Short-time regime propagator in fractals

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The propagator $P(r,t)$ for fractals in the short-time regime, i.e., the probability of finding at distance r at time t a particle that diffuses in a fractal substrate when $\xi = r/\sqrt{2D}t^{1/d_w} \gg 1$, is studied in order to elucidate its full functional form. For finitely ramified fractals it is shown (and, for any other self-similar media, conjectured) that the short-time propagator is given by $P(r,t) \approx P_0 t^{-d_s/2}\xi^{\alpha}\exp(-c\xi^{\nu})$ where $\nu = d_w/(d_w-1)$ and $\alpha = \nu/2 - d_f$, d_f and d_w being the fractal and random walk dimension of the medium, respectively. The value for ν agrees with that generally accepted. However, our result for the as yet not well established value of α differs from other recent proposals. We have checked these various short-time propagator proposals by comparing them to the short-time propagator calculated numerically for the Sierpinsky gasket. Our numerical results are precise enough to clearly support the validity of the short-time propagator proposed here (in particular, the validity of our relation for α) and to rule out the others. [S1063-651X(98)11305-3]

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I. INTRODUCTION

The behavior of many physical systems can be described in terms of the diffusion of a random walker either on a Euclidean or on a fractal medium [1–4]. This last type of diffusion is usually termed ''anomalous'' because it does not exhibit the characteristic classical features of the diffusion on Euclidean media. For example, the mean-square displacement of the diffusing particle is given by

$$\langle r^2 \rangle \approx 2Dt^{2/d_w}, \tag{1}$$

$d_w \neq 2$ being the anomalous diffusion exponent (or random walk dimension) and D the diffusion coefficient. The ''nonanomalous'' or classical relation is recovered when $d_w = 2$. If the medium is a random fractal (i.e., self-similar in a statistical sense, such as disordered media, for example) the analytical study of the diffusion process is very difficult. Fortunately, many of its properties can be understood by studying the diffusion in deterministic fractals. The strict self-similarity of these structures makes it possible to find rigorous analytical results by means of renormalization techniques. For example, by means of the renormalization procedure developed by Van den Broeck [5,6], one can find the probability density for the time spent by a diffusing particle to first reach a given distance r, i.e., the first-passage-time density, $\psi(r,t)$. In particular, in the short-time (or large-ξ) regime in which $\xi \equiv r/\sqrt{2D}t^{1/d_w}$ is large, it can be proved [7] that this quantity is given by

$$\psi(r,t) \approx A\xi^{\nu/2+d_w}\exp(-C\xi^{\nu}), \tag{2}$$

where $\nu = d_w/(d_w-1)$ and A and C are characteristic constants of the fractal medium (for example, $A \simeq 1.82$ and $C \simeq 0.98$ for the two-dimensional Sierpinski gasket [6,7]).

However, even for deterministic fractals, there are other important statistical quantities concerning the diffusion process whose behavior is as yet not well known. A prominent example is the quantity termed propagator or Green function, $P(r,t)$, defined as the (configurational averaged) probability of finding the random walker at time t on a given site of the fractal separated by a distance r from the starting site:

$$P(r,t) = \langle \mathcal{P}(\mathbf{r}_f,t;\mathbf{r}_i,t=0)\rangle_{\mathbf{r}_f,\mathbf{r}_i,|\mathbf{r}_f-\mathbf{r}_i|=r}, \tag{3}$$

where $\mathcal{P}(\mathbf{r}_f,t;\mathbf{r}_i,t=0)$ is the probability that the random walker starting from a site with position vector $\mathbf{r}_i$ at time $t=0$ arrives at a site with position vector $\mathbf{r}_f$ at time t. The configurational average is performed over all possible pairs of starting and destination sites separated by distance r [8]. This Green function is of central importance in diffusion theory because almost any other statistical quantity related to the diffusion process can be derived from it [1,2].

For many years even the basic form of the propagator on fractals was a subject of discussion, but it is now clear that the origin of the discrepancies stemmed from the lack of identification of the existence of two very different regimes for the propagator: the short- and long-time regimes (or large- and small-ξ regimes, respectively) [3,6,9]. Numerical and theoretical approaches have been employed in order to know the anomalous diffusion behavior in these two regimes.

From a theoretical perspective, there is at present a degree of consensus about the validity of a stretched Gaussian form

$$P(r,t) \approx P_0 t^{-d_s/2}\xi^{\alpha}\exp(-c\xi^{\hat{\nu}}), \tag{4}$$

for the short-time propagator, where

$$\hat{\nu} = \nu = d_w/(d_w-1), \tag{5}$$

$\xi = r/t^{1/d_w}$, $d_s = 2d_w/d_f$ is the spectral dimension and d_f is the fractal dimension. However, the expression for the exponent α of the power-law correction to the dominant exponential term is still an open question and different approaches to the problem lead to different predictions [9–15]. In this paper we improve previous arguments [7] to strengthen the validity of our prescription for α, namely,

$$\alpha = \nu/2 - d_f. \tag{6}$$

An obvious way to approach this question is to resort to numerical studies of the diffusion process. For example, O'Shaughnessy and Procaccia [16] and Klafter, Zumofen, and Blumen [9] have numerically studied the propagator for the short- and long-time regimes, respectively, on the Sierpinski gasket (the fractal typically used for testing). It should be noted that numerical study of this short-time regime (the regime in which we are interested in this paper) is especially difficult due to the fact that one must allow the particle to travel for a time long enough to reach the diffusive limit and, simultaneously, short enough to be inside the large-ξ regime. This implies the use of very large fractal lattices in the numerical simulations and, above all, requires a procedure to check whether the large ξ values are reached at the expense of using a time so short that it leads us to work not close enough to the diffusive limit, which hence could invalidate our conclusions. Therefore, it is crucial to have a criterion to gauge this closeness, especially if one is interested, as in this paper, in numerically elucidating the faint subdominant behavior of the propagator. The criterion used in this paper is largely inspired by the comparison of a numerically obtained mortality function for finite lattices to the known theoretical mortality function for infinite lattices [7]. (The mortality function is a quantity closely related to the propagator that will be defined in Sec. II A.) This way of controlling the quality of our numerical study makes (we believe) the numerical results reported here much more reliable.

