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LETTER TO THE EDITOR

Diffusion on fractal lattices and the fractal Einstein relation

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Abstract. Finitely ramified fractal lattices show anomalous diffusion with $\langle r^2 \rangle \propto t^{2H}$. There is a hierarchy of transit times which are shown by Monte Carlo simulation to satisfy $\langle \tau_n \rangle \propto \alpha^n$ for large n, where $\alpha = b^{1/H}$ and b is the base of the lattice. The lattice resistivity scales with size as $\rho \propto R^n$ where R is characteristic of the lattice. Exact renormalisation group methods yield α and R analytically and verify the Einstein relation for fractals $\alpha = RN$.

The main reason for investigating transport properties on fractal lattices (Mandelbrot 1982) is that solution of many important equations of physics on these lattices adds to our understanding of the geometric and topological properties that are relevant to modelling the corresponding physical processes. We develop and test an especially simple fractal form of the Einstein relation between the transient or diffusive and steady-state or conductive solutions of the potential equation on these lattices. This report extends and illustrates some ideas that have been developed in a study of conduction and diffusion in random networks such as percolation clusters (see the 'ant in the labyrinth problem' in de Gennes (1976), Straley (1980), Mitesku *et al* (1979), Roussenq (1980), Vicsek (1981); see also Gefen *et al* (1981), Ben-Avraham and Havlin (1982), Angles d'Auriac *et al* (1983), Alexander and Orbach (1982), Rammal and Toulouse (1983)). The same diffusion properties are verified here for a class of deterministic fractal lattices.

Figure 1 depicts the generators of the fractal lattices we consider, and table 1 lists their geometric and physical properties, determined both analytically and by Monte Carlo simulation. All these lattices are constructed by hierarchical extrapolation. Each stage of construction takes N copies of the order-n lattice, reduces them in the ratio $r = 1/b$, where b is an integer called the base, and connects them following a 'generating tie scheme' (see figure 2).

The profound qualitative differences between fractal lattices of finite and infinite ramification (Mandelbrot 1982, ch 16, and Gefen *et al* 1980) also prove critical to diffusion, hence infinitely ramified fractals are not treated in this paper.

In Monte Carlo simulations of random walks on fractal lattices, a starting point was selected at random, and each trial proceeded either until a prescribed number of steps was reached, or until the walk reached an absorbing boundary. The lattice size and the number of steps satisfy two goals. (1) The average walk diffuses long enough to be affected by the lattice structure (tremas or water sheds) over several levels of the fractal hierarchy. (2) A negligible fraction of the walks are absorbed by the boundary. By construction, any lattice vertex lies in a nested sequence of successively higher-order copies of the lattice. The corner vertices of an order-n lattice lie a

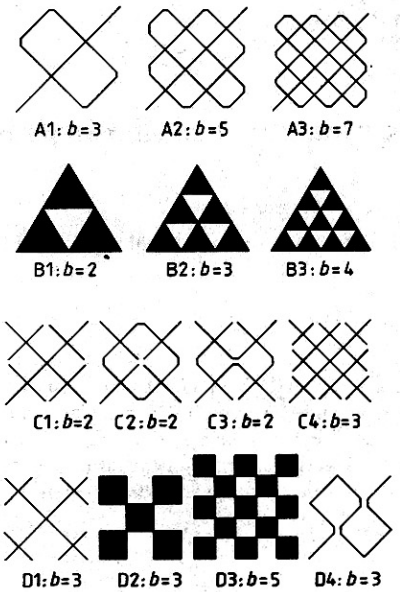

Figure 1. Generators (atoms) of our lattices.

Table 1.

Base	α	R	N	H (calc)	H (MC)
		Plane-filling 'Phi lattices' (*e.g. figure* 1(*A*))			
3	117/5	13/5	9	0.348 46	0.352
5	7175/87	287/87	25	0.364 75	0.367
7	897925/4901	18 325/4901	49	0.373 45	
9	329.148	4.0636	81	0.379 06	
11	522.878	4.3213	121	0.383 09	
13	765.1965	4.5278	169	0.386 27	
21	2270.200	5.1478	441	0.393 98	
		Sierpiński gaskets (*e.g. figure* 1(*B*))			
2	5	5/3	3	0.430 7	0.431
3	90/7	15/7	6	0.430 2	
4	1030/41	103/41	10	0.430 0265	
5	8315/197	1663/591	15	0.430 0306	
		Plane-filling 'X-lattices' (*figure* 1(*C*))			
2	8	2	4	1/3	0.333
2	$4+2\sqrt{2}$	$1+\sqrt{2}/2$	4	0.3608	0.365
2	7.2769	1.8192	4	0.3492	
3	22.457	2.495	9	0.3531	
		'X-lattice'; checkerboards; Peano curve (*figure* 1(*D*))			
3	15	3	5	0.405 68	
3	15	3	5	0.405 68	
5	51.54	3.96	13	0.4082	0.407
3	81	9	9	0.250	0.250

Figure 2. To construct our fractal lattices, copies of the initiator 'atom' are connected according to the generating tie scheme to yield the second-order lattice.

