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LETTER TO THE EDITOR

Scaling behaviour for excitation trapping on fractals

G Zumofen†, A Blumen‡ and J Klafter§

† Laboratorium für Physikalische Chemie, ETH-Zentrum, CH-8092 Zürich, Switzerland
‡ Lehrstuhl für Theoretische Chemie, Technische Universität München, D-8046 Garching, West Germany
§ Corporate Research Science Laboratories, Exxon Research and Engineering Co, Clinton Township, Annandale, New Jersey 08801, USA

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Abstract. We study the decay behaviour of a nearest-neighbour random walker which gets trapped at the first encounter of a sink. As underlying structures we consider fractals (Sierpinski gaskets) and regular lattices and establish the scaling behaviour of the decay law with respect to $x = -n^{\tilde{d}/2} \ln(1-p)$, where n is the number of steps, p the sink concentration and $\tilde{d}$ the spectral dimension. The decay scales well for x large. For small x, scaling is reasonable for the gaskets and the linear chain, and rather poor for the square lattice.

Recently, the topic of random walks on random media is enjoying growing interest, as witnessed by the large body of related research reviewed for instance in Weiss and Rubin (1983) and Hughes and Ninham (1983). Many stochastically disordered structures, like percolation clusters at criticality (Alexander and Orbach 1982), linear and branched polymers (Havlin and Ben-Avraham 1982), aggregates constructed by diffusion-limited growth (Witten and Sander 1983, Vicsek 1983), epoxy resins (Alexander *et al* 1983) and porous surfaces (Avnir *et al* 1983), are dilatationally invariant. These structures, while lacking translational symmetry, are self-similar under geometrical (length) scaling, and are thus fractals in the nomenclature of Mandelbrot (1977, 1982). Fractals, on the other hand, need not be stochastic: a well known example is the deterministically built Sierpinski gaskets (Sierpinski 1974, Urysohn 1927).

In this letter we address the problem of trapping of a random walker by randomly distributed sinks (traps) on fractals (Sierpinski gaskets). Applications of this problem are the energy transfer in disordered media (Zumofen and Blumen 1982, Blumen *et al* 1983, de Gennes 1983, Evesque 1983, Klafter *et al* 1984a, b) and also mathematically related problems such as the dielectric relaxation by diffusion of defects (Shlesinger and Montroll 1984) and the partition function for self-attractive polymers (Stanley *et al* 1983). Here we investigate both analytically and numerically the dependence on time and on the sink concentration of the decay law. We extend our calculations over many orders of magnitude and find that below the maximal dimension of two the decay law scales with time and with the sink concentration. The marginal dimension is related to the *compact* exploration, a concept stressed by de Gennes (1983).

As in our previous investigations (Zumofen and Blumen 1982, Blumen *et al* 1983, Klafter *et al* 1984a, b) we study trapping in the framework of the distribution R_n of distinct sites visited in n steps on the trap-free lattice. The quantity R_n is a stochastic variable, which depends on the particular realisation of the random walk. In the case

of equal microscopic transfer rates between the sites and if the walker is eliminated at its first sink encounter, the decay laws due to trapping are

$$\tilde{\Phi}_n = \langle (1-p)^{R_n} \rangle \equiv \langle \exp(-\lambda R_n) \rangle \tag{1a}$$

or

$$\Phi_n = \langle (1-p)^{R_n - 1} \rangle = \mathrm{e}^{\lambda} \tilde{\Phi}_n \tag{1b}$$

depending whether one allows the origin of the walk also to be a sink, (1*a*), or excludes this possibility, (1*b*). In these equations the average is to be taken over all random-walk realisations, and we set $\lambda = -\ln(1-p)$. Former investigations have focused on Φ_n, whereas $\tilde{\Phi}_n$ corresponds to a homogeneous initial condition (Klafter and Silbey 1983).

The right-hand side of (1*a*) now allows a cumulant expansion (Zumofen and Blumen 1982)

$$\tilde{\Phi}_n = \exp\left(\sum_{j=1}^{\infty} K_{j,n} (-\lambda)^j / j! \right) \tag{2}$$

where the $K_{j,n}$ are the cumulants of R_n. Including only a finite number of terms in (2) leads to approximations whose quality, however, depends both on the magnitude of λ and R_n and also on the properties of the distribution R_n, i.e. basically on the dimension of the underlying lattice. Thus, the cumulant expansion works better at small λ (i.e. for small trap concentrations), for small values of R_n (i.e. at shorter times) and for higher dimensions.

