Escape Times of j Random Walkers from a Fractal Labyrinth

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The problem of the statistical description of the first passage time $t_{j,N}$ to a given distance r of the first j of a set of N noninteracting diffusing particles, all starting from the same origin on fractal substrates, is addressed. Asymptotic expressions (the main and two corrective terms) for large N of the (arbitrary) moments of $t_{j,N}$ are given. It is shown that, to first order and for $1 \leq j \ll N$, the mth moment of $t_{j,N}$ goes as $(\ln N)^{m(1-d_w)}$, and its variance as $(\ln N)^{-2d_w}$, d_w being the anomalous diffusion exponent of the fractal medium. [S0031-9007(97)04503-1]

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The random walk formalism has proven to be extremely fruitful in science [1,2]. Usually it is the random walk of only *one* particle which is studied, but the behavior of *many* random walkers is also presently an area of active research [3]. Thus, for example, Larralde *et al.* have recently found very nice results regarding the number of distinct sites, $S_N(t)$, visited by a set of $N \gg 1$ independent random walkers on Euclidean lattices of one, two, and three dimensions [4]. Shortly thereafter, these results were extended to fractal substrates [5]. Diffusion in these fractal media has attracted much attention because it exhibits new, qualitatively different properties (anomalous diffusion) also present in geometrically disordered media (indeed, fractals are considered good models for disordered media) which are unexplained by the classical theories of diffusion [6,7]. For example, the mean-square displacement of a random walker is given by $\langle r^2 \rangle \approx 2Dt^{2/d_w}$, $d_w \neq 2$ being the anomalous diffusion exponent (or fractal dimension of a random walk) and D the diffusion coefficient.

In this Letter we give an answer to another basic question about the diffusion of a group of particles in a fractal medium that, as we will see, is closely related to the problem of calculating $S_N(t)$. The question is: If a set of N independent random walkers (*ants,* in the language coined by de Gennes [1,8]) are initially placed (*parachuted*) onto a site of a fractal structure (*the labyrinth*), how long will it take the first j random walkers to reach a given distance r from the origin? In other words, if the exits of the maze are placed at a distance r, what are the escape times of the first j ants of this battalion of N members? (Notice that not only the first passage time of the first particle is important if more than one particle must arrive at a certain place in order to trigger some effect there.) Explicitly, in this Letter we give asymptotic expressions ($N \gg 1$) for the moments of the jth passage time, $t_{j,N}(r)$, i.e., of the time to first reach a given distance r of the jth random walker of a set of N independent diffusing random walkers all starting from the same origin on a fractal substrate. Or, in other words, we give an asymptotic description of the order statistics [9,10] of the diffusion process. Some results concerning the order statistics of a set of random walkers on Euclidean lattices are known [11]. However, for the diffusion limit there are rigorous asymptotic ($N \gg 1$) results only for one-dimensional processes (with only certain conjectures for higher dimensions [9,12]). In this Letter we extend these results to fractal substrates and, in passing, improve the one-dimensional results.

In what follows we take the mean time spent by a single random walker to reach the (arbitrary) distance r as the time unit. Let the mortality function $h(t)$ be the probability that a single diffusing particle has reached this distance r during the time interval $(0,t)$, and let $\psi(t) = dh(t)/dt$ be the first-passage-time density. The probability density $q_{j,N}(t)$ for the first passage time to a site situated at a distance r of the jth out of N noninteracting particles is [9,10] $q_{j,N}(t) = N!/[(N-j)!(j-1)!]\psi(t)h^{j-1}(t)[1-h(t)]^{N-j}$. The generating function $U_{N,m}(z) = \sum_{j=1}^{N} \langle t_{j,N}^m \rangle z^{j-1}$ of the mth moment of the jth passage time, $\langle t_{j,N}^m \rangle = \int_0^\infty t^m q_{j,N}(t)\,dt$, can be written as [9,12]

$$U_{N,m}(z) = \frac{m}{1-z} \int_0^\infty t^{m-1}[(1-h+hz)^N - z^N]\,dt\,. \tag{1}$$

