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LETTER TO THE EDITOR

A diffusion model for transport on loopless aggregates

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Abstract. We propose a diffusion equation for transport on a loopless aggregate. The relevant distance variable is the chemical distance and the spatially dependent coefficients of the diffusion equation are found in terms of $B(l)$, the number of bonds at chemical distance l from the vertex of the tree, and $B^s(l)$, the number of bonds on the skeleton of the tree. It is shown that the resulting motion can be modelled in terms of a biased one-dimensional random walk with a probability of remaining in place that approaches 1 as $l \to \infty$. This is interpreted as being due to motion along dead ends. An important consequence of the model is a simple derivation of the expressions relating the diffusion exponent and fracton dimension to the fractal dimension and the intrinsic dimensions of the tree and its skeleton. The mean first-passage time to go from the vertex to an arbitrary shell is also found.

The analysis of transport properties on fractal aggregates has attracted considerable recent attention (Alexander and Orbach 1982, Ben-Avraham and Havlin 1982, Gefen *et al* 1983, Mandelbrot 1982, Rammal and Toulouse 1983, Pandey and Stauffer 1983). In earlier papers we have considered the problem of establishing the relations that must exist between exponents that characterise the diffusive motion (Havlin *et al* 1984, 1985b). The argument presented in these earlier papers was based on the Einstein relationship which allows one to express the chemical diffusion exponent d_w^l, the spatial diffusion exponent d_w, and the fracton dimension d, in terms of the fractal dimension, d_f, the intrinsic dimension of the tree, d_l, and that of the skeleton, d_l^s. These relations were shown to be $d_w^l = 2 + d_l - d_l^s$, $d_w = d_f/[d_l(2 + d_l - d_l^s)]$ and $d = 2d_l/(2 + d_l - d_l^s)$. When the trees are finitely ramified $d_l^s = 1$. This special case was applied to the analysis of lattice animals (Havlin *et al* 1984) and diffusion limited aggregation (Havlin *et al* 1984, Witten and Kantor 1984). In this letter we suggest an alternative approach for the study of diffusion on loopless aggregates based on the properties of an appropriately constructed diffusion equation. The philosophy of this approach is somewhat similar to that found in a recent investigation by O'Shaughnessy and Procaccia (1985). In contrast to their work, which expresses results in terms of geometric distances, we will use the chemical distance l (Havlin and Nossal 1984). A heuristic derivation of our suggested equation will be given.

Let us therefore consider a loopless tree characterised by a vertex or origin, an infinite branched skeleton, and finite dead ends that branch from the skeleton. The resulting structure, for simplicity, will be assumed initially to be discretised in units

of Δl. Later we will pass to the continuum limit. The random walk is chosen to be unbiased, allowing steps to nearest neighbours only. Thus a random walker at l can move in a single step only to $l \pm \Delta l$ on the tree with probabilities denoted by $p_{\pm}(l)$. The probability at each node for moving along a particular branch feeding into it is assumed to be equal to $1/n$, where n is the number of such branches. If we consider the transition probabilities as a function of l then it is evident that the $p_{\pm}(l)$ are not necessarily equal, nor do they necessarily sum to one, since the tree is more richly branched as l increases. It will therefore also be necessary to define a probability for pausing at any given step, equal to $p_0(l) = 1 - p_+(l) - p_-(l)$. In order to derive expressions for these probabilities we need to define quantities that characterise the tree and whose properties are assumed to be known. These will be $B(l)$, the number of bonds at chemical distance l from the vertex, and $B^s(l)$, the number of bonds on the skeleton at l. The probabilities $p_0(l)$ and $p_{\pm}(l)$ are related to these quantities by

$$p_0(l) = 1 - p_+(l) - p_-(l) = 1 - B^s(l)/B(l) \tag{1a}$$

$$p_+(l)/p_-(l) = B^s(l+1)/B^s(l). \tag{1b}$$

The first of these relations indicates that the random walker pauses in its progress along the skeleton whenever it finds itself on a dead end. The second indicates that the relative probabilities of a step in the forward or backwards directions along the skeleton depend on the relative number of bonds allowing motion forward and backwards.

