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LETTER TO THE EDITOR

Absorption probability distribution for rough surfaces

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Abstract. We calculate the absorption probability distribution for particles diffusing onto perfectly absorbing boundaries. The boundaries studied are rough but not fractal; nevertheless, non-classical behaviour is evident in the singularities of the measure and their distribution.

The phenomenon of multifractality has recently attracted considerable attention. The existence of an infinite set of exponents characterising the moments of a measure has been discerned in many diverse problems including fully developed turbulence (Benzi *et al* 1984), localisation (Castellani and Peliti 1986), dynamical systems (Benzi *et al* 1984, 1985, Jensen *et al* 1985, Halsey *et al* 1986a), diffusion-limited aggregation (DLA) (Meakin *et al* 1985, Turkevitch and Scher 1985, Amitrano *et al* 1986, Halsey *et al* 1986b, Meakin 1986a) and resistor networks (de Arcangelis *et al* 1985, Blumenfeld *et al* 1986).

This activity has stimulated, and is partly a consequence of, a general theory for fractal measures (Kadanoff 1986, Halsey *et al* 1986a), of which we make use here. One imagines the object divided into N pieces of length L and the measure for the ith piece equal to p_i $(i = 1, \ldots, N)$. Then the qth moment of the probability measure is defined by

$$M_q = \sum p_i^q. \tag{1}$$

The dimension D_q associated with the moment M_q is defined by (Hentschel and Procaccia 1983)

$$D_q = \lim_{L \to 0} \frac{1}{q-1} \frac{\ln M_q}{\ln L} \tag{2}$$

and for the problem studied here this is equivalent to the D_q defined by Halsey *et al* (1986a). The singularities of the measure have strength

$$\alpha(q) = \frac{\mathrm{d}}{\mathrm{d}q}[(q-1)D_q] \tag{3}$$

and are distributed over sets of dimension

$$f(\alpha(q)) = q\alpha(q) - (q-1)D_q. \tag{4}$$

The form of these functions is characteristic of the problem under consideration.

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In this letter we calculate the absorption probability distribution $\{p_i\}$ for particles diffusing onto a perfectly absorbing boundary. The boundary is 'rough' and the probability of absorption at site i is a strong function of the site's position. To control the roughness, the boundaries considered here are the successive stages in the recursive construction of the well known Koch curve. There is, in consequence, no averaging over configurations as in, say, DLA. The level 1 recursion is shown in figure 1. The sites of our boundary are the vertices of the Koch construction. Periodic boundary conditions are imposed so that, in figure 1, A is a neighbour of B and site C is deleted. One imagines particles diffusing from a height $y = X$ along the bonds of a triangular lattice and onto the Koch boundary. If a particle diffuses above height X it is considered to have 'died'. (Naturally the choice of height X has some effect on the distribution $\{p_i\}$, although for large enough X the effect would be small; we will consider the influences of boundary conditions fully in a subsequent paper.) This model is pertinent to the study of DLA and also to catalysis (see below).

It is well known that the adjacency matrix of a graph raised to a power n results in a matrix whose elements are the number of distinct paths between the vertices of the graph. Using this fact one can easily determine $\{p_i\}$ by multiplying together matrices for a graph representing the whole lattice. More specifically, if $p_{ij}(n)$ is the probability that a diffusing particle initially at site i arrives, after n steps, at site j, then

$$p_i = \left\langle \sum_n p_{ki}(n) \right\rangle_{\text{starting points } k} \tag{5}$$

with

$$\{p_{ij}(n)\} = A^n \tag{6}$$

and A is the adjacency matrix normalised so that

$$\begin{aligned} &\sum_j a_{ij} = 1 && \text{for site } i \text{ not on boundary} \\ &a_{ij} = 0 && \text{for } i \text{ on boundary.} \end{aligned} \tag{7}$$