As we are looking for expressions for $\langle t_{j,N}^m \rangle$ when $1 \leq j \ll N$, it is immaterial whether we evaluate the integral of Eq. (1) or

$$U_{N,m}^*(z) = \frac{m}{1-z} \int_0^\infty t^{m-1} \exp\{N \ln[1-h(t)(1-z)]\}\,dt\,, \tag{2}$$

and it suffices to know $h(t)$ for small times. The main term of the asymptotic expression of $h(t)$ for small times has already been calculated for finitely ramified fractals [13] through the estimation of the main term of the first-passage-time density, $\psi(t)$, by means of a renormalization procedure due to Machta [14] and Van den Broeck [15]. However, as we will see below, we have to get this main term *and* the next corrective term in order to evaluate the main term of the variance of $t_{j,N}^m$. To this end we proceed as follows. We start from the main asymptotic term of the Laplace transform of the first-passage-time density, namely,

$$\tilde{\psi}(s) \approx \tilde{A} \exp(-\tilde{C} s^{1/d_w}) \tag{3}$$

for large s. Here $\tilde{C}$ is a constant that can be estimated numerically and $\tilde{A}^{\eta-1}$ is the probability that one random walker goes from a site to any of its nearest neighbors on the nth generation (fractal) lattice via any of the shortest paths traced over the $(n+1)$th generation lattice, η being the number of steps of this path [13]. Values of these constants for several fractals are given in Table I. Next, we get $\psi(t)$ for small t by Laplace inversion of $\tilde{\psi}(s)$, which can be done by means of the saddle-point method [16], obtaining

$$\psi(t) \approx \hat{A} t^{-(1+\beta/2)} \exp(-C/t^{\beta})(1 + \phi_1 t^{\beta}), \tag{4}$$

where $\hat{A} = \sqrt{\nu/(2\pi)}(\beta\tilde{C}/\nu)^{\nu/2}\tilde{A}$, $C \equiv t_0^{\beta} = \beta^{\beta}(\tilde{C}/\nu)^{\nu}$, $\phi_1 = (1-2d_w)(d_w-2)/24C$, $\beta = 1/(d_w-1)$, and $\nu = \beta + 1$. From here one easily deduces that

$$h(t) \approx A t^{\beta/2} \exp[-(t_0/t)^{\beta}](1 + h_1 t^{\beta}) \tag{5}$$

for small t, with $A = \hat{A}/\beta C$ and $h_1 = \phi_1 - 1/2C$ (see Table I). Inserting this expression into Eq. (2) and after a lengthy derivation similar to that of Sect. 3 of Ref. [12] (details will be given elsewhere) we get

$$\begin{aligned} U^*_{N,m}(z) = \frac{1}{1-z}\frac{t_0^m}{\ln^{\alpha}\lambda}\Bigg\{1 &+ \frac{\alpha}{\ln\lambda}\left(\frac{1}{2}\ln\ln\lambda - \gamma\right) \\ &+ \frac{\alpha}{2\ln^2\lambda}\left[(1+\alpha)\left(\frac{\pi^2}{6}+\gamma^2\right) + \gamma - 2h_1 t_0^{\beta} - \left(\frac{1}{2} + (1+\alpha)\gamma\right)\ln\ln\lambda \right. \\ &\left. + \frac{1+\alpha}{4}\ln^2\ln\lambda\right] + \mathcal{O}\left(\frac{\ln^3\ln\lambda}{\ln^3\lambda}\right)\Bigg\}, \end{aligned} \tag{6}$$

where $\alpha = m/\beta = m(d_w - 1)$, $\gamma \simeq 0.577\,215$ is the Euler constant, and $\lambda = (1-z)NAt_0^{\beta/2}$.

