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Fractional diffusion equation on fractals: one-dimensional case and asymptotic behaviour

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Abstract. A fractional differential equation is studied and its application for describing diffusion on random fractal structures is considered. It represents the simplest generalization of the fractional diffusion equation valid in Euclidean systems. The solution of the fractional equation in one dimension is discussed, and compared with exact results for the fractional Brownian motion and the one-dimensional version of the 'standard' diffusion equation on fractals. In higher dimensions, it correctly describes the asymptotic scaling behaviour of the probability density function on random fractals, as obtained recently by using scaling arguments and exact enumeration calculations for the infinite percolation cluster at criticality.

1. Introduction

Transport phenomena in complex systems such as random fractal structures exhibit many anomalous features which are qualitatively different from the standard behaviour characteristic of regular systems [1, 2].

In the case of fractals, such anomalies are due to the spatial complexity of the substrate which imposes geometrical constraints on the transport process on all length scales (self-similarity). These constraints may be also seen as temporal correlations existing on all time scales. In the case of diffusion, for instance, these correlations lead to an anomalous behaviour of the mean-square displacement of a Brownian particle

$$R^2 \equiv \langle r^2(t)\rangle \sim t^{2/d_w} \tag{1.1}$$

where $d_w > 2$ is the anomalous diffusion exponent, and to a non-Gaussian shape for the *average* density function $P(r,t)$, describing the probability that the Brownian particle is found at time t at a distance r from its starting point [1, 2]

$$P(r,t) \sim t^{-d_f/d_w} \ \exp[-\mathrm{constant}(r/R)^u] \tag{1.2}$$

when $r/R \gg 1$ and $t \to \infty$, where $u = d_w/(d_w - 1)$ and d_f is the fractal dimension. Since $1 < u < 2$, the shape described by (1.2) is called a stretched Gaussian [3–5].

The asymptotic result (1.2) is exact for diffusion on topologically linear fractals such as paths generated by self-avoiding random walks (SAW) [1]. It is obtained by writing $P(r,t)$ as the convolution of the probability density $P(l,t)$, that the random walker is at chemical (topological) distance l [1] along the path from the origin, with the structural function $\Phi(r,l)$ giving the probability that two points at chemical distance l on the chain are at Pythagorian metric distance r. Since $P(l,t)$ is a Gaussian for linear fractals and the asymptotic behaviour of $\Phi(r,l)$ is known exactly for SAWs [6], a simple calculation based on the steepest descent method yields (1.2). The same result is obtained analytically for the infinite percolation cluster at criticality, since the structural function $\Phi(r,l)$ for percolation obeys a scaling form analogous to SAWs and $P(l,t)$ is well described by a stretched Gaussian similar to (1.2) [1, 2]. Extensive numerical calculations support these behaviours for $\Phi(r,l)$ [1, 7] and $P(l,t)$ [3–5] for percolation. Other analytical approaches based on scaling arguments and the Green function method also yielded (1.2) [8]. Moreover, (1.2) works equally well for describing the *envelope* decay of $P(r,t)$ on deterministic fractals such as the Sierpinski gasket [1, 9], thus it appears to be of general validity.

In view of the possible general validity of (1.2), one is tempted to search for a generic approach describing diffusion on fractals. Simple modifications of the standard diffusion equation valid in Euclidean systems have been proposed in the past [10,11] for describing the average behaviour of $P(r,t)$ (and of $P(l,t)$) on fractals, in which the characteristic anomalous behaviour (1.1) is explicitely taken into account. Such 'standard' diffusion equations can be solved exactly, but yield the result $u = d_w$ for $P(r,t)$, in contrast to the generally accepted stretched Gaussian behaviour (1.2). Thus, the problem of formulating a diffusion equation on fractals yielding (1.2) within an as simple as possible scheme is still open.

In this work, we pursue this 'macroscopic' approach further by discussing an alternative method for reformulating the diffusion equation on fractals in a very simple way within the framework of fractional calculus [12]. As in previous works [10, 11], our approach is aimed at describing the average behaviour of the physical quantities on fractals only. This means that the intrinsic singular character of a fractal structure leading to a lack of smoothness for $P(r,t)$ for a single configuration is averaged out, and the geometric and transport anomalies of the fractal are simply represented by the exponents d_f and d_w, respectively.

