

Fractal Behavior in Trapping and Reaction: A Random Walk Study

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We investigate the trapping of a random walker in fractal structures (Sierpinski gaskets) with randomly distributed traps. The survival probability is determined from the number of distinct sites visited in the trap-free fractals. We show that the short-time behavior and the long-time tails of the survival probability are governed by the spectral dimension \bar{d} . We interpolate between these two limits by introducing a scaling law. An extension of the theory, which includes a continuous-time random walk on fractals, is discussed as well as the case of direct trapping. The latter case is shown to be governed by the fractal dimension d .

KEY WORDS: Trapping; random walk; number of distinct sites visited; continuous-time random walk; Sierpinski gaskets; compact exploration.

1. INTRODUCTION

Random walks in lattices with randomly distributed trapping centers have been studied extensively^(1,2) with applications to problems such as mobile defects in crystals,⁽³⁾ electronic and vibrational energy transfer,⁽⁴⁻⁷⁾ and nuclear magnetic resonance.⁽⁸⁾ Recently, models of self-attracting polymers⁽⁹⁾ and for the Williams-Watts form of dielectric relaxation⁽¹⁰⁾ have also been mapped onto a trapping picture. All these studies have concentrated on models based on regular lattices. It has been recognized, however, that many structures in condensed matter physics appear to be of fractal nature (self-similar).⁽¹¹⁾ Examples are: linear and branched polymers,⁽¹²⁾ percolation clusters at criticality,^(13,14) aggregates constructed by diffusion-limited growth,⁽¹⁵⁾ epoxy resins,⁽¹⁶⁾ and porous surfaces.⁽¹⁷⁾ It would be of

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much interest therefore to extend the existing theories for regular lattices also to fractal structures.

In this paper we address the problems of trapping and reaction in fractals using the Sierpinski gaskets.⁽¹¹⁾ We focus on the decay functions and on the corresponding decay rates. We note that recent experiments on reactions of optical excitations in mixed molecular crystals have been interpreted in terms of migration and trapping in fractals.^(18,19) Moreover, the use of trapping of optical excitations for the characterization of polymer morphology has become widespread in recent years⁽²⁰⁾ and we believe that similar methods can be used for characterizing other complex structures.

In Section 2 we analyze the decay laws due to trapping in terms of the number of distinct sites visited. We study the mean number of distinct sites visited after n steps, S_n , and the variance σ_n^2 in Sierpinski gaskets and compare their values with those for regular lattices. This analysis is restricted to small and moderately large number of steps (short and moderate times). In Section 3 we extend these calculations to a very large number of steps (very long times). A scaling law is then proposed to describe the decay functions for all times and all trap concentrations. Section 4 compares the trapping results derived in previous sections with the direct transfer mechanism. It is demonstrated that different processes depend on different dimensions of the fractal. In Section 5 we relax the condition of a simple random walk with a fixed site-to-site stepping time by introducing a distribution of stepping times in the framework of the continuous-time random walk. This modification strongly affects the behavior due to trapping.

2. TRAPPING IN THE SHORT AND MODERATE TIME REGIMES

We consider a random walker in a fractal structure (Sierpinski gasket)⁽¹¹⁾ in which the traps are distributed randomly, occupying its sites with probability p . The microscopic transfer rates of the walker from a site to its neighboring sites are assumed to be equal. Furthermore, the walker gets trapped at the first encounter of a trap.

For a particular realization of the random walk on the trap-free fractal, let R_n denote the number of distinct sites visited in n steps. Note, as is usual in disordered systems, the difference from the regular lattice: here the stochastic variable R_n depends both on the starting point on the gasket, and on the sequence of directions of the steps; for a regular lattice the starting point is irrelevant. For the same realization of the walk let F_n denote the probability that trapping has not occurred up to the n th step in the ensemble of lattices doped with traps:

$$F_n = (1 - p)^{R_n - 1} \quad (1)$$

assuming the origin of the walk not to be a trap. The measurable survival probability is Φ_n , the average of F_n over all realizations of the random walk^(4,7,21,22) and over all starting points

$$\Phi_n = \langle F_n \rangle = \langle (1-p)^{R_n-1} \rangle \tag{2}$$

Introducing $\lambda = -\ln(1-p)$, Eq. (2) allows a straightforward cumulant expansion

$$\Phi_n = e^{-\lambda} \langle e^{-\lambda R_n} \rangle \equiv e^{-\lambda} \tilde{\Phi}_n \tag{3}$$

with

$$\tilde{\Phi}_n = \exp \left[\sum_{j=1}^{\infty} K_{j,n} (-\lambda)^j / j! \right] \tag{4}$$

where the $K_{j,n}$ are the cumulants of the distribution of R_n . As an example, the first two cumulants are

$$K_{1,n} = \langle R_n \rangle \equiv S_n \tag{5}$$

and

$$K_{2,n} = \langle R_n^2 \rangle - \langle R_n \rangle^2 \equiv \sigma_n^2 \tag{6}$$

where S_n and σ_n^2 are the mean and the variance of R_n .