Finally, we would like to point out here that numerical studies of the type carried out by Klafter *et al.* cannot resolve the question about the value of α because they analyze a quantity that, although almost equal to the true propagator, has a different power-law correction to the stretched exponential. This shall be discussed in Sec. IV.

The plan of the paper is as follows. Section II, which is divided into two subsections, is devoted to the (improved) theoretical derivation of the short-time propagator given by Eqs. (4)–(6). In Sec. II A we present some definitions and known results to be used later. Our theoretical argument for the short-time propagator is given in Sec. II B. Section III is devoted to the numerical study of the diffusion process in a two-dimensional Sierpinsky gasket in order to check the theoretical predictions. In Sec. III A we provide a detailed description of the simulation method. In Sec. III B we check the reliability of our numerical method by calculating the mortality function in the short-time regime for finite Sierpinsky lattices and comparing it to the exact (in the Laplace space) result. Also, these results are compared with the analytical mortality function corresponding to the infinite lattice. This allows us to know under what circumstances the method is reliable to the extent of being able to resolve the faint subdominant behavior of $h(r,t)$. In the first part of Sec. III C, we check a key relation used in the theoretical derivation of the propagator in Sec. II. In the second part we present the results of our simulation for the short-time propagator and conclude that these numerical results are precise enough to clearly support the validity of Eq. (4) with the dominant and subdominant exponents ν and α given by Eqs. (5) and (6), respectively. In Sec. IV we discuss the behavior of the function used by Klafter *et al.* [9] as propagator. It is proved theoretically, and verified numerically, that, though the dominant exponential term agrees with that of the ''true'' propagator, this is not the case for the exponent of the power-law subdominant term. We find that this exponent is in good agreement with the proposed in Ref. [9] for the ''true'' propagator. Finally, the results are summarized and discussed in Sec. V.

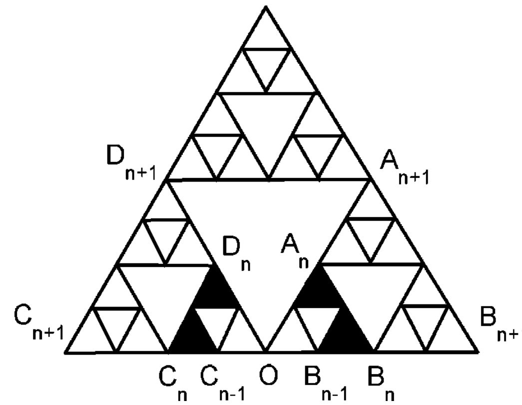

FIG. 1. The Sierpinski lattice with n generations. The labeled sites A_{n+1}, B_{n+1}, C_{n+1}, and D_{n+1} are the traps where the moving particle that starts from the origin 0 will be finally absorbed. On the sites A_n, B_n, C_n, and D_n the net probability fluxes are calculated at every time step in order to numerically compute the function $\hat{h}(r,t)$ with $r=2^n$. This figure would be the Sierpinsky lattice with $n=3$ generations if one assumes that there were no more internal triangles. The sites within the shaded area were used as destinations in order to compute the function $f(\xi)=\langle \mathcal{P}(\mathbf{r},t)t^{d_s/2}\rangle_{\mathbf{r},t,\xi=r/t^{1/d_w}}$. In this case the smallest triangles shown represent 8-generation lattices.

II. FIRST-PASSAGE TIME, SURVIVAL PROBABILITY AND PROPAGATOR

A. Definitions and some short-time results

It is well known that fractals are invariant under *decimation* due to their self-similarity. The decimation procedure in a deterministic fractal is the inverse process to its generation by means of an ''initiator'' and a ''generator'' [17]. For example, after one decimation, the portion of the Sierpinski lattice shown in Fig. 1 would become the same structure but without the internal triangles (triangles as the $OA_{n-1}B_{n-1}$). We will denote as zeroth decimated triangles the smallest triangles of the original (i.e., undecimated) lattice, as first decimated triangles the smallest ones after one decimation of the original lattice, and so on. Also, we will denote as the nth decimated Sierpinski lattice that formed by nth decimated triangles. Obviously, the zeroth decimated lattice is the original or ''microscopic'' lattice. We will say that the nth decimated lattice is formed by n connections (the sides of the nth decimated triangles) and n sites (the points of bifurcation or vertices). Finally, we will denote as Sierpinsky lattice with g generations or g generation Sierpinsky lattice the subset of the original lattice bounded by a gth decimated triangle. As usual, the ∞ generation Sierpinski lattice will be called the Sierpinski gasket. These definitions can be extended without difficulty to other fractals.

We describe the diffusion process as a continuous-time random walk. The diffusing particle goes (jumps) from a site of the original lattice to one of its nearest neighbors (of the original lattice, too) after a (waiting) time which is a random variable. It shall be assumed in this paper that the mean value of this random variable is finite. Let $\psi_n(t)$ be the first-passage-time (FPT) density of the random walker on the nth decimated lattice, i.e., the probability density that a diffusing particle starting at an n-site reaches, for the first time, at time t any of its nearest-neighbor n sites. We get the FPT density $\psi(t)$ of the fractal in the $n\to\infty$ limit: $\psi(t)=\lim_{n\to\infty}\psi_n(t)$.

