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Continuous-time random walks and the fractional diffusion equation

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Abstract. The average probability density $P(r,t)$ of random walks on fractals is revisited within the continuous-time random walks formalism. Corrections to the accepted asymptotic stretched Gaussian decay of $P(r,t)$ of the form r^α are discussed. It is shown that $P(r,t)$ obeys a diffusion equation with a fractional time derivative asymptotically, and predictions about the value of α are presented.

Transport phenomena on fractals display a variety of anomalous behaviours with respect to the standard counterparts valid on uniform systems (for recent reviews see, e.g., [1]). One of the questions of current interest regards the form of the probability density $P(r,t)$ of a random walker, at distance r at time t from its starting point at $t=0$, on such self-similar substrates (see also [2]).

Extensive numerical simulations on random fractals, supported by scaling arguments [2], suggest that, on average,

$$P(r,t) \sim \frac{1}{t^{d_s/2}} \exp[-\mathrm{const}\,(r/R)^u] \tag{1}$$

when $t \to \infty$ and $r \gg R$. Here, $R^2 = \langle (r(t) - r(0))^2 \rangle$ is the mean-square displacement of the random walker, $R \sim t^{1/d_w}$. The spectral dimension $d_s = 2d_f/d_w$, where d_f is the fractal dimension, and the exponent $u = d_w/(d_w - 1)$. When $d_w > 2$, $u < 2$ and $P(r,t)$ is called a stretched Gaussian [2]. We note that (1) is consistent with the normalization $\int_0^\infty \mathrm{d}r\, r^{d_f-1} P(r,t) = 1$.

A functional form similar to (1) is also obtained on deterministic fractals, such as Sierpinski gaskets [3]. Although the stretched Gaussian form in (1) is generally accepted, little attention has been drawn so far to the existence of a non-exponential prefactor in the asymptotic form of $P(r,t)$, i.e.

$$P(r,t) \sim \frac{1}{t^{d_s/2}} (r/R)^\alpha \exp[-\mathrm{const}\,(r/R)^u]. \tag{2}$$

In this paper we present some analytical results which indicate that (2) is a suitable generalization of (1) and give predictions about the value of the unknown exponent α. Our results are different to those discussed in [3], and are similar but complementary to those of [4]. The latter were based on a fractional diffusion equation (FDE) suggested recently for describing anomalous diffusion on fractals [5]. The aim of the present work is to motivate

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such FDE by revisiting the known continuous-time random walk (CTRW) formalism [6]. This formalism has also been applied to systems that mimic self-similar geometry (see e.g. [7]).

Let us start with a brief review of the CTRW formalism. We consider a random walker in a continuum d-dimensional space. Let $p(\boldsymbol{r})$ be the probability that a single-step of the walker falls in the interval $(\boldsymbol{r}+\mathrm{d}\boldsymbol{r})$ in any given step. Let $\psi(t)$ be the probability density for the time between two successive steps (waiting time distribution). In the CTRW formalism, the Fourier transform of $p(\boldsymbol{r})$

$$p(\boldsymbol{k}) = \int \mathrm{d}^d r \, \exp(-\boldsymbol{k}\cdot\boldsymbol{r}) p(\boldsymbol{r}) \tag{3}$$

and the Laplace transform of $\psi(t)$

$$\psi(s) = \int_0^\infty \mathrm{d}t \, \exp(-st)\psi(t) \tag{4}$$

are required for calculating the Laplace transform of $P(r,t)$, which can be written as [6]

$$P(r,s) = \frac{1-\psi(s)}{s}\frac{1}{(2\pi)^d}\int \mathrm{d}^d k \frac{\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})}{1-p(\boldsymbol{k})\psi(s)}. \tag{5}$$

To proceed further, we assume that $\psi(t) = \gamma(t_0/t)^\gamma/t$, when $t \geqslant t_0$, and $\psi(t) = 0$ otherwise. Here, t_0 represents the shortest elapsed time between two successive steps, and is taken as $t_0 > 0$ for normalization. The choice $\gamma = 2/d_\mathrm{w} < 1$, mimics the anomalous behaviour $R \sim t^{1/d_\mathrm{w}}$ mentioned above.