Making use of (2)-(4) one determines the 'multifractal' nature of this problem. Results are shown in figures 2 and 3. It is not easy, when we use the above method, to proceed to higher levels of recursion because of the computer resources required. We are presently assessing the feasibility of other approaches; our preliminary Monte Carlo results appear promising. The similarity between figure 3 and a corresponding graph for small DLA clusters (Amitrano *et al* 1986) should be noted. Notice that for large q

$$(q-1)D_q \to q \ln p_{\max}/\ln L = q\alpha_{\min} \tag{8}$$

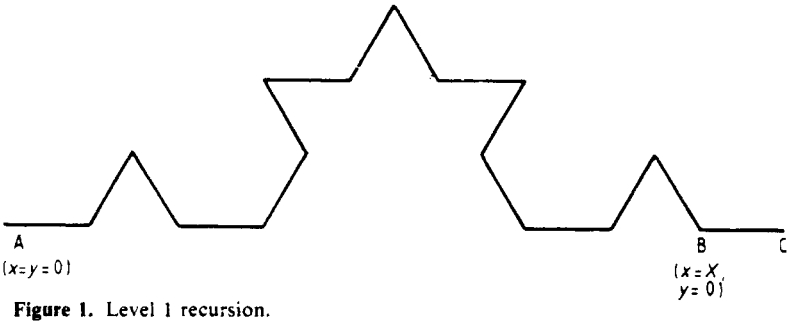

Figure 1. Level 1 recursion.

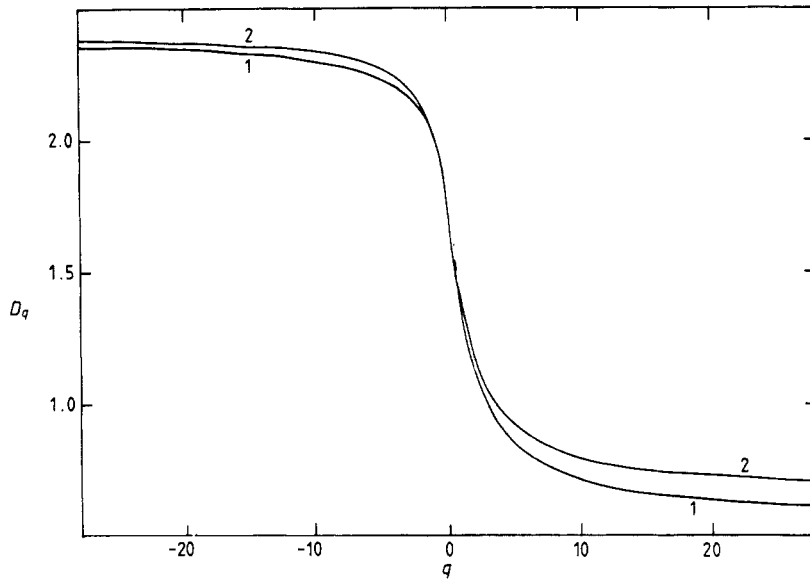

Figure 2. The exponent D_q. The labels 1 and 2 refer to the level of the Koch curve recursion.

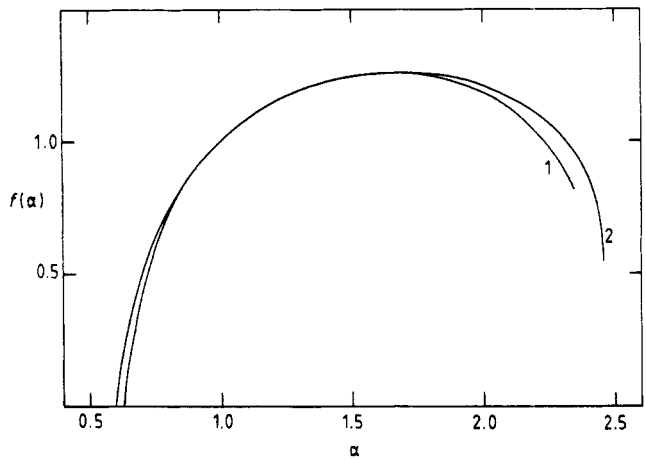

Figure 3. Dependence of dimension f on singularity strength α. Again labels 1 and 2 refer to the recursion level.

and for large negative q

$$(q-1)D_q \to q \ln p_{\min}/\ln L = q\alpha_{\max}. \tag{9}$$

A single power law singularity in the measure has $(q-1)D_q$ linearly dependent on q (Halsey *et al* 1986a). Meakin *et al* (1986) predict, on that basis, that a non-fractal object should show a linear dependence of $(q-1)D_q$ on q for q larger than some critical value and that $D_q = 1$ below. In contrast, our calculations show that $(q-1)D_q$ is, for intermediate q, not linear in q and there is a smooth crossover between the extreme linear behaviours ((8) and (9)). This difference arises because, although our boundaries are non-fractal, they are nevertheless associated with a range of power law