The idea of using fractional calculus as a mathematical description of dynamical processes in complex media is not completely new. Electrochemistry has been so far the most fertile field of application of fractional calculus, as in the study of the AC response of rough electrodes†. After the significant contribution of Oldham [14] regarding the mathematical developments of fractional calculus in electrochemistry, interesting results for complex RC networks were obtained by Jacquelin [15]. Le Mehaute proposed a fractional constitutive equation for describing transfer processes in fractal media [16]. His idea of representing the temporal anomalies in the transfer processes by a convolutional constitutive equation between fluxes and driving forces is interesting, but the approach lacks a clear physical meaning and cannot be applied to the more general problem of diffusion on fractals.

This paper is organized as follows. In section 2, we briefly review the application of fractional calculus to standard Brownian motion. In section 3, we discuss one-dimensional fractional Brownian motion and the extent to which it can be described

† The frequency behaviour of the impedance $Z(\omega)$ of electrochemica eletrodes is well described by the relation $Z(\omega) \sim 1/\omega^\eta$, with $\eta < 1$. The current voltage relation is given in the frequency domain by $I(\omega) = V(\omega)/Z(\omega)$, which implies $I(t) \sim \mathrm{d}^\eta V(t)/\mathrm{d}t^\eta$ (see e.g. [13]).

by a fractional differential equation. In section 4, a detailed analysis of the relaxation function corresponding to the one-dimensional fractional equation is given and its analogy with the electrochemical response of rough electrodes is discussed. In section 5, we analyse the standard diffusion equation for fractals [10], and derive the corresponding fractional equations. In section 6, a one-parameter family of fractional differential equations is developed, which reproduces the asymptotic behaviour of fractional Brownian motion and the standard model of section 5 exactly. An approximate expression for the fractional diffusion equation valid for homogeneous fractals is then proposed and its solutions discussed. In section 7, some concluding remarks are presented.

2. Fractional calculus and standard Brownian motion

Let us briefly summarize the basic ideas of fractional calculus which are illustrated here for standard Brownian motion in one dimension [12]. In the standard approach to diffusion, the starting point is the continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}M(r,t) = -I(r,t) \tag{2.1}$$

where $M(r,t) = \int_0^r \mathrm{d}r\, P(r,t)$ and $I(r,t)$ is the total probability current at distance r from the origin. Here, the normalization condition $M(\infty,t) = 1$ for $P(r,t)$ has been used. Equation (2.1) must be supplemented by a *constitutive* equation relating the current to $P(r,t)$. This is achieved by defining a second quantity $j(r,t)$, which we denote as the radial probability current, as

$$j(r,t) = -D_0\frac{\partial P(r,t)}{\partial r} \tag{2.2}$$

where D_0 is the diffusion coefficient. Identifying I with j, (2.2) is traditionally denoted as the first Fick's law, which substituted into (2.1) (in its differential form) leads to the well known diffusion equation for $P(r,t)$, whose solution is a Gaussian. Denoting by

$$P(r,s) = \int_0^\infty \mathrm{d}t\, \exp(-st)P(r,t)$$

the Laplace transform of $P(r,t)$, $P(r,s) = (1/\sqrt{D_0 s})\exp(-r\sqrt{s/D_0})$, and using it in (2.2) one easily obtains

$$j(r,s) = \sqrt{sD_0}P(r,s) \tag{2.3}$$

where $j(r,s)$ is the Laplace transform of $j(r,t)$. According to the definition of a fractional derivative (see the appendix), (2.3) can be written in the time domain [12] as

$$j(r,t) = \sqrt{D_0}\frac{\partial^{1/2}P(r,t)}{\partial t^{1/2}}$$

where

$$\frac{\partial^{1/2} P(r,t)}{\partial t^{1/2}} = \frac{1}{\Gamma(1-1/2)} \frac{\partial}{\partial t} \int_0^t \mathrm{d}\tau \, \frac{P(r,\tau)}{(t-\tau)^{1/2}}$$

which, together with the constitutive equation (2.2), yields

$$\frac{\partial^{1/2} P(r,t)}{\partial t^{1/2}} = -\sqrt{D_0} \frac{\partial P(r,t)}{\partial r}. \tag{2.4}$$

Equation (2.4) is the fractional calculus version of the standard diffusion equation in one dimension. It relates the radial probability current, and through the constitutive equation (2.2) the radial derivative of $P(r,t)$, to the fractional time derivative of order $\frac{1}{2}$ of $P(r,t)$. In the following, we consider the applicability of fractional calculus to non-standard Brownian processes. We start with the known case of fractional Brownian motion.