Expanding $U^*_{N,m}(z)$ in a power series of z one finds, after lengthy algebraic manipulation, the moment of order m of the mean first passage time for the first j out of N particles:

$$\langle t^m_{j,N}\rangle = \langle t^m_{1,N}\rangle + \frac{t_0^m}{\ln^{\alpha+1}\lambda_0 N}\sum_{n=1}^{j-1}\frac{\Delta_n(\alpha)}{n} \tag{7}$$

with

$$\begin{aligned} \langle t^m_{1,N}\rangle = \frac{t_0^m}{\ln^{\alpha}\lambda_0 N}\Bigg\{1 &+ \frac{\alpha}{\ln\lambda_0 N}\left(\frac{1}{2}\ln\ln\lambda_0 N - \gamma\right) \\ &+ \frac{\alpha}{2\ln^2\lambda_0 N}\left[(1+\alpha)\left(\frac{\pi^2}{6}+\gamma^2\right) + \gamma - 2h_1 t_0^{\beta} - \left(\frac{1}{2} + (1+\alpha)\gamma\right)\ln\ln\lambda_0 N \right. \\ &\left. + \frac{1+\alpha}{4}\ln^2\ln\lambda_0 N\right] + \mathcal{O}\left(\frac{\ln^3\ln\lambda_0 N}{\ln^3\lambda_0 N}\right)\Bigg\}, \end{aligned} \tag{8}$$

and where

$$\Delta_n(\alpha) = \alpha + \frac{\alpha(\alpha+1)}{2\ln\lambda_0 N}\left[(-1)^n\frac{2S_n(2)}{(n-1)!} + \ln\ln(\lambda_0 N) - \frac{1}{\alpha+1} - 2\gamma\right] + \mathcal{O}\left(\frac{\ln^2\ln\lambda_0 N}{\ln^2\lambda_0 N}\right), \tag{9}$$

$\lambda_0 \equiv \lambda(z=0)/N = At_0^{\beta/2}$, and $S_n(2)$ are Stirling numbers of the first kind [17]. In Fig. 1 we compare $\langle t_{1,N}\rangle$ calculated through the numerical integration of $\int_0^{\infty} t\, q_{1,N}(t)\,dt = \int_0^{\infty}[1-h(t)]^N$ with the values given by Eq. (8) for four subtrates. We see that the asymptotic formula is in good agreement with the numerical results even for N not too large, say, for $N \gtrsim 16$.

From Eq. (7) we can estimate the flux of particles, $\phi(t) = dj/dt$, that leaves a ("spherical") surface placed at the distance r (i.e., the flux of trapped particles if this spherical boundary is absorbent):

$$\phi(t) \sim \frac{1}{\langle t_{j+1,N}\rangle - \langle t_{j,N}\rangle} \approx \frac{\ln^{d_w}\lambda_0 N}{t_0(d_w-1)}\, j\,,$$

where we have approximated $\Delta_j(d_w-1)$ by $d_w - 1$. This means that initially (i.e., for short times) the number of absorbed particles at time t, $j(t)$, grows exponentially with time, $j(t) \sim \exp(t/\tau)$, the characteristic time $\tau = t_0(d_w-1)/(\ln^{d_w}\lambda_0 N)$ being smaller for larger d_w.

The variance $\sigma^2_{j,N} \equiv \langle t^2_{j,N}\rangle - \langle t_{j,N}\rangle^2$ can be deduced from Eqs. (7) and (8):

$$\sigma^2_{j,N} \approx \frac{t_0^2(d_w-1)^2}{\ln^{2d_w}\lambda_0 N} \times\left[\frac{\pi^2}{6} - \left(\sum_{n=1}^{j-1}\frac{1}{n}\right)^2 + \sum_{n=1}^{j-1}(-1)^n\frac{2S_n(2)}{n!}\right]. \tag{10}$$

Notice that it is necessary to know the main and two corrective terms of $\langle t_{j,N}\rangle$ and $\langle t_{j,N}\rangle^2$ to get only the main term of the variance. We see that to lowest order in $\ln N$, the coefficient of variation $t_{j,N}/\sigma_{j,N}$ goes as $\ln N$ independently of the fractal substrate (including the

TABLE I. Parameters appearing in the asymptotic expression of the mortality function, Eq. (5), the first-passage-time density, Eq. (4), and its Laplace transform, Eq. (3), for four substrates: The symbol 1D refers to the one-dimensional lattice, Sd to the d-dimensional Sierpinsky lattice, and GM to the Given-Mandelbrot curve.