Let us now consider the cumulant expansion (2). We remark that for regular lattices the asymptotic behaviour with n of the first cumulants $S_n \equiv K_{1,n} = \langle R_n \rangle$ and $\sigma_n^2 \equiv K_{2,n} = \langle R_n^2 \rangle - \langle R_n \rangle^2$ is known (see Weiss and Rubin 1983):

$$d = 1: \quad S_n = c_1 n^{1/2} + \ldots, \qquad \sigma_n^2 = c_2 n + \ldots, \tag{3a}$$

$$d = 2: \quad S_n = c_1 n / \ln n + \ldots, \qquad \sigma_n^2 = c_2 n^2 / \ln^4 n + \ldots, \tag{3b}$$

$$d = 3: \quad S_n = c_1 n + \ldots, \qquad \sigma_n^2 = c_2 n \ln n + \ldots. \tag{3c}$$

In (3), c_1 and c_2 are constants which depend on the lattice type. In former works (Blumen and Zumofen 1982 and citations therein) we have analysed these expansions and have established additional terms to (3) for different lattice types. On the other hand, for Sierpinski gaskets one finds (Blumen *et al* 1983, Angles d'Auriac *et al* 1983)

$$S_n = c_1 n^{\tilde{d}/2} + \ldots, \qquad \sigma_n^2 = c_2 n^{\tilde{d}} + \ldots. \tag{4}$$

In (4), $\tilde{d}$ is the spectral dimension of a gasket strictly embedded in a d-dimensional Euclidean space, $\tilde{d} = 2\ln(d+1)/\ln(d+3)$ (Alexander and Orbach 1982, Rammal and Toulouse 1983); this dimension is distinct from the Hausdorff dimension $\bar{d} = \ln(d+1)/\ln 2$ of the gasket (Mandelbrot 1977, 1982), which measures the density of lattice sites. Equation (4) is reminiscent of the regular one-dimensional case (or, equivalently, of the $d = \tilde{d} = 1$ Sierpinski gasket), for which all cumulants obey (see Weiss and Rubin 1983)

$$K_{j,n} \sim c_j n^{j/2} \tag{5}$$

with c_j being constants. For the Sierpinski gaskets $\tilde{d}$ always lies between 1 and 2, and (4) is a natural extension of (5) to this region. We note that in two dimensions, because of the presence of logarithmic terms in (3*b*), the extension (4) does not hold. *A fortiori*, of course (4) does not hold in three dimensions.

Inserting now (4) into the cumulant expansion (2) leads to

$$\Phi_n = \exp[-\lambda(S_n - 1) + \lambda^2\sigma_n^2/2 - \ldots] \approx \exp[-c_1\lambda n^{\tilde{d}/2} + (c_2/2)\lambda^2 n^{\tilde{d}} - \ldots]. \tag{6}$$

We thus find $\Phi_n \approx \exp[-f(x)]$, where the function $f(x)$ stands for the (possibly asymptotic) series $\Sigma_j c_j(-x)^j/j!$ and where we set $x \equiv \lambda n^{\tilde{d}/2} = -n^{\tilde{d}/2}\ln(1-p)$. Note, however, that the dependence of Φ_n on x cannot be expected to hold strictly, since in the derivation forms valid in the moderate- and long-time limit, (3)–(5), were inserted into (2), which is a short-times expansion. That this result for fractals still provides a good qualitative picture is due to the fact that the domains of validity of (4) are reached very quickly ($n \geq 10$) (Blumen *et al* 1983). The regions in which the decay law scales with x will become evident from the numerical results for Φ_n, presented below.

Turning now to the long-time limit, we notice that for the gaskets one has asymptotically for n large (Klafter *et al* 1984a,b)

$$\Phi_n \approx \exp(-C\lambda^{2/(\tilde{d}+2)} n^{\tilde{d}/(\tilde{d}+2)}) = \exp[-f(x)] \tag{7}$$

where again $x \equiv \lambda n^{\tilde{d}/2}$ and now $f(x) = Cx^{2/(\tilde{d}+2)}$, where C is a constant. As discussed in the derivation of (7), this expression is a generalisation of the long-time survival probability in Euclidean spaces (Balagurov and Vaks 1973, Donsker and Varadhan 1975) and reduces to the Euclidean result by replacing $\tilde{d}$ by d. For Sierpinski gaskets the derivation of (7) is facilitated by using the concept of compact exploration, as stressed by de Gennes (1983).