Since we are interested in the asymptotic form of $P(r,t)$, we need to study the $s \to 0$ behaviour of $P(r,s)$. In this limit, it is easy to show that $\psi(s) \cong 1 - bs^\gamma$, where $b = \gamma\Gamma(1-\gamma)t_0^\gamma$. Similarly, since we are interested in the asymptotic case $r \to \infty$, the main contribution to the integral in (5) will come from values $k \to 0$. For an isotropic walk with finite variance σ, $p(k) \cong 1 - \sigma^2 k^2/2$, when $k \to 0$, and equation (5) can be written as

$$P(r,s) = \frac{1}{\beta^d} Q_d(s) I_d(a) \tag{6}$$

when $r \to \infty$ and $s \to 0$, where $\beta = \sigma/\sqrt{2b}$, $Q_d(s) = s^{-(1-d/d_\mathrm{w})}$, $a = rs^{1/d_\mathrm{w}}/\beta$ and

$$I_d(a) = \frac{1}{(2\pi)^d}\int \mathrm{d}^d q \frac{\exp(-\mathrm{i}\boldsymbol{q}\cdot\hat{\boldsymbol{r}}a)}{1+q^2}. \tag{7}$$

Equation (7) can be solved easily in spherical coordinates, yielding $I_d(a) = \frac{1}{2}(2\pi/a)^\kappa \exp(-a)$, with $\kappa = (d-1)/2$, which is exact when $d = 1$ and $d = 3$, and only asymptotically exact when $d = 2$. Thus, equation (6) becomes

$$P(r,s) = A(\beta,d) Q_d(s) a^{-\kappa} \exp(-a) \tag{8}$$

where $A(\beta,d) = \frac{1}{2}(2\pi)^{-\kappa}\beta^{-d}$. The probability density may be normalized such that $\int_0^\infty \mathrm{d}r \, r^{d-1} P(r,t) = 1$, according to the assumption that the random walk takes place in a continuum d-dimensional space. Our asymptotic result (8) is consistent with this condition, as can be easily checked, but not with the normalization of $P(r,t)$ in (1). This discrepancy has further consequences, as we immediately see.

Let us discuss the asymptotic behaviour of $P(r,t)$ implied by (8). Following [4], one can show that (8) yields a power-law correction factor with an exponent α given by

$$\alpha = u\left(\tfrac{1}{2}(d_\mathrm{s}' - 1) - \kappa\right) \tag{9}$$

with $d_\mathrm{s}' = 2d/d_\mathrm{w}$. The fact that the spatial dimension d appears in (9) is a direct consequence of the normalization of $P(r,t)$. On fractals, we would expect, instead, that d_f would play the role of d. Thus, our approach leading to (8) and (9) needs to be generalized by incorporating the fractal dimension d_f explicitly in the formalism. To do this, it is instructive to analyse our result (8) from a different point of view, i.e. by working out the differential equation that $P(r,t)$ satisfies.

Such an equation is obtained simply by calculating the partial derivative of $P(r,s)$ with respect to r. The result is $\partial P/\partial r = -s^{1/d_w} P/\beta - \kappa P/r$, which, using the known properties of the Laplace transform for fractional derivatives [8], can be written as

$$\frac{\partial^{1/d_w} P(r,t)}{\partial t^{1/d_w}} = -\beta \left(\frac{\partial P}{\partial r} + \frac{\kappa}{r} P \right). \tag{10}$$

Equation (10) describes the behavior of $P(r,t)$ asymptotically. This equation corresponds to the standard diffusion equation when $d_w = 2$ [8]. A similar equation has been proposed in [4, 5], and derived more recently in [9].

The analogy between the CTRW and the fractional diffusion equation (FDE) approach is clearly manifested by our result (10). This analogy is actually not surprising, since in the FDE approach the 'anomalies' of the random walk are also governed by the 'temporal' variable in the formalism (see [5]). The parameter κ was introduced in [4] to reproduce the known FDE valid for standard Brownian motion in d-dimensions. On fractals, the value

$$\kappa = \frac{d_f - 1}{2} \tag{11}$$

was suggested on an empirical basis [4]. In what follows, we attempt to motivate the plausibility of the choice (11), by generalizing (6) and (7) to the case in which the fractal geometry of the medium is explicitly taken into account.

