First-passage time, survival probability and propagator on deterministic fractals

1995 J. Phys. A: Math. Gen. 28 7027

(http://iopscience.iop.org/0305-4470/28/24/004)

J. Phys. A: Math. Gen. 28 (1995) 7027–7038. Printed in the UK

First-passage time, survival probability and propagator on deterministic fractals

S Bravo Yuste

Departamento de Física, Universidad de Extremadura, 06071 Badajoz, Spain

Received 2 August 1995

Abstract. The first-passage time density, $\psi(r,t)$ (defined as the probability density for the time spent by a random walker to travel (for the first time) the distance r that separates the starting site from its nearest neighbours), and the survival probability $S(r,t)$ (i.e. the probability that a random walker who starts at a site has not been absorbed by traps located on its nearest neighbours at distance r in the time interval $(0,t)$), were calculated for the class of deterministic fractals in which sites are isolated from the rest of the lattice by their nearest neighbours. The large $\xi \equiv r/(\sqrt{2D}t^{1/d_w})$ asymptotic expressions for these quantities are $\psi(r,t) \approx A\xi^{\nu/2+d_w}\exp(-C\xi^\nu)$ and $h(r,t) = 1 - S(r,t) \approx (A/C)(d_w - 1)\xi^{-\nu/2}\exp(-C\xi^\nu)$ with $\nu = d_w/(d_w-1)$, A and C being characteristic constants for each fractal. The asymptotic expression for $S(r,t)$ is used to justify that, for this class of deterministic fractals, the propagator or Green function is given asymptotically by $P(r,t) \sim t^{-d_s/2}\xi^\alpha\exp(-C\xi^\nu)$ for large ξ, with $\alpha = \nu/2 - d_f$. This value of α differs from others proposed recently.

1. Introduction

Transport in disordered systems displays many qualitatively different properties with respect to transport in uniform systems [2, 3]. For example, such systems exhibit anomalous diffusion which is usually [1] manifested in the behaviour of the mean-square displacement of a random walker:

$$\langle r^2\rangle \approx 2Dt^{2/d_w} \tag{1.1}$$

where $d_w > 2$ is the anomalous diffusion exponent and D is the diffusion coefficient. Because fractal structures also show these anomalous properties, they have been regarded as models for geometrically disordered systems.

The key property of fractal structures is their dilation symmetry (self-similarity) which allows, in some cases, one to find analytic results by means of renormalization schemes. For example, the anomalous diffusion exponent [3] or the first-passage time to a nearest neighbour [4, 5] may be obtained in this way. Some other analytic results concerning the function $\hat{P}(\boldsymbol{r},t) \equiv r^{d_f-d}P(r,t)$, defined as the (configurational averaged) probability density to find the random walker at time t at a distance $\boldsymbol{r}$ from its starting point, are known. The constant d_f is the fractal dimension and d is the dimension of the Euclidean space in which the fractal is embedded. Both $\hat{P}$ and P are called the propagator or Green function of the diffusion. From the definition of $\hat{P}$, one has that $r^{d_f-d}P(r,t)\,\mathrm{d}^d\boldsymbol{r}$ is the probability of finding the random walker in the volume $\mathrm{d}^d\boldsymbol{r}$ at distance $\boldsymbol{r}$ from its starting point, and thus

$$\langle r^2\rangle = \int r^{d_f-d+2}P(r,t)\,\mathrm{d}^d\boldsymbol{r}\,. \tag{1.2}$$

0305-4470/95/247027+12$19.50

For loopless fractals (such as self-avoiding walks) and for the infinite percolation cluster at criticality, the propagator has the form of a stretched Gaussian [3]

$$P(r,t) \sim t^{-d_s/2} \exp\left(-\bar{c}\xi^{\hat{\nu}}\right) \tag{1.3}$$

for $\xi \gg 1$, where

$$\xi \equiv \frac{r}{\sqrt{2D}t^{1/d_w}} . \tag{1.4}$$

Here $d_s = 2d_f/d_w$ is the spectral dimension, c is a constant and

$$\hat{\nu} = \nu \equiv \frac{d_w}{d_w - 1} . \tag{1.5}$$

The propagator given by (1.3) is also expected for fractals with loops, but the value of $\hat{\nu}$ for fractals has been a subject of controversy [3]. Guyer [6], by means of numerical renormalization in the Laplace space, and Van den Broeck, by analytical renormalization on first-passage times, have shown that $\hat{\nu} = \nu$ for the Sierpinsky gasket in two dimensions. Also, Klafter *et al* [7] have found that this value is in agreement with numerical results for d-dimensional Sierpinsky gaskets. To the best of my knowledge, these are the only deterministic fractals with loops for which the propagator of (1.3), with $\hat{\nu}$ given by (1.5), has been justified. Surprisingly, in spite of this weak support, equation (1.3) together with (1.5) is usually accepted to be of general validity for all kinds of fractals! In this paper I shall add reasons to maintain this belief by giving arguments to support that $P(r,t)$ is described by (1.3) and (1.5), not only for Sierpinsky gaskets, but for a whole class of deterministic fractals (to which the d-dimensional Sierpinsky gasket belongs). These fractals are those in which sites are isolated from the rest of the lattice by their nearest neighbours of the same generation (a detailed description of this class of fractals is given in section 2). Examples are the d-dimensional Sierpinsky gasket, the Given–Mandelbrot curve [8], the Cayley tree, the hierarchical percolation model, or the Mandelbrot–Viseck curve [9]. Furthermore, I claim that the propagator for all of these fractals is more precisely described by adding a potential factor to (1.3), i.e.

