
[5] Montroll E W and Schlesinger M F 1984 in *Non-Equilibrium Phenomena II* ed J L Lebowitz and E W Montroll (Amsterdam: North-Holland)
[6] Stinchcombe R B 1984 in *Static Critical Phenomena in Inhomogeneous Systems* (*Lecture Notes in Physics* **206**) ed A Pękalski and J Sznajd (Berlin: Springer)
[7] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
[8] Gefen Y, Aharony A and Alexander S 1983 *Phys. Rev. Lett.* **50** 77
[9] Harris C K and Stinchcombe R B 1983 *Phys. Rev. Lett.* **50** 1399
[10] Kirkpatrick S 1973 *Solid State Commun.* **12** 1279
[11] Gefen Y to be published