Equation (1), together with known scaling properties of $B(l)$ and $B^s(l)$ at large l, allows us to find asymptotic expressions for the transition probabilities. The exponents d_l and d_l^s characterise the mass of the tree and the skeleton respectively, through the relations $M(l) \sim l^{d_l}$ and $M^s(l) \sim l^{d_l^s}$. These lead to

$$B(l) \sim \mathrm{d}M(l)/\mathrm{d}l \sim l^{d_l - 1}, \qquad B^s(l) \sim \mathrm{d}M^s(l)/\mathrm{d}l \sim l^{d_l^s - 1} \tag{2}$$

which, together with equation (1) leads to explicit expressions for the transition probabilities. These are

$$p_{\pm}(l) = (A/2l^{\alpha})(1 \pm B/2l), \qquad p_0(l) = 1 - A/l^{\alpha} \tag{3}$$

where A is a constant related to the proportionality factors in the asymptotic expressions for $M(l)$ and $M^s(l)$, and the parameters α and B are related to d_l and d_l^s by

$$\alpha = d_l - d_l^s, \qquad B = d_l^s - 1. \tag{4}$$

Equation (3) implies that as the random walker moves further from the origin it is increasingly likely to remain stationary. This is reasonable from the consideration that the random walker is increasingly likely to be caught in a dead end as it moves away from the origin. The origin of the terms in parentheses in equation (3) is the fact that when the skeleton branches, or $d_l^s > 1$, the random walk is biased in the direction of the more richly branched section.

Our assumption that the random walk moves to nearest neighbours only, allows us to write a recursion relation for the state probabilities $U_n(l)$ at step n:

$$U_{n+1}(l) = p_+(l - \Delta l)\, U_n(l - \Delta l) + p_-(l + \Delta l)\, U_n(l + \Delta l) + p_0(l)\, U_n(l) \tag{5}$$

or equivalently, in terms of the difference operators $\Delta_l f(l) \equiv f(l+1) - f(l)$, $\Delta_n g(n) \equiv g(n+1) - g(n)$,

$$\Delta_n U_n(l) = \Delta_l^2 p_-(l - \Delta l)\, U_n(l - \Delta l)) + \Delta_l [(p_-(l - \Delta l) - p_+(l - \Delta l))\, U_n(l - \Delta l)] \tag{6}$$

where $\Delta^2 \equiv \Delta(\Delta)$. At sufficiently large values of l this equation becomes

$$\Delta_n U_n(l) \sim \frac{A}{2}\Delta_l^2\left(\frac{U_n(l)}{l^\alpha}\right) - \frac{AB}{2}\Delta_l\left(\frac{U_n(l)}{l^{\alpha+1}}\right). \tag{7}$$

This form of the transport equation suggests a passage to the diffusion equation limit by replacing the difference operators by derivatives. Strictly speaking this can only be justified for $B=0$ but we have found, using numerical solutions of equation (6), that the resulting diffusion equation

$$\frac{\partial U}{\partial n} = \frac{A}{2}\frac{\partial^2}{\partial l^2}\left(\frac{U}{l^\alpha}\right) - \frac{AB}{2}\frac{\partial}{\partial l}\left(\frac{U}{l^{\alpha+1}}\right) \tag{8}$$

leads to results in good agreement with the solutions of the difference equation. This is illustrated by the results shown in figure 1. The results of this model will now be discussed.