We assume now that the random walk takes place in a subspace of non-integer dimension d_f, embedded in a d-dimensional continuum space. Accordingly, we argue that the integrations in spherical coordinates in q-space (7) should be performed using the form $\mathrm{d}q\, q^{d_f-1}$ in place of $\mathrm{d}q\, q^{d-1}$, while for the relevant angular part the form $\mathrm{d}\theta (\sin\theta)^{d_f-2}$ should be employed†. According to this, equations (6) and (7) become

$$P(r,s) = \frac{1}{\beta^{d_f}} Q_{d_f}(s) I_{d_f}(a) \tag{12}$$

where

$$I_{d_f}(a) = \frac{B_{d_f}}{(2\pi)^{d_f}} \int_0^\infty \mathrm{d}q \frac{q^{d_f-1}}{1+q^2} \int_0^\pi \mathrm{d}\theta (\sin\theta)^{d_f-2} \exp(-\mathrm{i}qa\cos\theta) \tag{13}$$

† The plausibility of our choice can be appreciated on a non-rigorous basis as follows. We note first that the integrand $\mathrm{d}q\, q^{d_f-1}$ implies that the support of the integral is a fractal. In this case, the Fourier transform of, say, a constant function on the fractal in r-space can be written as

$$\int_0^\infty \mathrm{d}r\, r^{d_f-1} \mathrm{const} \int_0^\pi \mathrm{d}\theta f(\theta) \exp(\mathrm{i}qr\cos\theta)$$

which scales as q^{-d_f}. Its inverse Fourier transform may then be defined as

$$\int_0^\infty \mathrm{d}q\, q^\beta q^{-d_f} \int_0^\pi \mathrm{d}\theta f(\theta) \exp(-\mathrm{i}qr\cos\theta)$$

where we see that the result is independent of r, provided that $\beta = d_f - 1$. The form of the integrand for the angular part, $f(\theta) = (\sin\theta)^{d_f-2}$, is the simplest possible one consistent with our assumption that the support is a homogeneous fractal, i.e. the angular variation of the mass is also determined by d_f, and with the requirement that it reduces to the known Euclidean results $f(\theta) = \sin\theta$ when $d_f = 3$, and $f = 1$ when $d_f = 2$.

and B_{d_f} can be determined from the normalization condition (for integral values of d_f, $B_3 = 2\pi$ and $B_2 = 2$). Here, $Q_{d_f}(s)$ is equal to $Q_d(s)$ with d replaced by d_f. Equation (13) can still be solved exactly, yielding

$$I_{d_f}(a) = \frac{B_{d_f}}{(2\pi)^{d_f}} 2^{\nu} \sqrt{\pi}\,\Gamma(\nu + \tfrac{1}{2}) a^{-\nu} K_{\nu}(a) \tag{14}$$

where $\nu = d_f/2 - 1$ and K_ν is a modified Bessel function (see, e.g., [10]). Using the asymptotic behaviour $K_\nu(a)$ for large a in (14), $K_\nu \sim \sqrt{\pi/2}a^{-1/2}\exp(-a)$, equation (12) can be written similarly to (8) as

$$P(r,s) = f_{d_f} A(\beta, d_f) Q_{d_f}(s) a^{-\kappa} \exp(-a) \tag{15}$$

where $f_{d_f} = (2\pi)^{-d_f} B_{d_f} \Gamma(\kappa)/(2\pi^{\kappa})$ and $\kappa = (d_f - 1)/2$ as in (11). We note that now $P(r,s)$ is consistent with the normalization condition $\int_0^\infty \mathrm{d}r\, r^{d_f-1} P(r,t) = 1$, i.e. with equation (1), without further modifications. The FDE corresponding to (15) is again of the form (10) with κ given by (11).

We can now come back to our discussion about the exponent α. The value (9) is now replaced by (see, e.g., [4])

$$\alpha = u\left(\tfrac{1}{2}(d_s - 1) - \kappa\right) \tag{16}$$

with d_s instead of d_s' and $\kappa = (d_f - 1)/2$, in agreement with the postulated value in [4]. We note that the value of α suggested in [3] corresponds to $\kappa = 0$, and was obtained by inverting the Laplace transform $P(r,s)$ proposed earlier in [11].

In conclusion, our derivation suggests that although power-law correction terms in the asymptotic form of $P(r,t)$ (cf (2)) are common to different formalisms studied, the value of the exponent α describing them depends sensitively on the approach used. We hope that the present work will stimulate further numerical work to test the prediction (16).

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