Extending now (6) and (7) to the whole x-range $x \equiv \lambda n^{\tilde{d}/2} = -n^{\tilde{d}/2}\ln(1-p)$, one assumes for the decay law a general scaling form

$$\Phi_n = \exp[-f(x)] \tag{8a}$$

with a universal function $f(x)$, which behaves in the small and large x limits as

$$f(x) = \begin{cases} \sum_j c_j(-x)^j/j!, & (8b) \\ Cx^{2/(\tilde{d}+2)}. & (8c) \end{cases}$$

Next we will compare this scaling assumption with decay laws Φ_n followed over 20 orders of magnitude over a very large time and trap-concentration domain. As we proceed to show, the scaling assumption performs well for Sierpinski gaskets ($\tilde{d} < 2$), and is not well obeyed for regular ($d \geq 2$) lattices.

In order to obtain the decay law Φ_n we followed the method of our previous works (Zumofen and Blumen 1982, Blumen *et al* 1983, Klafter *et al* 1984a, b). Thus the distribution of R_n-values was determined numerically for random walkers on *trap-free* structures. The decay was then computed as in (1), by averaging $\exp(-\lambda R_n)$ over the simulated walks. This method allows, due to the analytical pre-averaging over the sink positions, an increase in accuracy and a considerable decrease of numerical effort. For the determination of R_n, 50 000 realisations of walks were used. Note that for a mean number S_n of sites visited this corresponds to some $5 \times 10^4 \times 2^{S_n}$ walks on lattices with traps, i.e. to a very large number. As random-number generator we used the procedure RN1 of the ETH Computer Center, whose performance was checked in former works (Zumofen and Blumen 1982, Blumen and Zumofen 1982) through comparison with known analytical results and with other Fortran random-number generators.

We start our analysis with the short- and moderately long-decay regime and plot in figure 1 Φ_n for three Sierpinski gaskets. For the embedding Euclidean spaces we

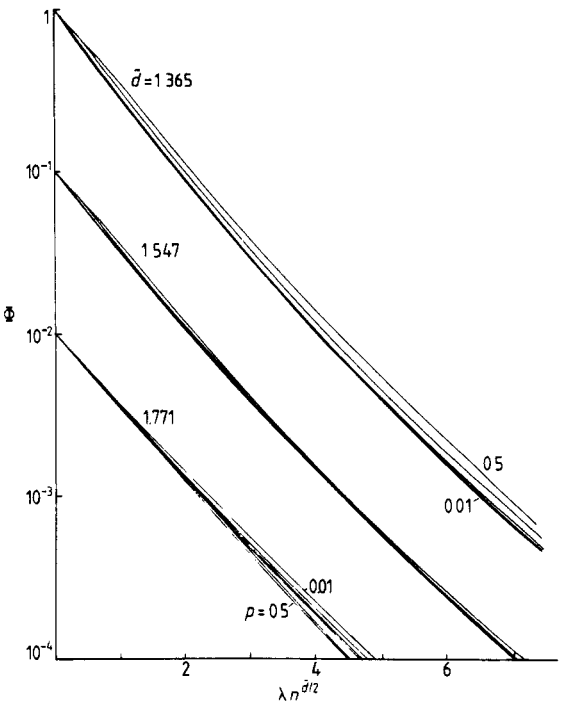

Figure 1. Decay law Φ_n due to randomly distributed traps on Sierpinski gaskets. The gaskets are embedded in two-, three- and six-dimensional Euclidean lattices and have (from above) the spectral dimensions $\tilde{d} = 1.365$, 1.547 and 1.771, respectively. The decay is plotted logarithmically and for clarity the curves are shifted by a factor of ten. The scaling form is $x = \lambda n^{\tilde{d}/2} = -n^{\tilde{d}/2} \ln(1-p)$, where p is the sink concentration which varies from 1 to 50%.

take $d = 2$, 3 and 6, so that the gaskets have the spectral dimensions $\tilde{d} = 1.365$, 1.547 and 1.771. For sink concentrations between 1% and 50% we follow the decay over the first two to three orders of magnitude. Since the goal is to check the behaviour $\Phi_n = \exp[-f(x)]$ for $x = \lambda n^{\tilde{d}/2}$, we plot Φ_n logarithmically over x. To facilitate the reference, in figure 1 the Φ_n which correspond to different values of $\tilde{d}$ are shifted with respect to each other by a factor of ten.