The solution to equation (8) that satisfies the initial condition $U(l,0)=\delta(l)$ is found to be

$$U(l,n) = \frac{\lambda^{(\alpha+1+B)/(2+\alpha)} l^{\alpha+B}}{\Gamma[(1+\alpha+B)/(2+\alpha)]} \frac{1}{n^{(\alpha+1+B)/(2+\alpha)}} \exp\left(-\frac{\lambda l^{2+\alpha}}{n}\right) \tag{9}$$

in which $\lambda = 2/[A(2+\alpha)^2]$. The expression for $U(l,n)$ allows us to deduce relations between the various exponents. The exponent d_w^l is readily found by calculating the mean square displacement $\sigma^2(l)$ from equation (9). Note that since l is always positive $\langle l\rangle > 0$. We find that the time dependence of $\sigma^2(l)$ is

$$\sigma^2(l) \equiv \langle l^2\rangle - \langle l\rangle^2 = Cn^{2/(2+\alpha)} \tag{10}$$

where C is a constant. This equation implies that $d_w^l = 2+\alpha = 2+d_l-d_l^s$. Furthermore, the behaviour of U for small but fixed l ($l=O(1)$) as $n\to\infty$ goes as $n^{-(1+\alpha+B)/(2+\alpha)}$ which implies that the fracton dimension is

$$\bar{d} = 2(1+\alpha+B)/(2+\alpha) = 2d_l/(d_l-d_l^s+2). \tag{11}$$

The exponents d_w^l and $\bar{d}$ are in agreement with those derived using an argument based on a calculation of resistance (Havlin *et al* 1984, 1985a, b), lending some confidence to the present results. One can observe that the term B representing the asymmetry of the structure does not appear in the exponential term in equation (9), but it does appear in the n-dependent term multiplying it and affects the fracton dimension in equation (11). That it should appear in the latter term is intuitively reasonable, since it represents the probability that the random walker is near the origin at step n. We have looked a little closer into the circumstances under which the B will appear in the exponent. Specifically we looked at the family of transition probabilities

$$p_\pm(l) = (A/2l^\alpha)(1 \pm B/2l^\beta) \tag{12}$$

finding that when $\beta \geqslant 1$, the parameter B does not appear in the exponent, in contrast to $\beta < 1$ when it does. This result was found by solving equation (5) numerically. No strictly analytic proof of its validity is known at present.

Our formula for $U(l,n)$ disagrees with that of O'Shaughnessy and Procaccia (1985), who derived a diffusion equation in the geometric distance, r, also based on scaling arguments. Although the average quantities and the scaling form represented by the exponents in equations (10) and (11) have been confirmed numerically (Havlin *et al*