$$P(r,t) \sim t^{-d_s/2}\xi^{\alpha} \exp\left(-c\xi^{\nu}\right) \tag{1.6}$$

with

$$\alpha = \nu/2 - d_f . \tag{1.7}$$

Expressions of the form (1.6) have been conjectured for any fractal in [10–12], but with different values for α. There, $P(r,t)$ is found as the solution of a fractional diffusion equation and several expressions for α are postulated on an empirical basis or from arguments of plausibility. The most recent proposal, due to Roman and Alemany [12], is $\alpha = \alpha_{\mathrm{RA}} \equiv (d_s - d_f)\nu/2$. This proposal has recently received additional support from Roman in [13], in which random fractals were studied analytically and numerically. Based on an entirely different approach and on numerical results for d-dimensional Sierpinsky gaskets, Klafter *et al* [7] have proposed $\alpha = \alpha_{\mathrm{KZB}} \equiv (d_f - d_w/2)/(d_w - 1)$.

In section 2, I calculate, following the procedure of van den Broeck [4, 5] and for those fractals with sites isolated by nearest neighbours, the probability density for the time spent by a random walker, initially on a site of the fractal lattice, to arrive for the first time at any of its nearest neighbours of the same generation, i.e. the first-passage-time (or waiting-time) density $\psi(t)$. Next, this quantity is reinterpreted as the probability density for the time spent by the random walker to travel, for the first time, the distance r that separates the starting site from its nearest neighbours. This shall be written as $\psi(r,t)$ in order to emphasize this interpretation. In this section it is proved that the first-passage-time density is given asymptotically by $\psi(r,t) \approx A\xi^{\nu/2+d_w}\exp(-C\xi^{\nu})$ for large $\xi \equiv r/(\sqrt{2D}t^{1/d_w})$. Here A and C are characteristic constants for each fractal. I provide their values for some significative cases below. Next, $\psi(r,t)$ is used to calculate the survival probability, $S(r,t)$, i.e. the probability that a random walker who starts at a site has not been absorbed by traps located on its nearest neighbours at a distance r in the time interval $(0,t)$. This is a fundamental quantity in the study of the so-called 'trapping problem' [14, ch 5] where it is required either directly, when the traps are placed at a fixed distance [15], or as a prior known magnitude when traps are randomly placed [16, 17]. Examples of this last case appear in the study of diffusion-limited reactions in fractal structures [18, and references therein] where, as is well known, the reaction kinetics is non-classical.

In section 3, it is argued that the functional form of $P(r,t)$, for large ξ, can be deduced from the functional form of $S(r,t)$ assuming, that $S(r,t) \sim \int_0^r P(x,t)x^{d_f-1}\,dx$ when t is small and r is large (i.e. large ξ). The expression for $P(r,t)$ so 'derived' is a stretched Gaussian corrected by a power-law factor whose exponent is given by $\nu/2 - d_f$ (see equation (1.6)). I think is worth noticing that the approach for this 'derivation', which goes through the concepts of first-passage time and survival probability, is, to the best of my knowledge, completely new. Finally, the results are summarized and discussed in section 4.

2. First-passage time and survival probability

As is well known, an easy way of generating deterministic fractals is by means of an iterative procedure that uses an 'initiator' and a 'generator' [8]. For example, we can generate a two-dimensional Sierpinsky fractal by means of a triangle as initiator and a generator formed by three triangles joined at their vertex. At each iteration (generation), every triangle equal (except for its size) to the initiator is replaced by the generator. Figure 1 shows a triangle of the nth generation and its internal triangles corresponding to the $(n+1)$th and $(n+2)$th generation. Of course, the fractal may be generated in the 'opposite direction'. One starts from the initiator (the zeroth triangle) and, at each iteration, the $(n+1)$th triangle is formed by means of the nth triangles (disposed in the same way that the zeroth triangles were arranged to form the generator (the first triangle)). I will call the zeroth decimated fractal or, simply, original lattice, the lattice formed by initiators, and the nth decimated fractal the lattice formed by the nth figures (triangles in our example). The $(n+1)$th decimated lattice is the decimated lattice of the nth decimated fractal.

For our purposes, we will see these geometrical constructions as lattices formed by connections (the sides of the triangles in our example) and sites (the points of bifurcations). The random walker goes (jumps) from a site to one of its nearest neighbours after a (waiting) time which is a random variable. It shall be assumed in this paper that the mean waiting time between jumps is finite. A property of the d-dimensional Sierpinsky lattice, shared by many other fractals (Given–Mandelbrot curve, Cayley tree, Mandelbrot–Viseck curve, hierarchical percolation model, ...), is that it is not possible to go from a site (say, O in figure 1) to a non-nearest neighbour on the $(n+2)$th decimated lattice (the site A, for example) via the connections of the $(n+1)$th decimated lattice without previously passing through its nearest neighbours on the $(n+2)$th decimated lattice (sites 1, 2, 3 and 4). It will be said that sites are isolated by their nearest neighbours in these fractals.