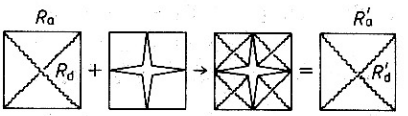

Figure 3. Construction of the renormalisation group for resistivity calculations; copies of the order-n universal graph are connected using the generating tie scheme. The $(n+1)$-order universal graph is then required to have identical two-point resistances.

distance $\propto b^n$ from an arbitrary vertex and serve as gates which must be crossed in order to diffuse further. Define the order-n transit time τ_n to be the first passage time to the corners of the order-n lattice from a random starting point inside it. Monte Carlo simulations show that $\langle\tau_n\rangle = K_1\alpha^n + K_2$, where the 'transit time' α is a characteristic of the lattice. Renormalisation group arguments yield K_1 and K_2 analytically and prove that differently defined transit times show the same scaling behaviour. The simplest ansatz consistent with the observed scaling for the τ_n is $\langle r^2(t)\rangle = t^{2H}$ with

$$H = \log b/\log\alpha \qquad \text{and} \qquad \alpha = \lim_{n\to\infty}\langle\tau_{n+1}\rangle/\langle\tau_n\rangle. \tag{1}$$

If the Einstein relation holds for self-similar structures, then (Gefen *et al* 1983)

$$\theta = -2 + 1/H = t/\nu - \beta/\nu \tag{2}$$

relates the exponents describing the power-law dependence on scale length L of the conductivity $\sim L^{-t/\nu}$ and the diffusion coefficient $\sim L^{-\theta}$. Here (Gefen *et al* 1983)

$$\beta/\nu = 2 - D = 2 - \log N/\log b; \qquad t/\nu = \log R/\log b, \tag{3}$$

where we define R by assuming that for large n the two-point resistance of an order-n lattice of unit resistors is $\propto R^n$. Substituting (1) and (3) into (2) yields

$$\alpha = RN, \tag{4}$$

which we call the fractal Einstein relation.

Using exact renormalisation group methods, we obtain exact values for α and R, although for convenience we sometimes use instead an iterative form of our renormalisation group which is easily adapted to computer solution and will also be presented. We model an order-n fractal lattice with a universal graph having a vertex for each gate of order n and identical physical properties. Linear equations are solved to yield recursively effective parameters for the equivalent universal graph. This procedure will be illustrated for figure 1(C2). Due to its Z_4 rotational symmetry, two effective parameters suffice to match either the resistivity or diffusion properties of the order-n lattice. The equivalent resistors connecting adjacent and diagonally opposite vertices will be denoted by R_a and R_d. The order-$(n+1)$ lattice connects copies of this graph according to the generating tie scheme of the lattice. The R'_a and R'_d of the resulting graph are then functions of R_a and R_d:

$$\begin{aligned} R'_a &= R_a(2R_d + R_a)/(R_d + R_a), \\ R'_d &= R_a(2R_d + R_a)(3R_d + R_a)/(R_d + R_a)^2. \end{aligned} \tag{5}$$

The unique positive fixed point yields $R'_a/R_a = R'_d/R_d = R = (1+\sqrt{2}/2)$. To calculate

α, the order-n lattice is modelled by a universal graph with bonds connecting each pair of gate vertices and effective transit 'step times' T_a(resp T_d) to an adjacent (resp diagonally opposite) gate vertex. Copies of this graph are connected to model random walk on the order-$(n+1)$ lattice. Average transit times to the corners of this lattice are then used as step times in the next-order universal graph. The relative probabilities of adjacent and diagonal steps on these equivalent graphs must also be calculated because they vary with n. Denote by $4P_a$ the probability that the next order-n gate is reached via sideways transition, and by $2P_d = 1-4P_a$ the probability that the next gate is reached via diagonal transition. Recursions for the corresponding order $(n+1)$ probabilities are obtained by using the Markov nature of these random walks to relate the conditional probabilities P'_{ak}, P'_{dk} for walks starting at any vertex in the graph to those for walks starting at its neighbours

$$P'_{ak} = P_a \sum_i P'_{ai} + P_d \sum_j P'_{aj}, \qquad P'_{dk} = P_a \sum_i P'_{di} + P_d \sum_j P'_{dj}, \tag{6}$$

sums over i, j being respectively those over adjacent and diagonal neighbours of vertex k. For this example

$$P'_a = P_a^2(4P_a^2-1)(2P_d+1)/\Delta, \qquad P'_d = -2P_a^2(2P_a^2+P_d)(2P_d+1)/\Delta, \tag{7}$$