The knowledge of all cumulants allows the exact determination of the decay function Φ_n via Eqs. (3) and (4). In general, however, one has to restrict oneself to the first cumulants, since the distribution of R_n is not known in great detail:

$$\tilde{\Phi}_{N,n} = \exp \left[\sum_{j=1}^N K_{j,n} (-\lambda)^j / j! \right] \tag{7}$$

The expression for $N = 1$

$$\tilde{\Phi}_{1,n} = \exp(-\lambda S_n) \tag{8}$$

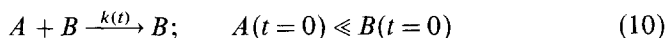
has been advanced in many areas^(4,6,18,23); in the random walk field it corresponds to the first-passage-time approximation;⁽⁶⁾ in the fractal field it was recently used by de Gennes.⁽²³⁾ For $N = 2$ one obtains from Eq. (7) the form⁽⁷⁾

$$\tilde{\Phi}_{2,n} = \exp(-\lambda S_n + \lambda^2 \sigma_n^2 / 2) \tag{9}$$

Let us point out that for three-dimensional regular systems Eq. (8) was found to be a good approximation over the main portion of the decay, and

that Eq. (9), which includes the variance, turned out to be very good both for three- and for two-dimensional regular lattices. On the other hand, in the one-dimensional regular case the cumulant expansion, Eq. (7), is very slowly convergent, so that at least $N=4$ is needed in order to describe well the decay over the first two orders of magnitude.⁽⁷⁾

According to formal chemical kinetics one obtains from Φ_n the decay rates $k_n = (\Phi_{n-1} - \Phi_n)/\Phi_n$, the discrete version of $k(t) = -\dot{\Phi}(t)/\Phi(t)$. The reaction scheme described here is



where B represents the traps. Equation (10) serves as a suitable model for describing energy transfer processes. The more general bimolecular case $A + B \rightarrow C$ will be discussed elsewhere.

We have simulated a series of different random walks on Sierpinski gaskets. For an embedding Euclidean space of dimension d the fractal dimension of the gasket is⁽¹¹⁾ $\bar{d} = \ln(d+1)/\ln 2$ and its spectral dimension is $\tilde{d} = 2 \ln(d+1)/\ln(d+3)$, so that $d \geq \bar{d} \geq \tilde{d}$.^(13,14,24) In the case that we are interested in, trapping of a walker, the fundamental quantity is the spectral dimension \tilde{d} (*vide infra* and Refs. 13 and 14). For these Sierpinski gaskets the spectral dimension is *always* less than 2; this allows us to analyze the performance of the cumulant expansion and the properties of the walker in the range below $\tilde{d}=2$. We have chosen gaskets of Euclidean dimension $d=2$, $d=3$, $d=4$, and $d=6$ which correspond to the spectral dimensions $\tilde{d}=1.365$, $\tilde{d}=1.547$, $\tilde{d}=1.654$, and $\tilde{d}=1.771$, respectively. The gaskets were generated iteratively, and were chosen to contain some 10,000 sites. Some 1000 to 5000 realizations of the walks were performed and both starting points and displacements were stochastically chosen using the random number generator RN1 of the ETH Computer Center.

In Fig. 1 we present the results for S_n in the range $0 \leq n \leq 1000$ for the four gaskets; we have also included S_n for the linear chain ($d=1$). The numerical results for S_n were fitted to

$$S_n = an^\alpha \quad (11)$$

with $\alpha = \tilde{d}/2$. On the scale of the figure the fit is excellent, and is indistinguishable from the numerical results, even for small n . Thus, for the gaskets, as in the one-dimensional regular case, the first term of the asymptotic expansion of S_n gives an adequate description for practically *all* n . The fit gives for the gaskets $a=1.295$ and $\alpha=0.685$ for $d=2$; $a=1.248$ and $\alpha=0.762$ for $d=3$; $a=1.205$ and $\alpha=0.809$ for $d=4$; and