The first-passage-time (FPT) density $\psi(t)$ of a fractal is, by definition, the probability that a diffusing particle starting at a site reaches, for the first time, at time t any of its

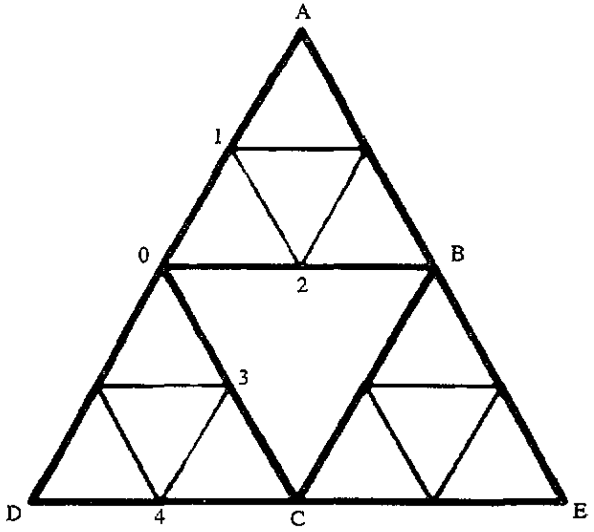

Figure 1. A triangle, AED, of the nth generation (decimation) and its internal triangles corresponding to the $(n+1)$th ($(n-1)$th decimation) and $(n+2)$th generation ($(n-2)$th decimation) of the two-dimensional Sierpinsky gasket. An example of the $(n+1)$th generation triangle is OAB, while one of the $(n+2)$th generation triangle is O12.

nearest neighbours on the many (ideally, infinitely) times decimated fractal. That is,

$$\psi(t) = \lim_{n\to\infty} \psi_n(t) \tag{2.1}$$

where $\psi_n(t)$ is the FPT density for the n-times decimated fractal. For fractals with sites isolated by their nearest neighbours it is possible to calculate $\psi(t)$ by means of the renormalization procedure of Van den Broeck [4, 5] (conceived initially by Machta [19] for a one-dimensional regular lattice). In this paper, I will consider FPT densities with a finite first moment (i.e. finite mean) that is taken to be equal to 1. This is equivalent to a setting of the time scale.

In [4, 5] van den Broeck has shown that, when $\psi(t)$ has finite first moment, its Laplace transform

$$\tilde{\psi}(s) \equiv 1/f(s) \tag{2.2}$$

may be obtained by solving the functional equation

$$f(\tau s) = \rho(f(s)) \qquad f(0) = f'(0) = 1 \tag{2.3}$$

where $\rho(x)$ is a characteristic function for each lattice and τ (time rescaling factor) is the factor by which the time to go from a site to one of its nearest neighbours grows (shrinks) in each decimation (generation). It is known that $\rho(x) = 16x^3 - 21x + 13/(2x) - 1/(2x^3)$ for the Given–Mandelbrot curve (notice that there was an erratum in the second term of $\rho(x)$ given in [5]) and that $\rho(x) = 4x^2 - 3x$ for the two-dimensional Sierpinsky gasket [5]. For the d-dimensional Sierpinsky gasket one has [20]

$$\rho(x) = 2dx^2 - 3(d-1)x + d - 2. \tag{2.4}$$

These characteristic functions will be needed to calculate the constant C that appears on the exponential term of the asymptotic form of $\psi(r,t)$ for large ξ (see equation (2.20)). The exact solution $f(s)$ of the functional equation (2.3) is generally unknown. Nevertheless, from this equation, one can find its Taylor-series expansion, information about its zeros and its asymptotic behaviour for large s.

Next shall be derived the asymptotic form, for large x, of $\rho(x)$ for fractals in which sites are isolated by their nearest neighbours (see equation (2.7)). The function $\rho(x)$ is defined by

$$\frac{1}{\rho(x)} = p \sum_{\alpha} \frac{1}{q_\alpha} x^{-N_\alpha} \tag{2.5}$$

where α labels every path that goes from the original site (say O in figure 1) to a specified nearest neighbour on the nth-generation lattice (A, for example), $1/q_\alpha$ is the probability of the random walker to go from O to that specified site along the path α (no matter what the arrival time), N_α is the number of steps or hops on the $(n+1)$th-generation lattice required to travel the path α, and p is the number of nearest neighbours of the original site ($p = 4$ in our Sierpinsky example). Equation (2.5) embodies the assumption that the random walker has an equal probability to go to any of its nearest neighbours from the original site. We can write (2.5) as

$$\frac{1}{\rho(x)} = x^{-\lambda} p \sum_{m} \frac{1}{q_m} + p \sum_{o} \frac{1}{q_o} x^{-N_o} \tag{2.6}$$

where the subscript m labels the shortest (minimum) path (or paths) that goes from the original site to the specified neighbour, λ is the number of steps of this minimum path, and the subscript o labels the other (non-minimum) paths. Continuing with the example of the two-dimensional Sierpinsky fractal (see figure 1), one sees that there exists only one minimum path between the site O and A (one of its nearest neighbours) through the next-generation lattice, namely, O $\rightarrow$ 1 $\rightarrow$ A. The length of this path is then $\lambda = 2$. Clearly, the probability of going from O to 1 is $\frac{1}{4}$, and the probability of going from 1 to A is also $\frac{1}{4}$, so the probability of going from O to A via the shortest path is $1/q_m = \frac{1}{16}$.