with

$$\Delta = P_a^4(16P_d-56) + P_a^2(8P_d^2-28P_d+16) - (2P_d-1)^2.$$

Eliminating P_d using the relation $4P_a+2P_d=1$ yields $P'_a = (2P_a+1)/(4P_a+6)$, with a single positive fixed point at $P_a = (\sqrt{2}-1)/2 = 0.207\,107$. (In the above, a matrix whose elements depend on two variables was inverted using the IBM symbolic calculation program SCRATCHPAD.) The expressions (7) for P'_a, P'_d are generating functions for random walks from a gate vertex to an adjacent, resp diagonally opposite, order-$(n+1)$ gate vertex: the coefficient of the term $P_a^m P_d^n$ yields the number of walks of this type consisting of m adjacent and n diagonal steps. Thus, defining $Q = T_a P_a \partial/\partial P_a + T_d P_d \partial/\partial P_d$, we have $T'_a = (1/P'_a)\,QP'_a$ and $T'_d = (1/P'_d)QP'_d$. The ratio of these equations yields the positive fixed point $T_d/T_a = (8+10\sqrt{2})/17$, hence the asymptotic scaling behaviour $T'_a/T_a = T'_d/T_d = 4+2\sqrt{2}$. The fractal Einstein relation is exactly verified.

In general, given limit values for P_a and P_d, the scaling parameter α for the diagonal and adjacent step times in the nth order universal graph is obtained non-iteratively by solving the Markov equations for $(n+1)$-order conditional transition times to a diagonally opposite gate vertex, similar to those for P_a and P_d:

$$T'_k = 4P_a\Big(\sum_i (T'_i + T_a)\Big/\sum_i 1\Big) + 2P_d\Big(\sum_j (T'_j + T_d)\Big/\sum_j 1\Big).$$

(The diagonal transition time from any vertex is a weighted average of those of its neighbours.) The solution for α is noniterative because the only independent transition time in the equations, $T_{aver} = 4P_aT_a + 2P_dT_d$, enters linearly and the diagonal transition time, which is one component of their solution, is $T'_{diag} = \frac{1}{2}(1-2P_a)T'_{aver}$.

Figure 1(C3) is a lattice whose generator lacks Z_k symmetry (k is the number of corner vertices)†. The recursion for the two independent resistor ratios (figure 4) is:

† If the renormalisation group is constructed by our scheme for a lattice having a general anisotropic three-corner atom and the tie generating scheme of figure 2(b), the only non-trivial fixed point corresponds to the Sierpiński gasket. The same is true for arbitrary values of the base b. This explains why this family of fractals attains scaling behaviour immediately. See Rammal and Toulouse (1983).

$$r_1' = \frac{(r_1+r_2)(3r_1+2r_1+2r_2+3r_1r_2)}{5r_1^2+2r_2^2+7r_1r_2+9r_1^2r_2+5r_2^2r_1+4r_1^2r_2^2},$$

$$r_2' = \frac{r_2(r_1+1)(3r_1+2r_2+3r_1r_2)}{4r_1^2+2r_s^2+5r_1r_2+9r_1^2r_2+7r_2^2r_1+5r_1^2r_2^2},$$

where $r_1 = R_H/R_D$ and $r_2 = R_V/R_D$. This renormalisation group, again, has only one non-zero stable fixed point in the physical regime: $(r_1, r_2) = (0.575\,458,\ 0.426\,970)$. It yields $R = 1.8192$.

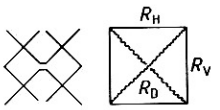

Figure 4. Universal graph for the asymmetric lattice C3.

The Markov equations for relative transition probabilities were iterated on the computer to yield $P_H = 0.17104$, $P_V = 0.230\,53$, $P_d = 0.098\,43$, where $2P_H + 2P_V + 2P_d = 1$. The equations for α contain only one independent transition time

$$T_{av} = 2P_HT_H + 2P_VT_V + 2P_dT_d,$$

and are solved non-iteratively as before via the diagonal transition time and the relation $T'_{av} = (1-2P_H)(1-2P_V)T'_d/(1+2P_d)$. In this case, $\alpha = T'_{av}/T_{av} = 7.2769$.

Note added in proof. Mandelbrot (*Proc. Stat Phys.* **15** to appear in *J. Stat. Phys.*) is relevant to the discussion in this paper, because it advances a formalism that applies both to diverse fractal diffusions in Euclidean spaces and to diffusions restricted to fractals. In this formalism, $1/H$ (as defined in this paper) is the diffusion's 'latent fractal dimension' and $D \times H$ (a ratio of latent dimensions) is the 'latent fractal co-dimension' of the instant when the diffusion recurs to its points of departure.

The examples in Table I all lie in the plane, $d = 2$. Comparing the diverse phi-lattices, the diverse Sierpinski gaskets, and the X-lattices of bases 3 and 5, we see that in each series taken separately H is nearly, but not quite, independent of the base.

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