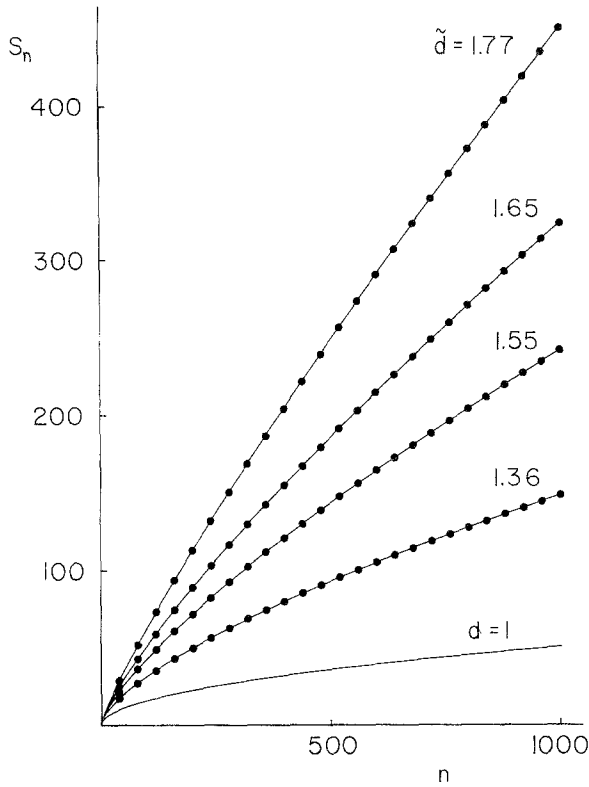


Fig. 1. Mean number of distinct sites visited in n steps, S_n , for four Sierpinski gaskets ($\tilde{d} = 1.365$, $\tilde{d} = 1.547$, $\tilde{d} = 1.654$, $\tilde{d} = 1.771$) as well as for the linear chain ($\tilde{d} = 1$). The points are the simulation results and the lines are the fit to Eq. (11).

$a = 1.138$ and $a = 0.865$ for $d = 6$. The result for a for $d = 2$ agrees with the result of Ref. 24. The difference between $2a$ and \tilde{d} is very small.

For the second cumulant σ_n^2 the results are presented in Fig. 2. We have fitted the numerical curves to the law

$$\sigma_n^2 = bn^\beta \tag{12}$$

since there is strong evidence that this should be the leading term of the corresponding expansion, with β being $\beta = \tilde{d} = 2a$.^(24,25) As may be seen from Fig. 2 the fit, Eq. (12), is very satisfactory. We obtain $b = 0.148$ and $\beta = 1.363$ for the gasket in $d = 2$, $b = 0.060$ and $\beta = 1.539$ for $d = 3$, $b = 0.053$ and $\beta = 1.60$ for $d = 4$, and $b = 0.041$ and $\beta = 1.67$ for $d = 6$. Equations (11) and (12) imply that for our fractals the ratio σ_n^2/S_n^2 should approach a constant independent of n , b/a^2 . b/a^2 equals 0.088 for $d = 2$, 0.039 for $d = 3$, 0.037 for $d = 4$ and 0.032 for $d = 6$. These values decrease

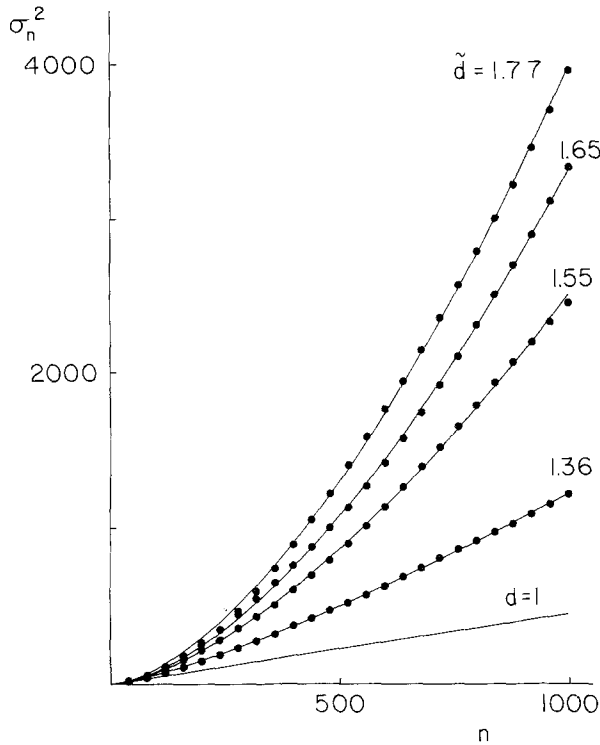


Fig. 2. The variance of the distribution of distinct sites visited in n steps, σ_n^2 . All symbols are as in Fig. 1 and the simulation results are fitted to Eq. (12).

monotonically with increasing \tilde{d} , which means that the distribution of R_n gets narrower for larger \tilde{d} .

How are these statistical properties in fractals related to the corresponding properties in regular lattices? The asymptotic behaviors of S_n and σ_n^2 for regular lattices are well known:^(1,2)

$$d = 1, \quad S_n = an^{1/2} + \dots, \quad \sigma_n^2 \sim 4(\ln 2 - 2/\pi)n, \quad \sigma_n^2/S_n^2 = \text{const} \quad (13a)$$

$$d = 2, \quad S_n = an/\ln n + \dots, \quad \sigma_n^2 \sim n^2/\ln^4 n, \quad \sigma_n^2/S_n^2 \sim 1/\ln^2 n \quad (13b)$$

$$d = 3, \quad S_n = an + \dots, \quad \sigma_n^2 \sim n \ln n, \quad \sigma_n^2/S_n^2 \sim \ln n/n \quad (13c)$$