Case	d_w	$\tilde{A}$	$\tilde{C}$	$\hat{A}$	ϕ_1	A	t_0	h_1
1D	2	2	$\sqrt{2}$	$\sqrt{2/\pi}$	0	$2\sqrt{2/\pi}$	1/2	−1
S2	ln 5/ ln 2	4	1.96	1.82	−0.050	2.46	0.97	−0.56
S3	ln 6/ ln 2	6	2.30	2.78	−0.078	3.36	1.53	−0.46
GM	ln 22/ ln 3	4	2.0	1.5	−0.14	2.5	1.2	−0.6

one-dimensional lattice). A check of this result for $j = 1$

$$\frac{t_{1,N}}{\sigma_{1,N}} \approx \frac{\sqrt{6}\,(d_w - 1)}{\pi} \ln N \tag{11}$$

is shown for the four example substrates in Fig. 2. It is clear that the numerically evaluated ratio $t_{1,N}/\sigma_{1,N}$ closely follows the theoretical prediction given by Eq. (11).

It should be kept in mind that we have chosen the mean time for a single particle to reach the distance r as a time unit. If we want this distance to appear explicitly in the above results, we have only to replace t by $t(\sqrt{2D/r}\,)^{d_w}$. For example, Eq. (8) to order zero and for $m = 1$ would become

$$\langle t_{1,N} \rangle \approx \frac{t_0}{\ln^{d_w - 1} \lambda_0 N} \left(\frac{r}{\sqrt{2D}} \right)^{d_w}. \tag{12}$$

It is instructive to use this formula to deduce an asymptotic expression for $S_N(t)$, the number of distinct sites visited by N particles diffusing on a fractal (which is the main result of Havlin *et al.* [5]). For media with spectral dimension $d_s = 2d_f/d_w$ less than two (d_f is the fractal dimension) the random walkers perform compact exploration in the sense of de Gennes [6,18] (most sites inside a compact region are visited before a new site outside this region is reached). If $R_N(t)$ is the mean longest distance reached by any of the N random walkers during the time t, the number of distinct sites visited by these particles is just the number of sites that are at distances smaller than R_N (i.e., the volume of the "sphere" of radius R_N), i.e., $S_N(t) \sim R_N^{d_f}(t)$. But we have found that the mean time to *first* reach the distance r by any of the N particles is given by $\langle t_{1,N}(r) \rangle \sim r^{d_w}/\ln^{d_w - 1} \lambda_0 N$ [cf. Eq. (12)], so that one expects that the mean *longest* distance reached by any of these particles should be given by $R_N(t) \sim (t \ln^{d_w - 1} \lambda_0 N)^{1/d_w}$. Therefore,

$$S_N(t) \sim t^{d_f/d_w} (\ln \lambda_0 N)^{d_f(d_w - 1)/d_w}, \tag{13}$$

in agreement with Havlin *et al.* [5].

In summary, we have answered the following basic problem about diffusion on fractals: Given a large number of particles all starting from the same place diffusing on a fractal, how long will it take (on average) for the first particle to cross a given distance? How long for the second one? And for the jth? In fact we have solved this (order