3. Fractional Brownian motion

Fractional Brownian motion (FBM) is the simplest mathematical model of a Gaussian stochastic process (random walk) whose variance does not scale linearly with time [17]. Its probability density function $P_{\mathrm{FBM}}(x,t)$ is defined, in one dimension, by [17]

$$P_{\mathrm{FBM}}(x,t) = \frac{1}{(4D\pi t^{2/d_w})^{1/2}} \exp\left(-\frac{x^2}{4D\ t^{2/d_w}}\right) \tag{3.1}$$

where $1 \leqslant d_w < \infty$ characterizes the time evolution of the mean-square displacement of the FBM, $\langle x^2(t)\rangle = 2Dt^{2/d_w}$, where D is a constant. In the following, we will only consider the diffusion regime $2 \leqslant d_w < \infty$.

According to its original definition [17], FBM can be described as an integral transform of Brownian motion (BM)

$$x_{\mathrm{FBM}}(t) = \int_{-\infty}^{t} K(t-\tau)\, \mathrm{d}x_{\mathrm{BM}}(\tau)$$

where $x_{\mathrm{FBM}}(t)$ and $x_{\mathrm{BM}}(t)$ are the positions of the particle undergoing the FBM and BM processes, respectively. The kernel $K(t-\tau)$ expressed by

$$K(t-\tau) = \begin{cases} (t-\tau)^{1/d_w-1/2} - (-\tau)^{1/d_w-1/2} & \tau < 0 \\ (t-\tau)^{1/d_w-1/2} & 0 < \tau < t \end{cases}$$

resembles the singular kernel in the definition of fractional derivatives (see the appendix). It seems interesting then, to compare the FBM results with the solution $P(x,t)$ of the extraordinary (fractional) differential equation

$$\frac{\partial^{1/d_w} P(x,t)}{\partial t^{1/d_w}} = -A \frac{\partial P(x,t)}{\partial |x|} \qquad A > 0 \tag{3.2}$$

which is the natural generalization of (2.4) to the case $d_w > 2$.

Indeed, the solution of (3.2) leads to $\langle x^2(t)\rangle \sim t^{2/d_w}$. Moreover, the return probability $P(0,t)$ for the initial condition $P(x,0) = \delta(x)$ and the whole hierarchy of moments $M_k = \langle x^k(t)\rangle$ have the same time dependence as for the FBM. To show this, we consider the Laplace transform $P(x,s)$ in (3.2) (see the appendix) and obtain

$$s^{1/d_w}\ P(x,s) = -A\frac{\mathrm{d}P(x,s)}{\mathrm{d}|x|}.$$

A simple integration yields,

$$P(x,s) = Q(s)\exp(-s^{1/d_w}|x|/A) \tag{3.3}$$

where $Q(s)$ is determined by the normalization condition $\int_{-\infty}^{\infty}\mathrm{d}x\,P(x,t) = 1$,

$$Q(s) = \frac{1}{2A}\frac{1}{s^{1-1/d_w}}.$$

It is easy to show from (3.3) that $P(0,t) \sim t^{-1/d_w}$. From (3.1), one has

$$M_{2k}^{\mathrm{FBM}}(t) = \frac{(4D)^k\Gamma(k+1/2)}{\sqrt{\pi}}t^{2k/d_w} \tag{3.4}$$

and from (3.3) we obtain,

$$M_{2k}(t) = \frac{A^{2k}\Gamma(2k+1)}{\Gamma(2k/d_\mathrm{w}+1)}t^{2k/d_w} \tag{3.5}$$

with $M_{2k+1}(t) = M_{2k+1}^{\mathrm{FBM}}(t) = 0$. Notice that (3.4) and (3.5) coincide when $d_\mathrm{w} = 2$ and $A^2 = D$.

From these results, we see that the proposed fractional equation (3.2) displays scaling properties similar to those of the FBM (hierarchy of moments and return probability). Nevertheless, the statistical features of the FBM and the stochastic process described by (3.2) are quite different. This can be seen by comparing the moments (3.4) and (3.5), which imply that $P(x,t) \neq P_{\mathrm{FBM}}(x,t)$. As we will see in section 6, $P(x,t)$ has a different asymptotic decay than $P_{\mathrm{FBM}}(x,t)$. The difference between the two processes is also manifested by studying the characteristic functions $P(k,t)$ and $P_{\mathrm{FBM}}(k,t)$ as described later.

4. Characteristic function and relaxation

The characteristic function $P(k,t)$ is defined as the Fourier transform of $P(x,t)$,

$$P(k,t) = \int_{-\infty}^{\infty}\mathrm{d}x\ \exp(-\mathrm{i}kx)P(x,t) \tag{4.1}$$

where $k \geqslant 0$. $P(k,t)$ is known as the intermediate scattering function in the theory of liquids [18] and represents the correlation of density–density fluctuations of wavevector k in the fluid. Its decay in time describes the relaxation of density fluctuations of wavevector k to equilibrium.