It is clear that for the family of the Sierpinski gaskets ($\tilde{d} \leq 2$) the moments of the distribution of distinct sites visited are situated between $d = 1$ and $d = 2$, Eqs. (13a) and (13b), respectively. The values of b/a^2 compare well with the exact result for the linear chain, $\tilde{d} = 1$, where $\sigma_n^2/S_n^2 = 0.088$. For two- and three-dimensional regular lattices $\sigma_n^2/S_n^2 \rightarrow 0$ for large n , Eqs. (13b)

and (13c). One may conjecture that for fractals the spectral dimension $\tilde{d} = 2$ replaces the Euclidean dimension $d = 2$ as the marginal dimension for the random walker; so that we expect⁽²⁴⁾ that asymptotically $S_n \sim n$ and $b/a^2 \rightarrow 0$ for $\tilde{d} \geq 2$.

The decay laws Φ_n are given in Fig. 3 for $\tilde{d} = 1.547$ and several values of the trap concentration ($p = 1\%$, 3% , 10% , and 30%). The Φ_n are plotted logarithmically versus n ; the full curves correspond to the exact decay, whereas the broken lines are the approximating forms $\Phi_{1,n}$ and $\Phi_{2,n}$, Eqs. (8) and (9). For the plot the formulas Eqs. (11) and (12) for S_n and σ_n^2 were used, obtaining thus approximate expressions with a minimal number of parameters. For all trap concentrations the decays are clearly *nonexponential*. We find a behavior much reminiscent of the decay laws for the square lattice: the mean number of sites visited, S_n , does not describe the decay well, whereas inclusion of the variance σ_n^2 considerably improves the agreement.⁽⁷⁾ We note⁽²⁶⁾ that the agreement is better for the higher-dimensional gaskets, a fact not surprising when remembering the one-

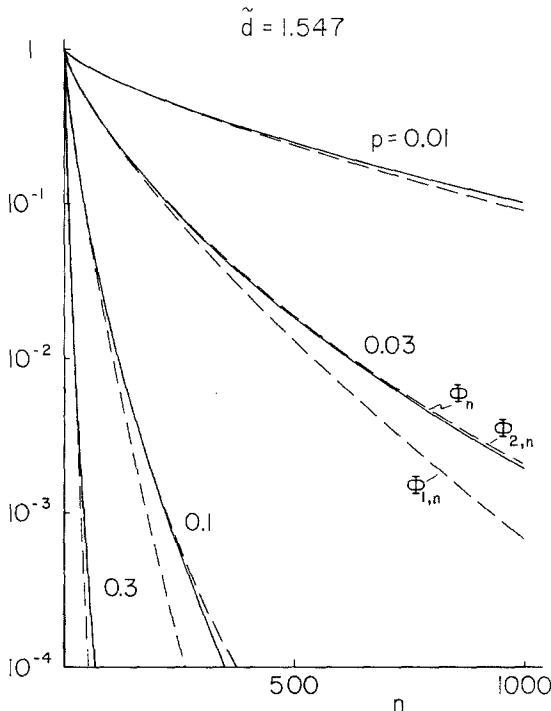


Fig. 3. The survival probability Φ_n for various trap concentrations p on a Sierpinski gasket $\tilde{d} = 1.547$, where n is the number of steps. The full lines denote the simulation data, whereas the dashed lines are the $\Phi_{1,n}$ and $\Phi_{2,n}$ approximations, Eqs. (8) and (9), respectively.

dimensional case, where four cumulants are necessary for a good description of the decay over two orders of magnitude. Thus the decay laws for the gaskets interpolate nicely between the linear chain and two-dimensional lattices, a result which is independent of the fractal dimension \bar{d} .

The dynamical quantities such as the moments of the distribution of distinct sites visited and also the decay, show a behavior which is situated between that which obtains for one- and for two-dimensional regular lattices. The unifying aspect is the *compact* exploration of the geometrical structures by the walker, a concept stressed by de Gennes.⁽²³⁾ As in the one-dimensional case, this leads to relations between the moments of the distributions, relations which appear from our numerical simulations.⁽²⁶⁾

3. LONG-TIME BEHAVIOR

In the previous section we have determined the survival probabilities Φ_n from the distribution R_n of distinct sites visited. We have concentrated on the short and moderately long times. In order to study the long-time regime we will have to treat the decay in a different manner.

As mentioned earlier, on fractal structures ($\bar{d} < 2$) the exploration is *compact*.⁽²³⁾ Already visited sites have a high probability of revisitation, so that, given a compact volume V which contains the walker, most points inside V are visited before a new site outside the volume is explored. Thus, if there is a trapping site inside V and the exploration is compact the survival probability is negligible.