Because $1 < \lambda < N_o$ and $\tilde{\psi}(s) \rightarrow 0$ for $s \rightarrow \infty$, one has that

$$\rho\left[\frac{1}{\tilde{\psi}(s)}\right] \approx \frac{[\tilde{\psi}(s)]^{-\lambda}}{p \sum_m 1/q_m} \tag{2.7}$$

for large s. For brevity's sake I will write $1/z$ instead of $p \sum 1/q_m$. Notice that $1/z$ can be interpreted as the probability that the random walker goes from a site to any of its nearest neighbours via any of the minimum paths. In our Sierpinsky example we have $1/z = \frac{1}{4}$. By using this definition of z and that of (2.2) for $f(s)$, together with (2.3), one finds that (2.7) becomes the functional equation

$$f(\tau s) \approx z f^{\lambda}(s) . \tag{2.8}$$

The solution of equation (2.8) is

$$f(s) \approx \frac{1}{A'} \exp\left(C' s^{\ln \lambda / \ln \tau}\right) \tag{2.9}$$

where

$$A' = z^{1/(\lambda - 1)} \tag{2.10}$$

and C' is a constant that can be evaluated numerically. It should be noticed that λ (which was defined as the number of steps of the minimum path that goes along the $(n+1)$th generation lattice between a site and any of its nearest neighbours on the nth generation lattice), is *also* the factor by which the distance between a site and any of its nearest neighbours grows (shrinks) in each decimation (generation). In other words, λ is the length rescaling factor in each generation or decimation. The definition of the anomalous diffusion coefficient by (1.1) implies that $d_w = \ln\tau/\ln\lambda$. Therefore, equation (2.9) is

$$f(s) \approx \frac{1}{A'} \exp\left(C' s^{1/d_w}\right). \tag{2.11}$$

The asymptotic behaviour of $\psi(t)$ for small times is obtained from the inverse Laplace transform of $\tilde{\psi}(s) \equiv 1/f(s)$, with $f(s)$ given by (2.11). It turns out that the Laplace transform of

$$I(t) = A t^{(\gamma-1)} \exp\left(-C/t^{\beta}\right) \tag{2.12}$$

can be obtained by means of the Laplace method [21] and is given by

$$\tilde{I}(s) \approx 2A \sqrt{\frac{\pi}{2(\beta+1)}} (C\beta)^{\frac{\gamma-1/2}{\beta+1}} s^{-\frac{\gamma+\beta/2}{\beta+1}} \exp\left[-\frac{\beta+1}{\beta}\left(C\beta s^{\beta}\right)^{\frac{1}{\beta+1}}\right] \tag{2.13}$$

for large s. Comparing this result with $\tilde{\psi}(s) = 1/f(s) \approx A' \exp(-C' s^{1/d_w})$ for large s, one finds that $\psi(t)$, for small t, should be given by

$$\psi(t) \approx A t^{-(\beta/2+1)} \exp\left(-C/t^{\beta}\right) \tag{2.14}$$

with

$$\beta = \frac{1}{d_w - 1} \tag{2.15}$$

$$C = \beta^{\beta} \left(\frac{C'}{\nu}\right)^{\nu} \tag{2.16}$$

$$A = \sqrt{\frac{\nu}{2\pi}} \left(\frac{\beta C'}{\nu}\right)^{\nu/2} A' \tag{2.17}$$

and where the relation $\nu = \beta + 1$ has been used. Values of A', C' A, and C for several fractals are given in table 1. Away from the short-time regime, $\psi(t)$ is given by

$$\psi(t) = \sum_{i=1}^{\infty} \frac{e^{x_i t}}{f'(x_i)} \tag{2.18}$$

with $x_i < 0$ being the ith largest root of $f(x) = 0$ [5].

Table 1. Constants appearing in the asymptotic expression of $\psi(s) = 1/f(s)$ for large s, equation (2.11), and $\psi(t)$ for small t, equation (2.14). The symbol 1D refers to the one-dimensional case, GM refers to the Given–Mandelbrot curve, and Sd to the d-dimensional Sierpinsky gasket.

Case	$d_w = \ln\tau/\ln\lambda$	A'	C'	A	C
1D	2	2	$\sqrt{2}$	$\sqrt{2/\pi}$	1/2
GM	$\ln 22/\ln 3$	4	2.0	1.5	1.1
S2	$\ln 5/\ln 2$	4	1.96[a]	1.82	0.98
S3	$\ln 6/\ln 2$	6	2.30[b]	2.78	1.31
S4	$\ln 7/\ln 2$	8	2.55[c]	3.69	1.56
S5	$\ln 8/\ln 2$	10	2.74	4.56	1.75
S6	$\ln 9/\ln 2$	12	2.90	5.42	1.91
S7	$\ln 10/\ln 2$	14	3.03	6.26	2.04

[a] In agreement with the value reported in [5].
[b] In agreement with the value reported in [7].
[c] A slightly different value of 2.56 was obtained in [7].