A property of the two-dimensional Sierpinsky gasket shared by many other fractals (the d-dimensional Sierpinsky gasket, the Given-Mandelbrot curve, the hierarchical percolation model, ...) is that it is not possible to go from an n site to a non-nearest-neighbor n site via the $(n-1)$ connections without previously passing through its nearest-neighbor n sites. In short, in these fractals sites are isolated by their nearest neighbors from the rest of the lattice. This property makes it possible to implement the renormalization procedure described by Van der Broeck [5,6] and, in this way, to evaluate $\widetilde{\psi}_{n+1}(s)$ in terms of $\widetilde{\psi}_n(s)$:

$$\widetilde{\psi}_{n+1}(s)=R[\widetilde{\psi}_n(s)], \tag{7}$$

$\widetilde{\psi}_n(s)$ being the Laplace transform of $\psi_n(t)$. The renormalization function R is known for several fractals [7]. For example, for the d-dimensional Sierpinsky gasket, $R(x)=x^2/[d-3(d-1)x+(d-2)x^2]$ [18]. The FPT density (with the first moment chosen as 1) can be obtained by solving the functional equation

$$\widetilde{\psi}(\tau s)=R[\widetilde{\psi}(s)], \tag{8}$$

with $\widetilde{\psi}(0)=\widetilde{\psi}'(0)=1$, and where $\tau=R'(1)$, or time rescaling factor, is the factor by which the time to go from a site to one of its nearest neighbors grows in each decimation. From this equation it is possible to deduce [7] that the probability density, $\psi(r,t)$, for a diffusing particle starting at a given site to reach, for the first time at time t, any other site of the medium separated by a distance r, is given by Eq. (2) for large $\xi=r/\sqrt{2D}t^{1/d_w}$.

Let $h_n(t)$ (or mortality function on the n-decimated lattice) be the probability that a random walker who starts at an n site is absorbed by traps located on its nearest-neighbor n sites in the time interval $(0,t)$. From the definitions of $\psi_n(t)$ and $h_n(t)$ one has $h_n(t)=\int_0^t\psi_n(t')dt'$ and therefore $\widetilde{h}_n(s)=\widetilde{\psi}_n(s)/s$, so that one can use Eq. (7) to recursively find $\widetilde{h}_n(s)$. Let $h(r,t)$, or mortality function of the fractal, be the probability that a random walker who starts at a site is absorbed by traps located on its nearest neighbors at distance r in the time interval $(0,t)$. Therefore $h(t,r)=\int_0^t\psi(t',r)dt'$, and, from Eq. (2) one finds that

$$h(r,t)\approx\frac{A(d_w-1)}{C}\xi^{-\nu/2}\exp(-C\xi^\nu) \tag{9}$$

for large ξ.

B. The propagator for large ξ

In this subsection we discuss the proposal of Ref. [7] for the short-time-regime propagator, i.e., Eqs. (4)–(6), and provide more arguments in its support. Let $\hat{h}(r,t)$ be the probability that the random walker that started at $r=0$ when $t=0$ is outside the region $\mathcal{R}$ of radius r after the time t when there exist no traps (free diffusion). It is clear from the above definitions that $\hat{h}(r,t)<h(r,t)$. In the argument of Ref. [7], the relation $\hat{h}(r,t)/h(r,t)=\text{const}$ for large ξ values, notwithstanding its crucial role, was a conjecture. Here we fill in this gap and go even further by predicting the value of this ratio. For simplicity's sake, let us assume that r is equal to the distance between the original site (site O) and one or more other fractal sites. For example, in Fig. 1, if r is the distance between O and A_n the region $\mathcal{R}$ is that limited by the triangles OA_nB_n and OC_nD_n. Let z_0 be the number of paths (connections) that a random walker placed on a site of the frontier of $\mathcal{R}$ (sites A_n, B_n, C_n, and D_n in our example) has available in order to exit this region, and let z be the total number of paths that the random walker can use. For example, $z_0=2$ and $z=4$ for the two-dimensional Sierpinsky gasket (see Fig. 1), $z_0=d$ and $z=2d$ for the d-dimensional Sierpinsky gasket, $z_0=3$ and $z=4$ for the Given-Mandelbrot curve and $z_0=1$ and $z=2$ for the one-dimensional lattice. It is clear from the definition of the mortality function that if N random walkers started at the site O when $t=0$, then $Nh(r,t)$ different particles arrive at the frontier of $\mathcal{R}$ during the time interval $(0,t)$. When arriving at the frontier, these particles have two options: either they re-enter $\mathcal{R}$ with probability $(1-z_0)/z$ or they exit with probability z_0/z. Thus, one could naively expect that the number of particles that are outside $\mathcal{R}$ at time t [i.e., $N\hat{h}(r,t)$] is $(z_0/z)Nh(r,t)$. But this is not (strictly) true because, for example, we are not counting those particles that, after arriving at the frontier, re-enter and finally exit from $\mathcal{R}$ by other sites. However, for short times, one expects that the number of particles with this behavior is negligible. We can go a step further and estimate this number. From the definition of $h(r,t)$ and because $h(r,t)\sim\exp(-\xi^\nu)$ for $\xi\gg1$, we know that if a number of order $(z_0/z)Nh(r,t)$ of particles start at a site of the frontier of $\mathcal{R}$, say the site A_n, and move into this region $\mathcal{R}$, then the number of these particles that arrive at any of the other sites of the frontier, which are separated by a distance of order r_* from A_n, after the time t_* (with $t_*<t$) is of order $(z_0/z)Nh(r,t)\exp(-\xi_*^\nu)$. This is an estimate of the number of particles that, for short times, exit from $\mathcal{R}$ in this indirect way. Therefore, taking into consideration that $r_*\sim r$ and $t_*\sim t$, we find that the number of particles outside $\mathcal{R}$, $N\widetilde{h}(r,t)$, should be $(z_0/z)Nh(r,t)\{1+O[\exp(-\xi^\nu)]\}$. This implies