For a given trap distribution around the origin of the walk there is a maximal trap-free volume V . Following Lifshitz,⁽²⁷⁾ Balagurov and Vaks,⁽²⁸⁾ and others⁽²⁹⁻³²⁾ we observe that the decay function is determined by the solution of the diffusion equation in V with absorbing boundaries, so that the long-time behavior is given by the lowest eigenvalue $\epsilon(V)$, and goes as $\exp[-t\epsilon(V)]$. The probability that the volume is trap-free is

$$(1 - p)^V \approx e^{-pV} \quad (14)$$

where we take the trap concentration to be small. To Eq. (14) corresponds the normalized Hertz distribution $p \exp(-pV)$. Averaging the decay over all compact volumes V one has asymptotically, for large t :

$$\Phi(t) \sim \langle \exp[-t\epsilon(V)] \rangle_V \sim \int p e^{-pV} e^{-t\epsilon(V)} dV \quad (15)$$

In Eq. (15) the dynamical decay law is expressed in terms of the geometrical

volumes V ; this allows now for fractals a straightforward scaling analysis. The volume of a fractal changes under dilatation by L as⁽¹¹⁾

$$V(L) \sim L^{\bar{d}} V(1) = C_1 L^{\bar{d}} \tag{16}$$

On the other hand, phonon modes scale as^(13,14,24)

$$\omega(V) \sim L^{-\bar{d}/\bar{d}} \omega(1) \tag{17}$$

and for the eigenvalues of the diffusion (or Schrödinger) equation one has the scaling:

$$\varepsilon(V) \sim L^{-2\bar{d}/\bar{d}} \varepsilon(1) = C_2 L^{-2\bar{d}/\bar{d}} \tag{18}$$

The exponent of L is by a factor of 2 larger than in Eq. (17), owing to the first (instead of second) time differential operator of the underlying differential equation. Inserting Eqs. (16) and (18) into Eq. (15) one obtains

$$\Phi(t) \sim \int \exp[-f(L)] dL \tag{19}$$

with, up to logarithmic corrections:

$$f(L) = pC_1 L^{\bar{d}} + tC_2 L^{-2\bar{d}/\bar{d}} \tag{20}$$

The leading term of Eq. (19) follows through a saddle-point analysis and is proportional to $\exp[-f(L_{\min})]$, where L_{\min} is the minimum of $f(L)$; corrections may be obtained by extensions of Watson's lemma.⁽³³⁾ From Eq. (20)

$$L_{\min} = (2tC_2/p\bar{d}C_1)^{\alpha/\bar{d}} \quad \text{with} \quad \alpha \equiv \bar{d}/(\bar{d} + 2) \tag{21}$$

so that

$$\Phi(t) \sim \exp[-f(L_{\min})] \sim \exp[-C_3 p^{2/(\bar{d}+2)} t^{\bar{d}/(\bar{d}+2)}] \tag{22}$$

We note the disappearance of \bar{d} from the final result, Eq. (22), which depends only on the spectral dimension \bar{d} . Equation (22) is a generalization of the long-time survival probability in Euclidean space⁽²⁸⁻³²⁾; it reduces to the Euclidean result by replacing \bar{d} by d . In fact, the exact Euclidean version of Eq. (22) is valid for all trap concentrations; thus p in Eq. (22) is substituted by $\lambda = -\ln(1 - p)$ [see Eq. (3)].

Now that we have derived the short-time decay laws in Sierpinski gaskets [$\bar{d} < 2$, Eqs. (9), (11)], and (12), and the long-time decay law, Eq. (22), we propose a scaling law for the survival probability Φ_n . This

interpolates between the two time regimes. Using Eqs. (3), (4), and (9) and an extension of Eq. (22) to all p (by introducing λ) we infer the following expression:

$$\Phi_n = e^{\lambda} \tilde{\Phi}_n \tag{23}$$

with

$$\tilde{\Phi}_n = \exp[-g(\lambda n^{\tilde{d}/2})] \tag{24}$$

where we transformed time t in Eq. (22) into number of steps n ($t = n\tau$, where τ is the stepping time). $g(x)$ is a universal function which reduces in limiting cases to

$$g(x) \sim \begin{cases} x & x \ll 1 \\ x^{2/(\tilde{d}+2)} & x \gg 1 \end{cases} \tag{25}$$

In order to check this scaling assumption we plot in Fig. 4 our results for Φ_n as a function of $\lambda^{2/\tilde{d}} n$ for three gaskets $\tilde{d} = 1.365$, $\tilde{d} = 1.547$, and $\tilde{d} = 1.771$.