We have defined $\psi(t)\,\mathrm{d}t$ as the probability that a diffusing particle starting at a site reaches any of its nearest neighbours of the same generation, for the first time, in the time interval $(t, t+\mathrm{d}t)$, unit time being the mean time spent by the diffusing particle to travel the distance between the original site and any nearest neighbour. This distance is, therefore, $\sqrt{2D}$. Thus, one can interpret $\psi(t)\,\mathrm{d}t$ as the probability that a diffusing particle starting at a site reaches another site separated by a distance r, for the first time, in the time interval $(t, t+\mathrm{d}t)$, unit time being the mean time to reach the distance r. This time is $(r/\sqrt{2D})^{d_w}$. In order to emphasize this interpretation, I will write this probability as $\psi(r,t)$, which can be explicitly stated in terms of $\psi(t)$:

$$\psi(r,t) = \psi\left[t(\sqrt{2D}/r)^{d_w}\right] = \psi\left(\xi^{-d_w}\right). \tag{2.19}$$

For the sake of simplicity and without loss of generality, in what follows I will choose the unit of length so as to make $2D = 1$. Using equations (2.19) and (2.14), one gets

$$\psi(r,t) \approx A\xi^{\nu/2+d_w} \exp(-C\xi^{\nu}) \tag{2.20}$$

for large $\xi = r/t^{1/d_w}$.

Let $h(t)$ be the probability that a random walker, who starts at $t = 0$ at a given site (say O), is absorbed during the time interval $(0, t)$ by traps placed on the nearest neighbours of O belonging to the same generation, unit time being the mean time spent by the diffusing particle to go to any of its nearest neighbours from the original site. I will call the mortality function the function $h(r,t)$ defined as the probability that a random walker who starts at a site is absorbed by traps located on its nearest neighbours at a distance r in the time interval $(0,t)$. It is clear from the definitions of $h(r,t)$ and $S(r,t)$ that $h(r,t) = 1 - S(r,t)$. Reasoning as after (2.18), one sees that, analogously to (2.19), $h(t)$ and $h(r,t)$ are related by

$$h(r,t) = h\left(\xi^{-d_w}\right). \tag{2.21}$$

From the definition of $\psi(t)$ and $h(t)$ we know that

$$h(t) = \int_0^t \mathrm{d}\tau\, \psi(\tau). \tag{2.22}$$

Inserting (2.14) in this equation, integrating, and using the resulting expression in (2.21), one finds that the mortality function of a random walker in fractals isolated by nearest neighbours is

$$h(r,t) \approx \frac{A(d_w - 1)}{C}\xi^{-\nu/2} \exp(-C\xi^{\nu}) \tag{2.23}$$

for large ξ. On the other hand, inserting (2.18) into (2.22) and using the relation

$$1 \equiv \langle t\rangle \equiv \int_0^\infty \psi(t)\,\mathrm{d}t = \sum_{i=1}^{\infty} \frac{-1}{x_i f'(x_i)} \tag{2.24}$$

one finds that

$$h(r,t) = 1 + \sum_{i=1}^{\infty} \frac{\mathrm{e}^{x_i/\xi^{d_w}}}{x_i f'(x_i)}. \tag{2.25}$$

Figure 2 plots the difference, ΔS, between the survival probability

$$S(r,t) = -\sum_{i=1}^{\infty} \frac{\mathrm{e}^{x_i/\xi^{d_w}}}{x_i f'(x_i)} \tag{2.26}$$

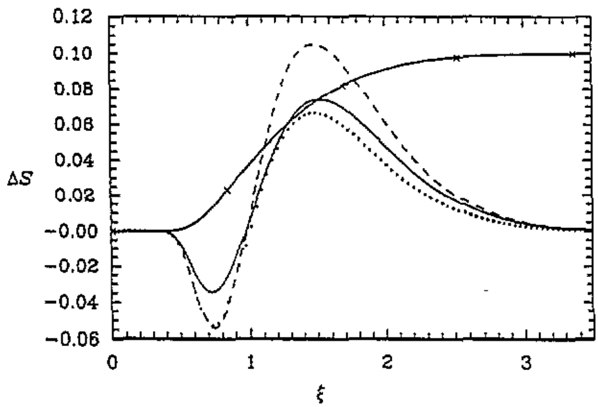

Figure 2. The difference, ΔS, between the survival probability corresponding to the two-dimensional Sierpinsky gasket (full curve), the three-dimensional Sierpinsky gasket (broken curve), and the Given–Mandelbrot curve (dotted curve) with respect to that corresponding to the one-dimensional lattice. As reference, also represented is one-tenth of the survival probability for the one-dimensional lattice (full curve with crosses).

corresponding to the two- and three-dimensional Sierpinsky lattice and to the Given–Mandelbrot curve with that corresponding to the one-dimensional lattice:

$$S(r,t) = \frac{1}{\pi}\sum_{n=1}^{\infty}(-1)^{n-1}\frac{2}{n-\frac{1}{2}}\exp\left[-\tfrac{1}{2}(n-\tfrac{1}{2})^2\pi^2 t^{1/2}\right]. \tag{2.27}$$

I have also plotted $S(r,t)/10$ for the one-dimensional lattice as a reference. We see that $S(r,t)$ is smaller for the three fractal examples than for the one-dimensional case when $\xi \lesssim 1$, and it is larger when $\xi \gtrsim 1$. Recall that $S(r,t)$ is the probability that the random walker has never gone further than r from its starting point at 0 along the time interval $(0,t)$, and that t^{1/d_w} is the ensemble average of the distance spanned by random walkers between their starting site and their positions at time t (cf equation (1.1)). Therefore, figure 2 means that the probability that over the time interval $(0,t)$ a random walker *never* goes further than the ensemble averaged (or mean) distance travelled by random walkers at time t is always smaller for our fractal examples than for the one-dimensional lattice. The opposite is true for $\xi \gtrsim 1$, i.e. the probability that during the time interval $(0,t)$ a random walker has gone further than the mean distance corresponding to this time is always larger for our fractal lattices than for the one-dimensional lattice. A remarkable fact is that the values of $S(r,t)$ for $\xi = 1$ are very similar; they are compressed between 0.37 and 0.38 in our four examples. Also notice that ΔS has a minimum close to $\xi = \frac{3}{4}$ and a maximum near $\xi = \frac{3}{2}$ for every fractal.