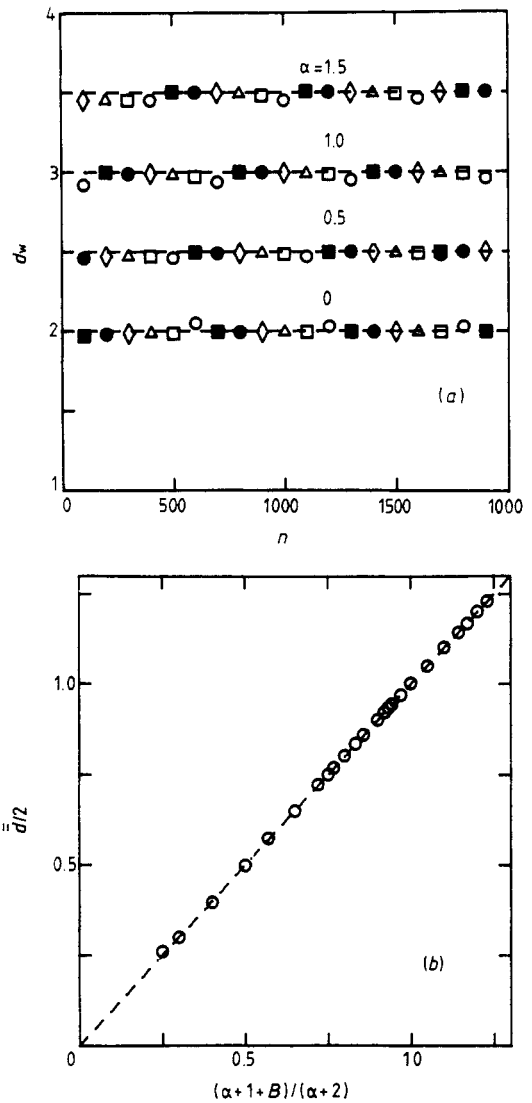

Figure 1. Results generated by a numerical solution of equation (5) for (*a*) d_w^l, (*b*) $\bar{d}$ for different values of the parameters α and B. These results are in agreement with equations (10) and (11). The different symbols in (*a*) represent different values of B: $B=-0.5$(○), $B=0.3$(□), $B=0.5$(△), $B=0.8$(◇), $B=1.0$(●), $B=1.5$(■). The symbols in (*b*) represent different (α, B) apirs in the ranges $0<\alpha\leqslant 1.5$, $-0.5\leqslant B\leqslant 1.5$.

1984, 1985b), we believe that the detailed form of equation (9) is not necessarily accurate for loopless aggregates or for other fractals. One might expect to have another exponent θ that characterises the random pausing time distribution caused by sojourns on dead ends. Thus, we conjecture that a more general treatment might lead to a change in the exponent in (9) to the form $\exp[-\lambda(l^{2+\alpha}/n)^{\theta}]$ with $\theta<1$. Very recent unpublished numerical results for several fractals are consistent with the identification $\theta=(d_w-1)^{-1}$. Such an effect has been found recently for diffusion on percolation clusters (Havlin *et al* 1985a).

If the diffusion equation in equation (8) is found in more detail to lead to an accurate description of transport on such loopless aggregates, then it is also possible to solve first-passage problems for the time to reach a shell at a specified value of the chemical distance. For example, if equation (8) is expressed as

$$\partial U/\partial n = MU \tag{13}$$

where M is the differential operator involving l, then the mean first-passage time to reach level L starting from level l is given as the solution to

$$M^{+}\langle n(l)\rangle = -1 \tag{14}$$

where M^{+} is the adjoint operator to M (Weiss 1967). This equation is to be solved subject to the boundary conditions

$$\langle n(L)\rangle = 0, \qquad \mathrm{d}/\mathrm{d}l\langle n(l)\rangle|_{l=0} = 0 \tag{15}$$

It is easy to show, using the combination of equations (8) and (13)-(15), that $\langle n(0)\rangle \sim L^{\alpha+1}$ which is the result one expects knowing that $\langle l\rangle \sim n^{1/(\alpha+2)}$.

References

Alexander S and Orbach R 1982 *J. Physique* **43** L625
Ben-Avraham D and Havlin S 1982 *J. Phys. A: Math. Gen.* **15** 2691
Gefen Y, Aharony A and Alexander S 1983 *Phys. Rev. Lett.* **50** 77
Havlin S, Djordjevicz Z V, Majid I, Stanley H E and Weiss G H 1984 *Phys. Rev. Lett.* **53** 178
Havlin S, Movshovitz O, Trus B and Weiss G H 1985a *J. Phys. A: Math. Gen.* **18** L719
Havlin S and Nossal R 1984 *J. Phys. A: Math. Gen.* **17** L427
Havlin S, Nossal R, Trus B and Weiss G H 1985b *Phys. Rev.* B **31** 7497
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
O'Shaughnessy B and Procaccia I 1985 *Phys. Rev. Lett.* **54** 455
Pandey R B and Stauffer D 1983 *Phys. Rev. Lett.* **51** 527
Rammal R and Toulouse G 1983 *J. Physique Lett.* **44** L13
Weiss G H 1967 *Adv. Chem. Phys.* **13** 1
Witten T A and Kantor Y 1984 *Phys. Rev.* B **30** 4093