$$\frac{\hat{h}(r,t)}{h(r,t)}=\frac{z_0}{z}\{1+O[\exp(-\xi^\nu)]\} \tag{10}$$

for $\xi\gg1$. One can explicitly check this relation for the one-dimensional lattice. In this case, $\hat{h}(r,t)=\text{erfc}(\xi/\sqrt{2})$ and $h(r,t)=2\Sigma_{m=1}^{\infty}(-1)^{m+1}\text{erfc}[(2m-1)\xi/\sqrt{2}]$ with $\xi=r/\sqrt{2Dt}$. But $\text{erfc}(x)\approx\exp(-x^2)/(\sqrt{\pi}x)$ for $x\gg1$, so that, in agreement with Eq. (10), $\hat{h}(r,t)/h(r,t)=1/2+\exp(-4\xi^2)/3+\cdots$ for $\xi\gg1$. In summary, we conclude that the ratio $\hat{h}/h$ is equal to a constant (z_0/z) plus exponentially small terms.

With these results in hand we can now proceed to calculate the propagator for the short-time regime as in Ref. [7]. Because the propagator $P(r,t)$ is the probability of finding a particle at a site of the fractal separated by a distance r from the starting site at time t, and because the number of sites situated between r and $r+dr$ is given by $\Omega r^{d_f-1}dr$, it is clear that

$$\hat{h}(r,t)=\Omega\int_r^\infty P(x,t)x^{d_f-1}dx. \tag{11}$$

Assuming only that the propagator has the form of Eq. (4), this integral leads to

$$\hat{h}(r,t)\approx\frac{P_0\Omega}{\hat{\nu}c}\xi^{\alpha+d_f-\hat{\nu}}\exp(-c\xi^{\hat{\nu}}) \tag{12}$$

for large ξ. Comparing this expression with that obtained from Eq. (9) and Eq. (10), one finds that

$$c=C, \tag{13}$$

$$\hat{\nu}=\nu\equiv\frac{d_w}{d_w-1}, \tag{14}$$

$$P_0=\frac{z_0 d_w A}{z\Omega}, \tag{15}$$

$$\alpha=\frac{\nu}{2}-d_f, \tag{16}$$

where $\Omega=3d_f$ for the two-dimensional Sierpinski gasket. In the next section we shall check these expressions for $h(r,t)$ [cf. Eq. (9)], for $\hat{h}(r,t)$ [cf. Eq. (10)], and for $P(r,t)$ [cf. Eq. (4) with Eqs. (13)–(16)], by means of numerical simulation of the diffusion process in the two-dimensional Sierpinsky gasket.

III. NUMERICAL RESULTS FOR THE SIERPINSKY GASKET

A. Numerical solution of the CK equation

We carried out our simulations of the diffusion process numerically by solving the Champan-Kolmogorov (CK) equation. We considered Sierpinski lattices embedded in $d=2$ dimensions with a number $g=4$, 6, and 8 of generations. Notice that if we take the length of the base of the zeroth decimated triangle as the length unit, then 2^g is the length of the base of the triangle (the gth decimated triangle) in which the lattice is inscribed and 2^g is the distance from the origin O to the absorbing traps. The Sierpinski structures used in the simulations are a subset of a portion of a hexagonal lattice inside the main triangle. Two cordinates locate each site by taking the generators of the hexagonal lattice as a basis and the top vertex of the main triangle as the origin. Nevertheless, it is convenient to change to the orthogonal basis $\{\mathbf{e}_v,\mathbf{e}_h\}$ as in Fig. 2 because this divides the lattice into horizontal sets of sites with a fixed v coordinate. In order to update the probability distribution $P(v,h,t)$ at every time step we have to know the relative positions of the nearest neighbors of every site $\{v,h\}$. For this criterion, the sites on the lattice are classified into three different types: R, L, and C as shown in Fig. 2. Once the type of each site is known, the updating of the probability distribution $P(v,h,t)$ for finding the moving particle on site $\{v,h\}$ at time t is easily performed. If the coordinates and type of every site on a given generatrix lattice are found by direct enumeration, any lattice with an arbitrary number of generations may be constructed by a recursive procedure.

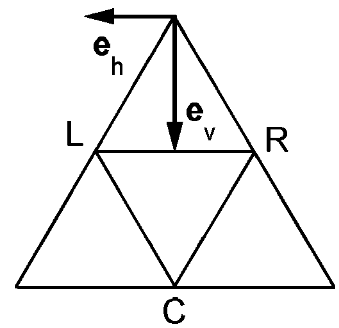

FIG. 2. Basis vectors used in the simulations to locate the sites of the two-dimensional Sierpinski lattice and the three site types according to the relative position of their neighbors R, L, and C.

The identification of every site by the two coordinates $\{v,h\}$ is not efficient because there are many coordinate pairs corresponding to no site in the finitely generated Sierpinski lattice. Better memory management is achieved if sites are numbered from top to bottom and from left to right, so that the top vertex of the main triangle is site number 1 and the right vertex is site number $N_{\max}=3(3^{g+1}+1)/2$. The one-particle distribution $P(N,t)$, N being the identification number of a given site, is updated in parallel following the simple rule (CK or master equation)

$$P(N,t+1)=\frac{1}{4}\sum_{\text{neighbors}}P(M,t). \tag{17}$$

In order to find the neighbor numbers M we still need the coordinates and types of all sites that have been stored on the corresponding vectors: $v(N)$, $h(N)$, and $T(N)$.