3. Propagator for large ξ

Let $\hat{S}(r,t)$ ($\hat{h}(r,t)$) be the probability that the random walker which started at $r = 0$ when $t = 0$ is inside (outside) the region of radius r after the time t when there exist no traps (free process). It is clear that $\hat{S}(r,t)$ and $S(r,t)$ are different. Moreover, it should be clear that $\hat{S}(r,t) > S(r,t)$ ($\hat{h}(r,t) < h(r,t)$) because in the free process the random walker can return to the inner region after walking in the outer region, whereas this is not possible when there exist (perfect) traps at distance r. However, I conjecture that

$$h(r,t) \approx k\hat{h}(r,t) \tag{3.1}$$

for large ξ (short times and/or large distances), k being a constant. This conjecture is supported by the fact that $h(r,t) \approx 2\hat{h}(r,t)$ for the one-dimensional lattice (cf the appendix). Moreover, it is expected that $1 < k < 2$ because for fractal structures the probability of return to the inner region should be smaller than for the one-dimensional lattice, in agreement with the fact that the probability to return to the origin, $P(0,t) \sim t^{-d_s/2}$, decays more slowly for the one-dimensional lattice ($d_s = 1$) than for fractal structures in which $d_s > 1$.

Next, it is proved that the quantity $\hat{h}(r,t)$ obtained from (3.2) by using the propagator of (1.6) satisfies (3.1), provided that $\alpha = \nu/2 - d_f$. It is clear from the definition of $\hat{h}(r,t)$ and $\hat{P}(r,t) \equiv r^{d_f-d}P(r,t)$ that

$$\hat{h}(x,t) = \Omega_d \int_x^\infty \hat{P}(r,t) r^{d-1}\,\mathrm{d}r \tag{3.2}$$

with $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$. Assuming that the propagator has the form

$$P(r,t) \approx at^{-d_s/2}\xi^\alpha \exp(-c\xi^{\hat{\nu}}) \tag{3.3}$$

for large ξ (cf equation (1.6)), one gets from (3.2) that

$$\hat{h}(x,t) \approx \Omega_d a t^{-d_s/2} \int_x^\infty r^{d_f-1}\xi^\alpha \exp(-c\xi^{\hat{\nu}})\,\mathrm{d}r \tag{3.4}$$

$$\approx \Omega_d a \int_{\xi_x}^\infty \xi^{\alpha+d_f-1} \exp(-c\xi^{\hat{\nu}})\,\mathrm{d}\xi \tag{3.5}$$

$$\approx \frac{\Omega_d a}{\hat{\nu}} \left(\frac{1}{c}\right)^{(\alpha+d_f)/\hat{\nu}} \Gamma\left(\frac{\alpha+d_f}{\hat{\nu}}, c\xi_x^{\hat{\nu}}\right) \tag{3.6}$$

with $\xi_x = x/t^{1/d_w}$. Using the asymptotic expansion of the incomplete gamma function [22] one finds that

$$\hat{h}(r,t) \approx \frac{a\Omega_d}{\hat{\nu}c}\xi^{\alpha+d_f-\hat{\nu}} \exp\left(-c\xi^{\hat{\nu}}\right) \tag{3.7}$$

for large ξ. Equation (3.1) together with (2.23) and (3.7) implies that the propagator is given by (3.3) with

$$c = C \tag{3.8}$$

$$\hat{\nu} = \nu \equiv \frac{d_w}{d_w - 1} \tag{3.9}$$

$$a = \frac{Ad_w}{k\Omega_d} \tag{3.10}$$

$$\alpha = \frac{\nu}{2} - d_f\,. \tag{3.11}$$

Notice that although I have assumed that k is a constant, this is not strictly necessary. The above results are valid even if k depends on ξ provided that $k(\xi)$ is subdominant with respect to ξ^α (for example, $k(\xi)$ could change logarithmically).

It should be clear that it has not *been* proved *that the propagator is given asymptotically* by (3.3) with α and $\hat{\nu}$ given by (3.9) and (3.11), respectively. However, I think that this result is quite plausible because it is derived from the reasonable assumption that $h(r,t)/\hat{h}(r,t)$ is subdominant with respect to a power of ξ. As said before, this argument leads to the correct values of α and $\hat{\nu}$ for the one-dimensional lattice. Furthermore, the agreement of this result for $\hat{\nu}$ with the widely accepted value $\nu \equiv d_w/(d_w - 1)$ reinforces the plausibility of our argument. On the other hand, there is no consensus about the value of α, with even the existence of the potential prefactor not being well established. The most recent proposal of Roman and Alemany [12], $\alpha_{\rm RA} = (d_s - d_f)\nu/2$, and the relation of Klafter *et al*, $\alpha_{\rm KZB} = (d_f - d_w/2)/(d_w - 1)$, differ significantly from the present result $\alpha = \nu/2 - d_f$. For example, for the Given–Mandelbrot curve ($d_f = \log 8/\log 3$, $d_s = 2\log 8/\log 22$) one finds $\alpha = -1.117$, whereas $\alpha_{\rm RA} = -0.425$ and $\alpha_{\rm KZB} = 0.268$; for the two-dimensional Sierpinsky fractal ($d_f = \log 3/\log 2$, $d_s = 2\log 3/\log 5$) one has $\alpha = -0.707$, whereas $\alpha_{\rm RA} = -0.193$ and $\alpha_{\rm KZB} = 0.321$. We see in these examples (other examples could be given) that the expression for α proposed in this paper leads to negative values less than $\alpha_{\rm RA}$, which are also negative, and $\alpha_{\rm KZB}$, which are positive. This means that the potential term ξ^α has the effect of decreasing $P(r,t)$ when the value of α proposed in this paper is used or that proposed by Roman and Alemany, the decrement being smaller in the last case; the effect is the opposite when $\alpha_{\rm KZB}$ is used.