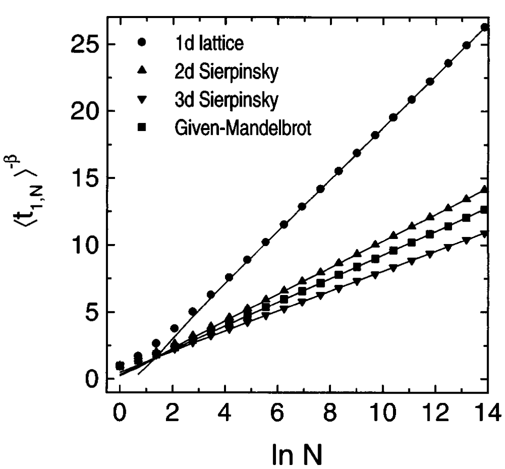

FIG. 1. The dependence on N of the first passage time of the first particle out of N, $\langle t_{1,N} \rangle$, for the one-dimensional lattice, the two- and three-dimensional Sierpinsky lattices, and the Given-Mandelbrot curve. Here $\beta = 1/(d_w - 1)$. The symbols correspond to the numerical estimate for $N = 2^n$ with $n = 0, 1, \ldots, 20$, and the solid lines to Eq. (8) with $m = 1$. Times are expressed in units of the mean first passage time of a *single* random walker.

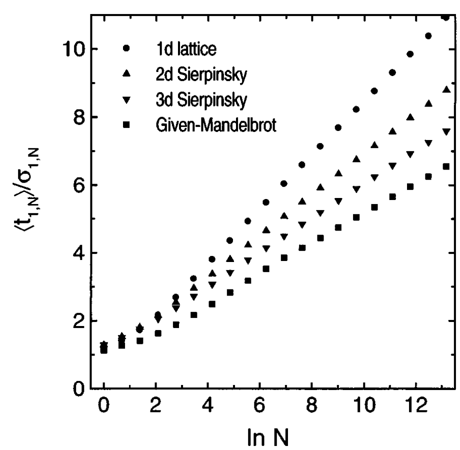

FIG. 2. The ratio $\langle t_{1,N} \rangle / \sigma_{1,N}$ evaluated numerically for $N = 2^n$ with $n = 0, 1, \ldots, 20$ for the same substrates as in Fig. 1. The slopes of linear fits to the last ten points (N from 2^{11} to 2^{20}) are 0.783 for the one-dimensional lattice, 0.596 and 0.497 for the two- and three-dimensional Sierpinsky lattices, respectively, and 0.433 for the Given-Mandelbrot curve. These values are in good agreement with the corresponding asymptotic values given by Eq. (11), i.e., $\sqrt{6}\,(d_w - 1)/\pi$, which are 0.780, 0.590, 0.492, and 0.430, respectively.

statistics) problem in a more general way because we have found expressions (although asymptotic) for the arbitrary moments of these quantities, namely, the first passage time $t_{j,N}$ of the jth particle out of a total of $N \gg j$. The solution is condensed in Eq. (6), in which the main and two asymptotic corrective terms of the generating function of these moments are given. We have seen that this is the minimum number of terms needed to obtain the main term of the variance. We have discovered the extremely mild dependence of the first passage time of the first walkers on the number N of walkers: these times are (to first order) inversely proportional to a power of $\ln N$, the power being the anomalous diffusion exponent, d_w, characteristic of the medium in which the diffusion is taking place. The results of this Letter open up an alternative route for experimentally determining d_w for self-similar media (for example by means of the experimental evaluation of the ratio $\langle t_{1,N}\rangle/\sigma_{1,N}$; see Fig. 2). Because a *set* of particles is used (typically with $N \sim 10^{23}$) this kind of experiment should be easier to carry out than any experiment involving a single molecule.

At this point it is natural to ask whether the results we have found are valid for all self-similar media (disordered media included). I think that the answer is affirmative for the following reasons. Knowledge of the mortality function $h(t)$ for short times [cf. Eq. (5)] is crucial in obtaining the key formula of this Letter, Eq. (6). This function has been rigorously derived by means of a renormalization procedure for finitely ramified deterministic fractals, but is unknown for other types of self-similar media (percolation clusters at criticality, for example). However, there are arguments to support the validity of the expression used in this Letter, Eq. (5), for these other media also [13]. Moreover, the fact that from the results presented in this Letter we were able to reobtain the expression found by Havlin *et al.* [5] for the number of distinct sites visited by N random walkers [cf. Eq. (13)], which is valid for the percolation cluster at criticality, also supports this conjecture.

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