In Eq. (17) we have assumed the microscopic first passage distribution is $\psi_0(t)=\delta(t-1)$. No influence of this particular distribution on the statistical quantities of the infinite (or fractal) lattice is expected, as has been analytically proved by renormalization methods [5,6], but in the finitely generated lattices used in the numerical solutions unavoidable finite size effects dependent on $\psi_0(t)$ appear.

B. The mortality function

In this subsection we test our implementation of the numerical method described in the previous subsection by checking to what extent we are able to reproduce known results on the mortality function for finite and infinite lattices. Moreover, this test will serve to decide under what conditions one should expect that our numerical results describe the short-time propagator for an infinite lattice.

To this end a Sierpinski lattice with $g=4$, 6, 8 generations was considered. The particle starts moving from site O and is finally absorbed by traps placed on sites A_g, B_g, C_g, and

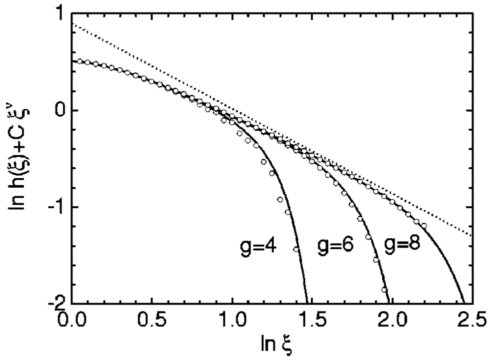

FIG. 3. The mortality function subdominant behavior $h(r,t)\exp(C\xi^\nu)$ as obtained from simulation against ξ for Sierpinski lattices with $g=4$, 6, and 8 generations (continuous line), besides the exact asymptotic behavior in the large ξ limit for the Sierpinski gasket (dotted line). The circles correspond to results obtained numerically inverting the exact Laplace transform $\widetilde{h}_g(s)$.

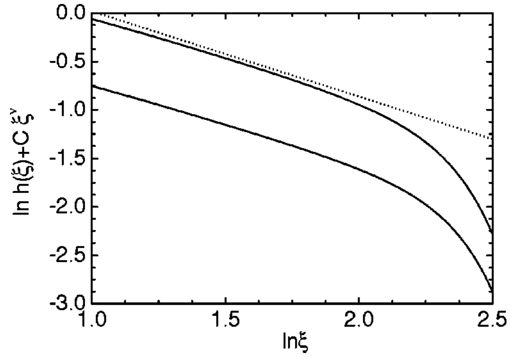

FIG. 4. The subdominant behavior of the mortality function $h(r,t)$ (the upper curve) and the function $\hat{h}(r,t)$ (the lowest curve) for the Sierpinski lattice with $g=8$. The dotted line is the exact asymptotic behavior of $h(r,t)$ for the Sierpinski gasket.

D_g, with the nearest neighbors of the origin belonging to the same decimation (see Fig. 1). Hence, the following initial conditions are satisfied by the probability distribution $P(N,t)$:

$$P(N,t=0)=\begin{cases}1, & N=N_0\\ 0, & N\neq N_0,\end{cases} \tag{18}$$

where $N_0=N_{\max}-2^g$ is the identifying number of the origin site.

The boundary condition imposed by the trap sites is taken into account by ignoring these sites in the sum of Eq. (17) when N corresponds to one of their neighbors. The probability flux towards the traps $F(r,t)$ is measured at every time step. Its sum from $t=1$ to a given t is the mortality function $h(r,t)$.

In Fig. 3 we have plotted on a double-logarithmic scale the results for $h(r,t)\exp(C\xi^\nu)$ against ξ as obtained (i) from simulations for Sierpinski lattices with $g=4$, 6, and 8; (ii) from the exact asymptotic expression for the large ξ limit for the infinite lattice

$$\ln h(\xi)+C\xi^\nu=\ln\frac{A(d_w-1)}{C}-\frac{\nu}{2}\ln\xi, \tag{19}$$

with $A=1.82$ and $C=0.98$ [7]; and (iii) from numerical Laplace inversion of $\widetilde{h}_g(s)=\widetilde{\psi}_g(s)/s$, which can be calculated exactly by means of renormalization equations as was shown in Sec. II A [cf. Eq. (7)]. (It is important to note that the agreement of our numerical results with the ''exact'' ones obtained by numerical Laplace inversion for the three finite lattices is a good test of the reliability of our simulations.) This figure clearly shows that, for example, it is not possible to use the Sierpinski lattice with four generations ($g=4$) to study the diffusion on the Sierpinski gasket for the large-ξ regime because the exact asymptotic behavior is never reached. However, we see that there exists an interval of ξ values (that we shall call interval of confidence), say $\ln\xi\in[1.3,1.8]$, where $\ln h_8(\xi)+C\xi^\nu$ vs $\ln\xi$ is almost a straight line that runs parallel and is almost coincident with the theoretically known subdominant behavior of the mortality function for the infinite lattice, i.e., almost coincident with $\ln h_\infty(\xi)+C\xi^\nu$, that is, with $\ln h(\xi)+C\xi^\nu$. Thus, one expects that, inside this interval of confidence, the behavior of the mortality function on the Sierpinski gasket is well approximated by the corresponding one on the Sierpinski lattice with eight generations given the fact that for this finite lattice and for this range of ξ we are able to resolve the exponent of its faint subdominant behavior. For example, a linear fit of $\ln h_8(\xi)+C\xi^\nu$ inside the confidence interval $[1.3,1.8]$ leads to the estimation of $\nu/2\simeq0.87$, in remarkably good agreement with the exact value for the infinite lattice $\nu/2=\ln 5/[2(\ln 5-\ln 2)]\simeq0.878$. On the other hand, the fact that the line for $h_8(\xi)$ is separate from $h(\xi)$ by an almost constant distance on the above interval means that diffusion on this finitely generated Sierpinski lattice cannot account for the amplitude $A(d_w-1)/C$ of the short-time-regime mortality function (see also Fig. 4). Obviously, this distance shrinks as the number of generations is increased.