4. Conclusions

In this paper I have studied some fundamental quantities that describe statistically the diffusion of a random walker on a particular class of fractals. These quantities are the first-passage time, the survival probability and the Green function or propagator. The fractals considered were those in which it is not possible for the random walker to go from a site, say O, to a non-nearest neighbour on the decimated lattice through the original (non-decimated) lattice, without passing through nearest neighbours of O that belong to the decimated lattice.

For all of these fractals I have found that the asymptotic expression for the first-passage-time density for $\xi \gg 1$ can be written in terms of the anomalous diffusion coefficient d_w as: $\psi(r,t) \approx A\xi^{\nu/2+d_w}\exp(-C\xi^\nu)$ where $\nu = d_w/(d_w + 1)$. The constants A and C were calculated numerically for the Given–Mandelbrot curve and for the two- to seven-dimensional Sierpinsky gasket and compared with reported estimations when available.

I also calculated the survival probability for this class of fractals. It was shown for the Given–Mandelbrot curve and for the two- and three-dimensional Sierpinsky gasket that this quantity is smaller than that corresponding to the one-dimensional lattice for $\xi \lesssim 1$ (with the minimum at $\xi \sim \frac{3}{4}$), larger for $\xi \gtrsim 1$ (with the maximum at $\xi \sim \frac{3}{2}$), and almost coincident for $\xi \simeq 1$. In any case, the differences are always small. The asymptotic expression of the survival probability for large ξ was also obtained in terms of the anomalous diffusion coefficient: $S(r,t) \approx 1 - (A/C)(d_w - 1)\xi^{-\nu/2}\exp(-C\xi^\nu)$.

From this last expression I have 'derived' the asymptotic form of the propagator for $\xi \gg 1$: $P(r,t) \approx at^{-d_s/2}\xi^\alpha\exp(-C\xi^{\hat{\nu}})$. The value obtained for $\hat{\nu}$ is $\nu = d_w/(d_w + 1)$, which is precisely the widely accepted value. However, the value obtained for α, namely $\alpha = \nu/2 - d_f$, differs from others suggested recently. Therefore, it would be convenient to have simulation results precise enough to be able to resolve this discrepancy.

As said before, it is well known that for fractals without loops the propagator decays as $\exp(-C\xi^\nu)$ for $\xi \gg 1$. This is also true for the percolation cluster at criticality. Moreover, it was argued in this paper that this result is also true for all fractals (with and without loops) belonging to a given (and broad) class. Thus, it is a natural step to conjecture that the propagator would exhibit this behaviour for all media with self-similarity. Another natural, although admittedly more risky, step along this line of reasoning would lead us to conjecture that the potential factor ξ^α appearing in the propagator is also universal.

This paper has been concerned with the study of the diffusion of a random walker on fractals generated deterministically so that they are strictly self-similar. I think it would also be interesting to carry out this study for random fractals (which are self-similar only in a statistical sense), and analysing to what extent the results provided in this paper remain valid or change. Work is in progress along this line.

Acknowledgments

I gratefully acknowledge support from the Dirección General de Investigación Científica y Técnica (Spain) through grants no 93-063 and PB94-1021 and the hospitality of the Department of Chemistry and Biochemistry of the University of California, San Diego, during my sabbatical stay.

Appendix

In this appendix it shall be proved that (3.1) holds in one dimension with $k = 2$. Let $h(x, t)$ be the probability that the random walker who starts at x will be absorbed by traps placed at $x = -r$ and $x = r$ in the time interval $(0, t)$, let $H(x, t) = 1 - h(x, t)$ be the probability that he will *not* be absorbed, and let $g(x)$ be the initial probability density function. Then, the mortality function is given by

$$h(r, t) = \int_{-r}^{r} g(x) h(x, t)\, \mathrm{d}x = 1 - \int_{-r}^{r} g(x) H(x, t)\, \mathrm{d}x. \tag{A.1}$$

It is well known [23, section X.5] that $H(x, t)$ is given by

$$\begin{aligned} H(x, t) = \sum_{m=-\infty}^{\infty} \Bigg[& \phi\left(\frac{4mr + 2r - x}{\sqrt{2Dt}}\right) - \phi\left(\frac{4mr - x}{\sqrt{2Dt}}\right) \\ & - \phi\left(\frac{4mr + 2r + x}{\sqrt{2Dt}}\right) + \phi\left(\frac{4mr + x}{\sqrt{2Dt}}\right)\Bigg] \end{aligned} \tag{A.2}$$

where $\phi(x)$ is the standard normal distribution

$$\phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \mathrm{e}^{-u^2/2}. \tag{A.3}$$