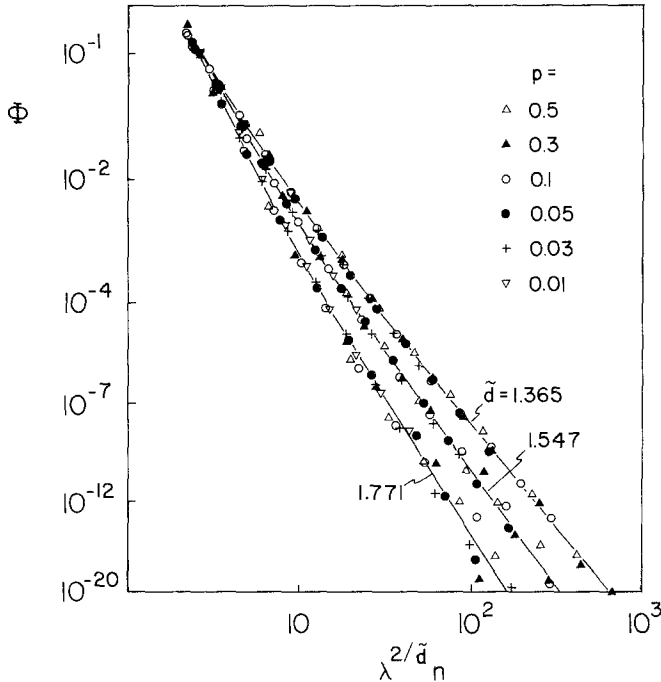


Fig. 4. Scaling behavior of Φ_n : $\ln \Phi_n$ is plotted vs. $\lambda^{2/\tilde{d}} n$ for three gaskets ($\tilde{d} = 1.365$, $\tilde{d} = 1.547$, and $\tilde{d} = 1.771$).

We see that for each of these spectral dimensions Eq. (24) describes the survival probability relatively well over many orders of magnitude of Φ_n . For a more detailed analysis see Ref. 35. Similar behavior has been recently suggested for one-dimensional ($d = 1$) trapping.^(35,36) For a square lattice ($d = 2$) such a scaling proposal fails.⁽³⁵⁾ One concludes then that Eq. (24) fits the decay laws for $\bar{d} < 2$ corresponding to the compact exploration case.

In order to find where the asymptotic behavior given by Eq. (22) is reached we performed numerical simulations⁽³⁴⁾ on a Sierpinski gasket with $\bar{d} = 1.365$. However, in the range $10^{-20} \leq \Phi_n \leq 1$ we could not fit the results to Eq. (22), $\Phi(t) \sim \exp(-ct^\alpha)$ with $\alpha = \bar{d}/(\bar{d} + 2)$. For all trap concentrations we find the same *form* but with α larger than the predicted one. We have also studied regular lattices,⁽³⁴⁾ where one expects the same expression as in Eq. (22) to hold, with \bar{d} replaced by d . The regular cases also display similar behaviors: For example, in two dimensions we could not observe the expected long-time tails ($\alpha = 1/2$) over many orders of magnitude of the survival probability.

4. DIRECT TRAPPING

A different mechanism for trapping of an excitation in fractals is the direct, one-step trapping. In this case an excited donor decays to randomly distributed acceptors in a structure of fractal dimension \bar{d} .

Direct trapping in regular lattices has been studied both theoretically^(5,37,38) and experimentally.^(5,38) Also charge recombination in amorphous materials has been described in the same framework.^(39,40) Here we generalize the direct trapping results to include fractal structures.

We start our considerations by assuming that the donor and the acceptors are embedded in a fractal. The survival probability $\Psi(\mathbf{K}; t)$ of the excited donor (assumed at the origin) for a fixed acceptor configuration \mathbf{K} is exponential⁽³⁷⁾

$$\Psi(\mathbf{K}; t) = \exp \left[-t \sum_{j \in \mathbf{K}} W(\mathbf{R}_j) \right] = \prod_{j \in \mathbf{K}} \exp[-tW(\mathbf{R}_j)] \quad (26)$$

where $W(\mathbf{R}_j)$ denotes the transfer rate to an acceptor at position \mathbf{R}_j and the sum and product extend over all acceptors. As an example we choose the multipolar interactions:

$$W(\mathbf{R}_j) = \frac{\alpha_m}{R_j^s} \quad (27)$$

The quantity of experimental interest is not $\Psi(\mathbf{K}; t)$ but its ensemble average over all possible configurations of the acceptors distributed on the

fractal, $\Psi(t)$, where $\Psi(t) = \langle \Psi(\mathbf{K}; t) \rangle_{\mathbf{K}}$. If the fractal sites are randomly occupied with probability p one obtains from Eq. (26)^(5,37)

$$\Psi(t) = \prod_i' \{1 - p + p \exp[-tW(\mathbf{R}_i)]\} \quad (28)$$

Here the product extends over *all* sites of the fractal structure with the exception of the donor site. This means that the ensemble average reproduces the details of the structure (it also depends on the donor site) and in the process of the direct transfer the whole fractal structure is being sampled.