Outside the confidence interval and for larger values of $\ln\xi$ we see that the line loses its straightness and begins to curve. We attribute this behavior to the appearance of finite-size effects, i.e., as a manifestation of the fact that the diffusion is really taking place on a finite lattice. The figure clearly shows that these finite-size effects appear earlier (i.e., for smaller values of ξ) for the smaller lattices. Inside these regions of ξ values, the simulation results are not reliable in the sense that they are not able to describe the behavior of the mortality function on the infinite lattice, i.e., on the Sierpinski gasket. For example, if we had used the values of $h_8(\xi)$ around $\xi=2.5$ to predict the power-law correction exponent of $h(\xi)$ we would wrongly find a much lower value than $-\nu/2$.

Finally, it is worthy of note that there exists a maximum ξ value beyond which $h_g(\xi)$ is equal to zero. This value is the one assigned to a (ballistic, nondiffusive) particle traveling from the origin to a trap along an straight line, that is, the first particle to reach the traps. These particles arrive at the traps in a minimum time equal to the value of the distance 2^g from the origin to the traps, so that $\xi_{\max}=2^{g(1-1/d_w)}\equiv2^{g/\nu}$, where $\nu=d_w/(d_w-1)$. This implies that the width of the interval of ξ values where one can confidently extrapolate to the asymptotic large ξ regime grows exponentially with g.

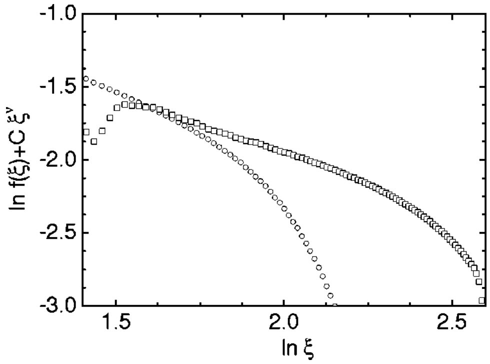

FIG. 5. Subdominant behavior of the propagator $P(r,t)$ obtained from an average over all sites within the shaded area in Fig. 1 and $t<2\times10^5$. The square (circle) symbols denote the simulation results when the shaded triangle is an 8-generation (6-generation) lattice.

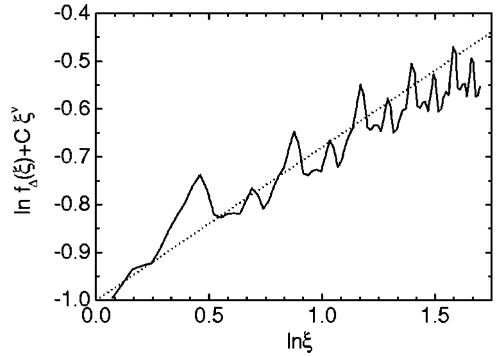

FIG. 6. Subdominant behavior of $P_{\triangle}(r,t)$ at $t=1000$. Here $f_{\triangle}(\xi)$ denotes $P_{\triangle}(r,t)t^{d_s/2}$. Simulations were carried out on an 8-generation lattice. The straight line has a slope of $\alpha_{\mathrm{KZB}}\simeq0.321$.

C. The propagator $P(r,t)$ and the $\hat{h}(r,t)$ function

In Sec. II B we have shown that starting from the general form of the propagator given in Eq. (4) and taking into account the key result of Eq. (10), it can be proved that $\alpha=\nu/2-d_f$ and that $\hat{\nu}$ coincides with the widely accepted value $\nu=d_w/(d_w-1)$. In this subsection we present numerical evidence supporting the validity of Eq. (10) and simulation results for the propagator itself, which shows that α adjusted values indeed agree with our proposal for the Sierpinski gasket embedded in two dimensions.

In order to compute a numerical value for the probability of finding the moving particle at a distance from the origin larger than r at time t, $\hat{h}(r,t)$, we have calculated the net flux entering the border sites A_n, B_n, C_n, and D_n (see Fig. 1) at every time step t. Then a numerical integration of this flux leads to approximate values for $\hat{h}(r,t)$, $t=1,2,\ldots$ with $r=2^g$, where g is the number of generations of the triangles formed by the vertices O, A_n, and B_n or O, C_n, and D_n. In Fig. 4 we have plotted the subdominant behavior of the mortality function and the function $\hat{h}(r,t)$ in the $g=8$ case (the entire lattice used in $\hat{h}(r,t)$ simulation was a $g=11$ Sierpinski lattice). The plotted curves are almost parallel straight lines in the ξ value region where extrapolation to the infinite lattice is significant. This means that $\hat{h}(r,t)$ and $h(r,t)$ are proportional in the large ξ asymptotic limit. At very short times, i.e., for $\xi\simeq\xi_{\max}$, the two functions $\hat{h}(r,t)$ and $h(r,t)$ tend to zero. The relation $\hat{h}(\xi)/h(\xi)\approx(z_0/z)\xi^{\alpha+d_f-\nu/2}$ follows from Eqs. (9), (10), and (12) [notice that $\hat{\nu}=\nu$ by Eq. (14)]. A linear fit of the numerical data for $\hat{h}(\xi)/h(\xi)$ on a double-logarithmic scale using the confidence interval $\ln\xi\in[1.3,1.8]$ gives us numerical estimations for the exponent $\epsilon=\alpha+d_f-\nu/2$ and the proportionality constant z_0/z. We have found that latter exponent is indeed small ($\epsilon=0.02$) as expected, which in turn means that our proposal $\alpha=\nu/2-d_f$ is probably correct in the infinite-generation lattice as the difference found on the finite-generation lattice has its origin in finite-size effects already described in the previous subsection. It is also noteworthy that $\hat{h}(\xi)/h(\xi)$ is equal, within the error bars, to the theoretically expected constant $z_0/z=1/2$, where ξ is taken as a typical value inside the extrapolation interval.