Table 1.

	ln S	
ln k_1/k_f	level 1	level 2
−20	17.227 441 3	15.841 121 8
−19	16.227 441 4	14.841 123 3
−18	15.227 441 7	13.841 127 4
−17	14.227 442 5	12.841 138 4
−16	13.227 444 7	11.841 168 5
−15	12.227 450 7	10.841 250 1
−14	11.227 466 8	9.841 471 97
−13	10.227 510 7	8.842 073 82
−12	9.227 629 84	7.843 701 29
−11	8.227 953 53	6.848 063 25
−10	7.228 831 27	5.859 484 79
−9	6.231 201 78	4.887 702 59
−8	5.237 533 74	3.949 040 31
−7	4.253 966 54	3.056 090 08
−6	3.293 674 92	2.202 094 66
−5	2.375 876 49	1.373 444 00
−4	1.507 411 60	0.561 343 50
−3	0.665 641 32	−0.252 611 70
−2	−0.180 834 71	−1.097 381 98
−1	−1.056 565 25	−1.993 053 75
0	−1.974 521 58	−2.936 611 46
1	−2.930 979 39	−3.911 085 79
2	−3.911 684 68	−4.900 781 64
3	−4.903 995 06	−5.896 846 73
4	−5.901 075 86	−6.895 378 41
5	−6.899 989 15	−7.894 835 36
6	−7.899 587 60	−8.894 635 20
7	−8.899 439 63	−9.894 561 51
8	−9.899 385 17	−10.894 534 4
9	−10.899 365 1	−11.894 524 4
10	−11.899 357 8	−12.894 520 7
11	−12.899 355 0	−13.894 519 4
12	−13.899 354 0	−14.894 518 9
13	−14.899 353 7	−15.894 518 7
14	−15.899 353 5	−16.894 518 6
15	−16.899 353 5	−17.894 518 6
16	−17.899 353 5	−18.894 518 6
17	−18.899 353 5	−19.894 518 6
18	−19.899 353 5	−20.894 518 6
19	−20.899 353 5	−21.894 518 6
20	−21.899 353 5	−22.894 518 6

singularities. As the recursion level goes to infinity the boundary becomes fractal and one would expect a continuous distribution of singularities. The closeness of the curves in figure 3 intimates that the distribution of singularities for the limit Koch curve may not be too dissimilar from the low-level approximations obtained after only a few recursions.

We now briefly discuss a practical application of the calculated distribution $\{p_i\}$. Following Meakin (1986b), we consider the reaction scheme

$$A + S \rightarrow A_a \tag{10a}$$

$$A_a \rightarrow B \tag{10b}$$

$$A + A_a \rightarrow C. \tag{10c}$$

(10*a*) represents the adsorption of an A molecule onto a catalyst surface (S). Reaction (10*b*) is the conversion of adsorbed A molecules into B molecules with rate constant k_1. The B molecules are, on their formation, immediately desorbed. Reaction (10*c*) represents the interaction of an A molecule with a previously adsorbed A molecule to produce a C molecule, which we assume is also desorbed promptly. Classically, the selectivity (i.e. ratio of C to B produced) of the catalyst should be inversely proportional to k_1. Meakin found that for a particular fractal catalyst $S \propto k_1^{-0.79}$. In terms of the $\{p_i\}$, S is given by (see Meakin 1986b)

$$S = \frac{k_f \Sigma p_i^2/(k_1 + 2p_i k_f)}{k_1 \Sigma p_i/(k_1 + 2p_i k_f)} \tag{11}$$

where k_f is the input flux of particles. This function is given in table 1. Note the region in the centre of the range where S is not linearly dependent on $1/k_1$. Outside this central region S is proportional to $1/k_1$, as expected for a smooth catalyst.

It is apparent from the above discussion that the transition from 'rough' behaviour to genuine fractal behaviour is a gradual one. In this context it is worthwhile recalling that even the largest simulated DLA clusters (for example) only have 'fractal' properties over appropriate length scales. The surprise is that incipient multifractal behaviour can be observed even for very low levels of recursion when the boundary is only *beginning* to look fractal. Figure 3 is both an extrapolation and interpolation and it is interesting that there appears to be only a small dependence on the level of recursion. We intend to go on and further investigate the crossover between rough and fractal boundaries.

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