For low density of acceptors, $p \ll 1$, an approximate form to $\Psi(t)$ can be derived from Eq. (28). Distinct from Eq. (28) this form does not depend anymore on the position of the donor. In the continuous description one obtains

$$\Psi(t) \simeq \exp \left(-p \int d\mathbf{R} \rho(R) \{1 - \exp[tW(\mathbf{R})]\} \right) \quad (29)$$

where $\rho(R)$ is the density of sites on the fractal structure⁽¹¹⁾:

$$\rho(R) = \rho_0 R^{\bar{d}-d} \quad (30)$$

where ρ_0 is a proportionality constant. Equation (29) is then, for isotropic interactions $W(R)$,

$$\Psi(t) \simeq \exp \left(-p\rho_0 V_d \int dR R^{\bar{d}-1} \{1 - \exp[-tW(R)]\} \right) \quad (31)$$

where V_d is the volume of the d -dimensional unit sphere. We now insert the form (27) into Eq. (31) and obtain for multipolar interactions⁽⁴¹⁾

$$\Psi(t) = \exp(-pAt^{\bar{d}/s}) \quad (32)$$

where A is time independent. Unlike the decay laws derived in previous sections for a random walker and which depend solely on the spectral dimension \bar{d} , here we encounter a situation where the decay is given by the fractal dimension \bar{d} . Thus, for each mechanism a different dimension of the fractal is decisive. In this sense, trapping on fractals shows a richer behavior than in the case of regular lattices where $d = \bar{d} = \bar{d}$.

Equation (32) is an extension of a known result for Euclidean dimension d ^(37,38) to fractal dimension \bar{d} (by replacing d by \bar{d}). Experimentally, the change from the direct to the indirect mechanism may be monitored by changing the concentration of the molecules involved.

5. CONTINUOUS-TIME RANDOM WALK (CTRW) ON FRACTALS

We return to the case of trapping of a random walker, Sections 2 and 3. However we now relax the condition used in these sections that the walker hops from site to site with a *fixed* stepping time. We introduce a distribution of stepping times $\psi(t)^{(42)}$ which mimics an additional disorder superimposed on the geometric (fractal) disorder. Thus, we encounter a case where two independent random processes affect the survival probability due to trapping.

Introducing the distribution of stepping times $\psi(t)$ in the framework of the CTRW has been proven to be a powerful approach toward the understanding of transport in amorphous materials.⁽⁴³⁾ Generally the distribution of stepping times is a function in which spatial and temporal processes are coupled.^(44,45) Here we assume a decoupled version of the CTRW.

In order to introduce the continuous-time aspect to the trapping problem one has to translate the number of steps of Section 2 into time. Let $\chi_n(t)$ be the probability of having performed *exactly* n steps in time t , then the survival probability after time t is^(21,47)

$$\Phi(t) = \sum_n \Phi_n \chi_n(t) \tag{33}$$

where Φ_n is given by Eq. (2). In our model all steps occur with a common stepping time distribution $\psi(t)$, so that $\chi_n(t)$ can be obtained from $\psi(t)$. We denote by $f(u)$ the Laplace transform of $f(t)$; $f(u) = \mathcal{L}[f(t)]$, then^(42,46)

$$\chi_n(u) = [\psi(u)]^n [1 - \psi(u)]/u \tag{34}$$

From Eqs. (33) and (34) the Laplace transform of $\Phi(t)$ in the CTRW framework is given by

$$\Phi(u) = \frac{1 - \psi(u)}{u} \sum_n \Phi_n [\psi(u)]^n \tag{35}$$

$\Phi(t)$ strongly depends on the nature of the distribution of stepping times $\psi(t)$. As discussed by us before^(46,47) two cases are of particular interest. In the first case all moments $\tau_j = \int t^j \psi(t) dt$ of $\psi(t)$ are finite; then for small u

$$\psi(u) = 1 - u\tau_1 + \dots \tag{36}$$

In the second case, $\psi(t)$ has a long-time tail⁽⁴³⁾ $\psi(t) \sim t^{-1-\beta}$ ($0 < \beta < 1$) so that $\int t\psi(t) dt$ diverges. In this case

$$\psi(u) = 1 - \Gamma(1 - \beta)u^\beta/\beta + \dots \tag{37}$$

$\Gamma(x)$ is the Euler gamma-function. As an example for the first case where all moments exist we choose^(46,47)

$$\psi(t) = -\frac{d\Psi}{dt} \tag{38}$$

where $\Psi(t) = e^{-At^\gamma}$ ($0 < \gamma < 1$). $\Psi(t)$ describes the probability of the walker to remain on the site occupied at time $t = 0$, while $1 - \Psi(t)$ is the probability of transfer during time t to other available sites. For more detailed discussions of Eq. (38) see Refs. 21, 44, and 46–48. Figure 5 represents the survival probability $\Phi(t)$ in the CTRW framework with $\psi(t)$ as in Eq. (38). $\Phi(t)$ has been obtained from the inverse Laplace transform of Eq. (35),⁽⁴⁸⁾ where Φ_n were taken from the calculations in Section 2 for $\tilde{d} = 1.36$. γ has been given the value 0.14 so that the corresponding $\psi(t)$ is broad enough to demonstrate the effect of the CTRW.⁽⁴⁷⁾ The dashed curves in the figure