An additional check of these results was obtained from a direct simulation of the propagator. We took into account that the propagator $P(r,t)$ is a structure-averaged quantity. Thus, we define a function $f(\xi)$ including all the ξ dependence of the propagator as

$$f(\xi)=\langle\mathcal{P}(\mathbf{r},t;r=0,t=0)t^{d_s/2}\rangle_{\mathbf{r},t,\xi=r/t^{1/d_w}}, \qquad (20)$$

where the average is performed over all destination lattice sites and time steps. A space-time average is necessary in order to eliminate the local space structure observed with the usual snapshot method (see Fig. 6).

The Chapman-Kolmogorov equation was solved in the 11-generation Sierpinski lattice (the largest lattice that our computer can work with) starting with the probability distribution $P(\mathbf{r}=\mathbf{0},t=0)=1$, $P(\mathbf{r},t=0)=0$ if $\mathbf{r}\neq\mathbf{0}$. Two cases were considered. In the first, the average was restricted to the time interval $t<2\times10^5$ and to the sites within the shaded triangles of Fig. 1, which are 8-generation triangles. We ignored the 8-generation triangles adjacent to the origin in order to allow the diffusive regime to be reached. In the second case, we carried out the same calculations but now with the shaded triangles being 6-generation triangles and the same time interval.

In Fig. 5 the simulation results for the subdominant behavior of $f(\xi)$ [i.e., $\ln f(\xi)+c\xi^{\nu}$ vs $\ln\xi$] are plotted for both cases. We find a behavior very close to that we have seen for the mortality function in Fig. 3 (which is not very surprising taking into account that, as was discussed in Sec. III B, the two quantities are closely related): a line that is almost straight within a certain interval and that becomes curved for larger values of ξ. We will interpret this behavior in the same way as was done for the mortality function. Thus, we take the interval of ξ values where the plot of $\ln f(\xi)+c\xi^{\nu}$ vs $\ln\xi$ is almost straight as the confidence interval in which the propagator (including its subdominant term) for an infinite lattice is well described by the propagator for the finite lattice. We interpret the fact that the line is curved for larger values (outside the confidence interval) as a manifestation of the fact that the diffusion is really taking place on a finite lattice; i.e., we are here seeing finite-size effects (notice that these effects appear for smaller values of ξ for the smallest lattice case). For the case in which 8-generation triangles are used, we see that inside a certain (confidence) interval, say $\ln \xi \in [1.7,2.1]$, the line is approximately a straight line. A linear fit within this interval, assuming the values of $\nu \simeq \ln 5/(\ln 5 - \ln 2)$ and $c \simeq 0.98$, leads to $\alpha \simeq -0.79$ and $P_0 \simeq 0.67$, which compare reasonably well with our theoretical predictions of Eq. (15) for the two-dimensional Sierpinski gasket ($\alpha = -0.707$, $P_0 = 0.444$). It is worth noting that the fitted values are very sensitive to the values used for c and ν. For example, if the improved value [19] $c \simeq 0.981$ is used, the linear fit leads to $\alpha = -0.74$ and $P_0 = 0.63$, which are even closer to our theoretical predictions. This sharply contrasts with other theoretical predictions such as those of Ref. [9] [$\alpha = \alpha_{\mathrm{KZB}} \equiv (d_f - d_w/2)/(d_w - 1) \simeq 0.321$], Ref. [12] [$\alpha = (d_s - d_f)\nu/2 \simeq -0.193$], or Ref. [15] ($\alpha = 0$), which are clearly ruled out.

The (relatively) large difference between our theoretically predicted P_0 and the numerically obtained value may be due, apart from the uncertainties in the linear fit in Fig. 5, to the fact that the amplitude of the propagator in the short-time regime for our 8-generation lattice case could be substantially different from that of the gasket, as is the case for the amplitude of the mortality function (this was discussed above in Sec. III B).

A feature in this figure not present in that of the mortality function (Fig. 3) is the irregular behavior of the subdominant propagator for $\ln \lesssim 1.5$ in the 7-generation lattice case. This irregularity does not appear in the 6-generation lattice case either. We attribute this behavior to boundary effects: for large times there is a small but non-negligible probability (notice that we are resolving subdominant terms) that the random walker that is inside our shaded 8-generation lattice has come to this region after visiting the boundary of our 11-generation lattice, thus ''realizing'' that he is moving inside a box, not an infinite lattice. For the 6-generation lattice case, the distance between the frontier and the region in which we are computing the propagator (i.e., the shaded triangle) is so large that these boundary effects are really negligible, only showing up for even larger times (i.e., for even smaller values of ξ). Obviously, because the mortality function is evaluated for absorbing boundary conditions, these boundary effects never appear in Fig. 3.

IV. THE PROPAGATOR $P_\triangle$

In this section we explain why our numerical simulations and those carried out by Klafter *et al.* [9] disagree with respect to the value of the power-law subdominant exponent of the short-time propagator. The key point is that those authors analyze a quantity that is not the true or configurationally averaged propagator. That quantity, which we will denote by $P_\triangle(r,t)$, is defined as the probability of finding at time t the diffusing particle at distance r *along the sides* of the main triangle, which has a vertex at the starting point of this diffusing particle. It should be noted that those authors are completely aware that this quantity is not the true or configurationally averaged propagator. However, it seems that they assume that the two quantities have the same asymptotic form. This is a risky assumption for a disordered medium because not all directions are equivalent due to the presence of holes that serve as obstacles to diffusion, and the function $P_\triangle(r,t)$ only describes the propagation up to the *very specific* sites, which lies on the sides $OA_n, OB_n, \ldots$ of the triangles in Fig. 1. In the particular case of the two-dimensional Sierpinski gasket it is intuitively clear that the propagation along the sides of the main triangle is faster than along a path forming an angle with them as a consequence of the triangular holes appearing in all scales that the diffusing particle must go around. As the propagator is defined as the structural average of the transition probability between two sites (3), it can be expected that $P(r,t) < P_\triangle(r,t)$.