As is evident by inspection, the overall shape of the decay is indeed universal. Plotting Φ_n as a function of $\lambda n^{\tilde{d}/2} = -n^{\tilde{d}/2} \ln(1-p)$, instead of letting Φ_n depend only parametrically on p (Blumen *et al* 1983, Klafter *et al* 1984a,b), renders very similar the decays which hold for different sink concentrations. Notice also the parallelity of the decays for different spectral dimensions $\tilde{d}$: if we had not shifted the Φ_n-bundles, they would be hardly distinguishable. Summarising, we find for all p and $\tilde{d}$ considered that for small and moderate x the decays Φ_n scale quite well.

However, as was also expected from the discussion above, in this x range, scaling is not quantitative. For instance, for $\tilde{d} = 1.365$ the difference at $\Phi_n = 10^{-3}$ between the $p = 0.01$ and the $p = 0.5$ curves is a factor of 1.5. One has also examples for better scaling behaviour, such as the Φ_n-bundle for $\tilde{d} = 1.547$. Here the decay scales better, due to an interplay between higher-order terms in the asymptotic forms for S_n and σ_n^2, equations (4). A feeling for this aspect may be gained from figure 1 by noticing that for $\tilde{d} = 1.365$ the scaled decay law for $p = 0.5$ lies above the one for $p = 0.01$,

whereas for $d = 1.771$ the opposite is true. In fact this trend extrapolates to random walks on linear chains ($d = \tilde{d} = 1$): here the decay forms Φ_n are known analytically (Movaghar *et al* 1982, Weiss and Rubin 1983) and behave similarly to the $\tilde{d} = 1.365$ case (Klafter *et al* 1984a,b). Plotting $\tilde{\Phi}_n$ instead of Φ_n renders even better the scaling behaviour in $d = 1$ (Anlauf 1984), but worsens the agreement for larger $\tilde{d}$ values.

We now turn to the large-x regime (long times), where for all dimensions scaling behaviour is obeyed in the asymptotic limit. In figure 2 we display for the three

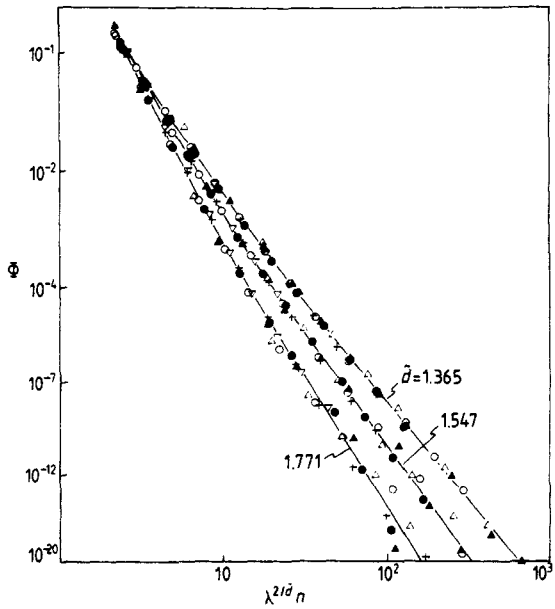

Figure 2. Long-time behaviour of the decay law Φ_n on Sierpinski gaskets. The gaskets used are as in figure 1 and the sink concentrations p are ▽, 1; +, 3; ●, 5; ○, 10; ▲, 30 and △, 50%. The scales used, $-\ln(-\ln \Phi_n)$ against $\ln(n\lambda^{2/\tilde{d}}) = (2/\tilde{d}) \ln x$, are discussed in the text.