Using the relation $\phi(-x) = 1 - \phi(x)$, one finds that $h(x, t) = 1 - H(x, t)$ is given by

$$h(x, t) = 2\left[1 - \phi\left(\frac{x}{\sqrt{2Dt}}\right)\right] + 2\sum_{m=1}^{\infty} (-1)^m \left[\phi\left(\frac{mL - x}{\sqrt{2Dt}}\right) - \phi\left(\frac{mL + x}{\sqrt{2Dt}}\right)\right]. \tag{A.4}$$

The initial probability density function is $g(x) = \delta(x - 0)$ when random walkers start at $x = 0$. In this case, inserting (A.4) into (A.1), one gets

$$h(r, t) = 2[1 - \phi(\xi)] + 2\sum_{m=1}^{\infty} (-1)^m \{\phi[(2m - 1)\xi] - \phi[(2m + 1)\xi]\} \tag{A.5}$$

where $\xi \equiv r/\sqrt{2Dt}$. Using the relation $\phi(x) = 1 - \mathrm{erfc}(x/\sqrt{2})/2$, equation (A.5) becomes

$$h(r, t) = 2\sum_{m=1}^{\infty} (-1)^{m+1} \mathrm{erfc}\big[(2m - 1)\xi/\sqrt{2}\big]. \tag{A.6}$$

But the function $\mathrm{erfc}(x)$ decreases quickly for large x so that, for large ξ, equation (A.6) yields

$$h(r, t) \approx 2\,\mathrm{erfc}\big(\xi/\sqrt{2}\big). \tag{A.7}$$

On the other hand, the propagator in one dimension is

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right). \tag{A.8}$$

Therefore, the probability that the random walker who starts at $x = 0$ and $t = 0$ is outside the region $[-r, r]$ after the time t when no traps exist is given by

$$\hat{h}(r,t) = \int_{-\infty}^{r} P(x,t)\,\mathrm{d}t + \int_{r}^{\infty} P(x,t)\,\mathrm{d}t \tag{A.9}$$

$$= 2\int_{r}^{\infty} P(x,t)\,\mathrm{d}t \tag{A.10}$$

$$= \frac{2}{\pi}\int_{\xi/\sqrt{2}} \mathrm{e}^{-y^2}\,\mathrm{d}y \tag{A.11}$$

$$= \mathrm{erfc}\big(\xi/\sqrt{2}\big). \tag{A.12}$$

Comparing (A.7) with (A.12), it is proved that $h(r,t) \approx 2\hat{h}(r,t)$ for $\xi \gg 1$ in one dimension.

References

[1] The existence of fractals where the diffusion exponent is non-anomalous, i.e. where $d_w = 2$, has recently been reported by Burioni R and Cassi D 1994 *Phys. Rev.* E **49** R1785; 1995 *Phys. Rev.* E **51** 2865
[2] Bunde A and Havlin S (ed) 1994 *Fractals in Science* (Berlin: Springer)
[3] Havlin S and ben-Avraham D 1987 *Adv. Phys.* **36** 695
[4] Van den Broeck C 1989 *Phys. Rev. Lett.* **62** 1421
[5] Van den Broeck C 1989 *Phys. Rev.* A **40** 7334
[6] Guyer R A 1984 *Phys. Rev.* A **29** 2751
[7] Klafter J, Zumofen G and Blumen A 1991 *J. Phys. A: Math. Gen.* **24** 4835
[8] Feder J 1988 *Fractals* (New York: Plenum)
[9] Mandelbrot B B and Vicsek T 1989 *J. Phys. A: Math. Gen.* **22** L377
[10] Giona M and Roman H E 1992 *J. Phys. A: Math. Gen.* **25** 2093
[11] Roman H E and Giona M 1992 *J. Phys. A: Math. Gen.* **25** 2107
[12] Roman H E and Alemany P A 1994 *J. Phys. A: Math. Gen.* **27** 3407
[13] Roman H E 1995 *Phys. Rev.* A **51** 5422
[14] Weiss G H 1994 *Aspects and Applications of the Random Walk* (Amsterdam: North-Holland)
[15] Weiss G H and Havlin S *J. Stat. Phys.* **63** 1005
[16] Donsker N D and Varadhan S R S 1979 *Commun. Pure. Appl. Math.* **32** 721
[17] Havlin S, Larralde H, Trunfio P, Kiefer J E, Stanley H E and Weiss G H 1992 *Phys. Rev.* A **46** R1717
[18] Anacker L W and Kopelman R 1987 *Phys. Rev. Lett.* **58** 289.
[19] Machta J 1981 *Phys. Rev.* B **24** 5260
[20] This formula agrees with previously calculated equations for $d = 2$ (see [5]), and $d = 3$ (see Parrondo J M R, Martinez H L, Kawai R and Lindenberg K 1990 *Phys. Rev.* A **42** 723). I have checked explicitly that this relation holds for $d = 4$ and $d = 5$. For higher dimensions it is only a conjecture.
[21] Wong R 1989 *Asymptotic Approximations of Integrals* (Boston, MA: Academic)
[22] Abramowitz M and Stegun I (ed) 1972 *Handbook of Mathematical Functions* (New York: Dover)
[23] Feller 1957 *An Introduction to Probability Theory and its Applications* 2nd edn, vol I (New York: Wiley)