We start by showing analytically that, although the two ''propagators'' are very close, they exhibit different power-law corrections to the same stretched exponential. In Refs. [5,6] Van den Broeck developed a renormalization scheme for $P_\triangle(2^n,t)$, the probability of finding the random walker precisely at the nearest neighbors of the origin after n decimations of the two-dimensional fractal lattice (see Fig. 1) at time t. He found that the following exact asymptotic relation in the Laplace space holds:

$$\frac{\widetilde{P}_\triangle(r,s)}{\widetilde{P}_\triangle(0,s)} \sim \exp[-crs^{1/d_w}]. \tag{21}$$

Taking into account that the probability distribution of return to the origin is $P_\triangle(0,t) = P(0,t) \sim t^{-d_s/2}$ and inverting the Laplace transform in Eq. (21) for $P_\triangle(r,t)$ we find that this pseudopropagator is in fact given by Eqs. (4) and (5), but with $\alpha = \alpha_{\mathrm{KZB}} \equiv (d_f - d_w/2)/(d_w - 1)$.

In order to check the above statements numerically, i.e., that the subdominant behavior of $P_\triangle(r,t)$ does not correspond to that of the true propagator, we have plotted $\ln P_\triangle(r,t) t^{d_s/2} + c\xi^\nu$ at $t = 1000$ against $\ln \xi$ in Fig. 6. A rough and almost periodic structure is observed, which is possibly an effect of the bottlenecks that occur at those sites corresponding to the transition between the n-generation and the $(n+1)$-generation lattice (such as the ones labeled in Fig. 1). Nevertheless, the general trend is well represented by a prefactor ξ^α with $\alpha \simeq 0.3$ in agreement with the theoretical prediction $\alpha_{\mathrm{KZB}} \simeq 0.321$ for the two-dimensional Sierpinski gasket, but in clear disagreement with the exponent $\alpha \simeq -0.8$ found numerically for the averaged propagator $P(r,t)$.

V. CONCLUSIONS

In this paper we have studied the Green function or propagator on deterministic fractals, which is one of the most fundamental quantities in the statistical description of the diffusion of random walkers. Starting from an exact result for the large-ξ limit (or short-time regime) of the mortality function on a fractal with traps, Eq. (9), and taking into account Eq. (10), we derived an expression for the propagator in the asymptotic regime $\xi \gg 1$: $P(r,t) \approx P_0 t^{-d_s/2} \xi^\alpha \exp(-c\xi^\nu)$ with $\alpha = \nu/2 - d_f$ and $\nu = d_w/(d_w - 1)$. The same functional form for the short-time propagator has recently been proposed by other authors but with very different relations between α and the characteristic parameters of the fractal structure in which the diffusion is taking place (fractal dimension d_f, spectral dimension d_s, random walk dimension d_w).

In order to elucidate this controversy we carried out simulations in a two-dimensional Sierpinski lattice. Specifically, we calculated numerically the mortality function, the closely related $\hat{h}(r,t)$ function, and the propagator. By comparing the simulation results for the mortality function with its exact asymptotic behavior we were able to delimit a range of ξ values where the diffusive behavior on a finite lattice is similar to that on the infinite Sierpinski gasket. The numerical results for $\hat{h}(r,t)$ in the 8-generation Sierpinski lattice showed that the relation $\hat{h}(r,t)/h(r,t)\approx 1/2$ is probably true for the large-ξ limit in the two-dimensional Sierpinski gasket. This gives indirect support to our proposed short-time propagator. More direct support came from numerical simulation of the propagator itself in the 11-generation Sierpinsky lattice. A structural average over a significant portion of this lattice was performed, and the numerical estimates found for α and P_0 were consistent with the theoretical predictions of this paper $[\alpha=\nu/2-d_f=-0.707,\quad P_0=z_0 d_w A/(z\Omega)\simeq 0.444]$, but clearly ruled out other recent theoretical proposals.

The function $P_\triangle(r,t)$, which describes the propagation along the sides of the main triangle, was also simulated and the results agreed with the same propagator form of Eq. (4) but with $\alpha=\alpha_{\mathrm{KZB}}=(d_f-d_w/2)/(d_w-1)\simeq 0.321$. We thus deduce from the above discussion that the probability of finding a random walker at a given site at time step t, provided that it started from another given site at time $t=0$, depends explicitly on the positions of those two sites as a consequence of the local microscopical disorder. Only its average over the whole lattice (the propagator) is a meaningful statistical quantity with a simple analytical behavior.

Simulations showed that the dominant term $\exp(-c\xi^\nu)$ appears in the propagator $P(r,t)$ and in the pseudopropagator $P_\triangle(r,t)$ (and also in the mortality function and first-passage-time density) in a Sierpinski lattice, but that the subdominant power-law exponent takes very different values. The analytical results of Sec. II suggest that the same is true in any deterministic fractal.

An extension of these results to other deterministic fractals (e.g., Given-Mandelbrot curve, Sierpinski gaskets embedded in higher dimensions) or even random fractals (e.g., percolation aggregates) is necessary in order to check the possible universality of the (short-time) propagator expression proposed in this paper. Work along this line is in progress.

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