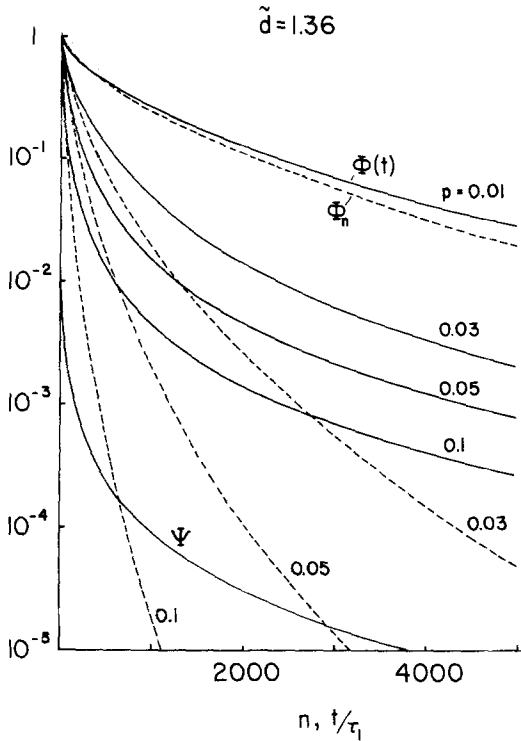


Fig. 5. Decay laws $\Phi(t)$ for walks on a gasket ($\tilde{d} = 1.36$) with $\psi = -\dot{\Psi}$, $\Psi(t) = e^{-At^\gamma}$, $\gamma = 0.14$. The trap concentrations are as indicated. The dashed curves are the decay laws which obtain for a fixed stepping time. Also plotted is the corresponding $\Psi(t)$.

describe the decay laws in the fractal with a fixed stepping time. The full curves give $\Phi(t)$ in the presence of $\psi(t)$. One sees that for short times $\psi(t)$ does not change $\Phi(t)$; however, at longer times the decay laws are much slower owing to the broad distribution of stepping times. The fractal nature is completely masked by the temporal disorder. It is interesting to note that for long times the full curves are parallel to each other and to $\Psi(t)$ of Eq. (38). This is due to an avoided crossing effect⁽⁴⁷⁾: trapping cannot be more efficient than the probability of remaining on the initial site, $\Psi(t)$. Thus, for long times $\Phi(t) \sim \Psi(t) = e^{-At^\gamma}$. For the stepping time distribution with long-time tails $\psi(t) \sim t^{-1-\beta}$ we find⁽⁴⁸⁾ that $\Phi(t)$ deviates from the regular fractal behavior even earlier than in Fig. 5. In this case for long times $\Phi(t) \sim 1/t^\beta$ which again corresponds to the avoided crossing argument. The same result was obtained for regular lattices.^(46,47) Namely, for broad $\psi(t)$ the decay due to trapping is determined by the distribution of stepping times rather than by the fractal dimensions.

The CTRW version of the mean number of distinct sites visited in a fractal (Sierpinski gasket) can be readily obtained from $\psi(t)$ as in Eq. (33)

$$S(t) = \sum_n S_n \chi_n(t) \tag{39}$$

where $S_n = an^{\tilde{d}/2}$ (see Section 2). For Eq. (39) we have derived the following results.⁽⁴⁸⁾ With $\psi(t)$ having all moments the asymptotic behavior of $S(t)$ is

$$S(t) \sim t^{\tilde{d}/2} \tag{40}$$

which preserves the fractal nature of S_n in Section 2. However, for the $\psi(t)$ of Eq. (37)

$$S(t) \sim t^{\beta\tilde{d}/2}, \quad 0 < \beta < 1 \tag{41}$$

Here the exponent shows the effect of subordination: the two processes behave asymptotically in a multiplicative manner. In the compact case, $\tilde{d} < 2$, Eqs. (40) and (41) are related to the mean-squared displacement of the walker $\langle R^2(t) \rangle$ and therefore to the diffusion coefficient in the fractal structures^(13,14)

$$\langle R^2(t) \rangle \sim |S(t)|^{2/\tilde{d}} \tag{42}$$

From Eqs. (40) and (41) we then have

$$\langle R^2(t) \rangle \sim t^{\tilde{d}/\tilde{d}} \tag{43a}$$

and

$$\langle R^2(t) \rangle \sim t^{\beta\tilde{d}/\tilde{d}} \tag{43b}$$

respectively. Equation (43b) is a generalization of the Alexander–Orbach⁽¹³⁾ result for broad distributions of stepping times. In this case the diffusion does not depend only on \bar{d} and \tilde{d} for the given structure, but is sensitive to the disorder parameter β . We note that in this case the survival probability $\Phi(t) \sim 1/t^\beta$ is related to $S(t)$ in an interesting way:

$$\Phi(t) \sim \frac{1}{[S(t)]^{2/\bar{d}}}, \quad \tilde{d} < 2 \quad (44a)$$

$$\Phi(t) \sim \frac{1}{S(t)}, \quad \tilde{d} > 2 \quad (44b)$$

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