Sierpinski gaskets the decay law over 20 orders of magnitude. Since the decay goes asymptotically as $\exp(-Cx^{\alpha})$, we plot $-\ln(-\ln \Phi_n)$ against $(2/\tilde{d}) \ln x$ so that in these scales the asymptotic form is a straight line. The factor $2/\tilde{d}$ is introduced for convenience only: plotting the decay as a function of $\lambda^{2/\tilde{d}} n = x^{2/\tilde{d}}$ instead of $\lambda n^{\tilde{d}/2} = x$ allows us to distinguish the Φ_n corresponding to different $\tilde{d}$. As is apparent from figure 2, the long-time behaviour scales for all concentrations (1% to 50%) considered; this fact establishes the universal behaviour of Φ_n in this x range. On the other hand, even for $10^{-20} < \Phi_n < 10^{-12}$ the decay laws do not follow straight lines. Thus, as remarked by us earlier for the $\tilde{d} = 1.365$ gasket (Klafter *et al* 1984a,b), the domain of validity of the asymptotic law, equation (7), is reached very slowly, and may even be inaccessible to experimental observation. We thus find that quantitative scaling sets in *long before* the domain of validity of (7) is reached.

In order to present a *counterexample* to smooth scaling behaviour, we show in figure 3 the decay law Φ_n for a square lattice ($d = 2$). Here we follow again Φ_n over 20 orders of magnitude, and plot $-\ln(-\ln \Phi_n)$ against $\ln x$. Direct inspection of the

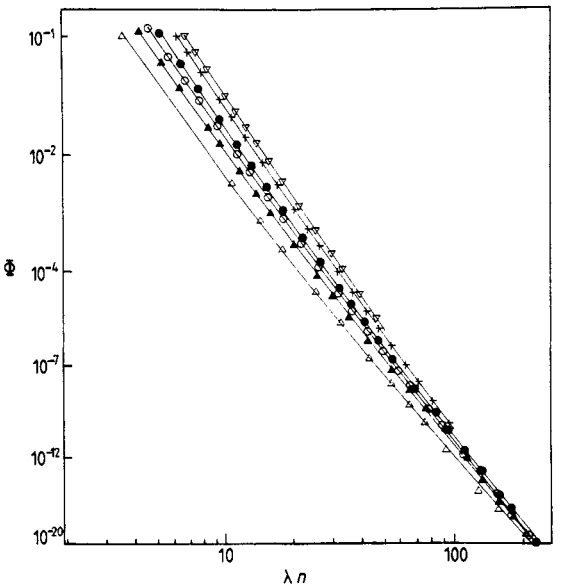

Figure 3. Long-time behaviour of the decay law Φ_n on a square lattice ($d = 2$), for sink concentrations ▽, 0.5; +, 1; ●, 3; ○, 5; ▲, 10 and △, 30%. The scales correspond to those of figure 2.

figure shows that in two dimensions scaling obtains only asymptotically and that in the intermediate range ($10 < \lambda n < 30$) for different trap concentrations the *scaled* decay law varies by many orders of magnitude. Thus $d = 2$ turns out to be a marginal random-walk dimensionality also with respect to scaling. We note that below $d = 2$, say on Sierpinski gaskets, the exploration is *compact* in the sense of de Gennes (1983), since already visited sites have a high revisitation probability by the walkers. Thus for a given compact volume V around the origin of the walk most points inside V are visited before a new site outside the volume is explored. As discussed by us (Klafter *et al* 1984a, b), the probability for such volumes to be trap free and the average number of steps needed for their exploration are connected. Thus scaling and compactness appear as different aspects of an underlying relation between sink density and temporal behaviour.

In this letter we have studied for several fractal lattices both analytically and numerically the decay law due to trapping. From the analytical forms a universal scaling law was inferred, which combines the trap concentration, the number of steps (i.e. time) and the spectral dimension of the fractal. The numerical results show the domain of validity and the limitations of this scaling law. For all structures investigated, the law is quantitatively obeyed in the long-time (large number of steps) limit. Deviations appear in the short- and moderately long-decay regime, where scaling is reasonable for the Sierpinski gaskets. For comparison we have also reported results for regular structures. With respect to scaling, the linear chain behaves similarly to the low-dimensional $\tilde{d} = 1.365$ gasket, whereas for short and moderately long decays, scaling is poor for the square lattice. Sierpinski gaskets bridge the gap between $d = 1$ and $d = 2$: the optimal (fractional) dimension for scaling lies around $\tilde{d} = 1.5$ for Φ_n and around $\tilde{d} = 1$ for $\tilde{\Phi}_n$, whereas the marginal dimension is $d = 2$.

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