The characteristic function $P(k,t)$ corresponding to the fractional equation (3.2) can be evaluated from the hierarchy of moments $\{M_n(t)\} = \{\langle x^n(t)\rangle\}$ given in (3.5). It can be shown that

$$P(k,t) = \Psi_{d_w}(A^2k^2t^{2/d_w}) \tag{4.2}$$

where

$$\Psi_{d_w}(x) = \sum_{n=0}^{\infty} \frac{(-x)^n}{\Gamma(2n/d_w+1)}. \tag{4.3}$$

The series (4.3) is absolutely convergent since, for large n,

$$\frac{|u_{n+1}(x)|}{|u_n(x)|} \leqslant \frac{|x|e^{2/d_w}}{[2(n+1)/d_w+1]^{2/d_w}} \to 0$$

where $u_n(x) = (-x)^n/\Gamma(2n/d_w+1)$. For $d_w = 2$, $\Psi_2(x) = \exp(-x)$.

To derive the asymptotic behaviour of Ψ_{d_w} for $d_w > 2$, we consider the Fourier transform of (3.3), and obtain

$$\frac{1}{s^{1-2/d_w}(A^2k^2+s^{2/d_w})} = \int_0^{\infty} dt\, \exp(-st)P(k,t). \tag{4.4}$$

This can be expressed in terms of the universal function $\Psi_{d_w}(x)$, which satisfies the integral equation

$$\frac{1}{1+x} = \int_0^{\infty} e^{-y}\Psi_{d_w}(xy^{2/d_w})dy \tag{4.5}$$

where $x = A^2k^2s^{-2/d_w}$. From (4.5), we find that for $x \to \infty$ and $d_w > 2$

$$\Psi_{d_w}(x) \sim 1/x \tag{4.6}$$

while when $d_w = 2$, $\Psi_2(x) = \exp(-x)$ in accordance with (4.3). Thus, for the anomalous case $d_w > 2$ we obtain the power law decay

$$P(k,t) \sim \frac{1}{A^2k^2t^{2/d_w}}$$

in contrast to the stretched exponential decay characteristic of the FBM [17]

$$P_{\mathrm{FBM}}(k,t) = \exp(-Dk^2t^{2/d_w}).$$

Notice that for $d_w = 2$, the latter reduces to the exponential decay of regular Brownian motion. We conclude that (3.2) does not correspond to one-dimensional FBM and a more general fractional equation is required to describe it.

Nevertheless, it is interesting to see how the asymptotic behaviour of the relaxation function $\Psi_{d_w}(x)$ is achieved for $x \to \infty$. Figure 1 shows the behaviour of the universal function $\Psi_{d_w}(x)$ for different values of d_w. Notice that for $d_w > 2$, $\Psi_{d_w} \cong \exp(-x)$ for small x, which corresponds to the stretched exponential behaviour of

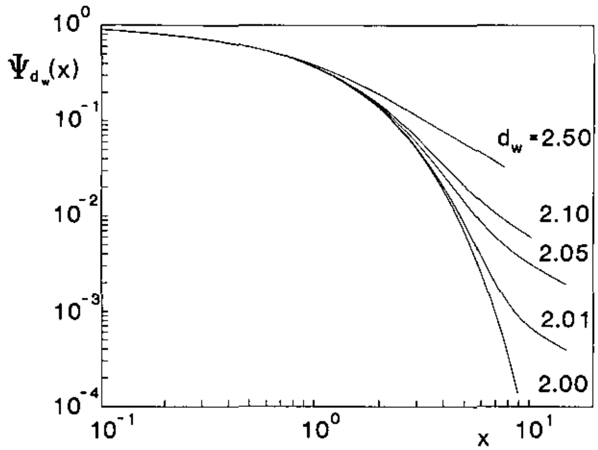

Figure 1. Plot of the 'universal' function $\Psi_{d_w}(x)$ against x, for different values $d_w = 2.5, 2.1, 2.05, 2.01$ and 2. Notice that for sufficiently large x, the curves tend to the asymptotic result $\Psi_{d_w}(x) \sim 1/x$, while for sufficiently small x they coincide with the standard result $\Psi_2(x) = \exp(-x)$.

$P_{FBM}(k,t)$ as a function of t. Asymptotically, $\Psi_{d_w}(x) \sim 1/x$ as expected from (4.6).

The result (4.3) has been obtained recently in the study of the electrochemical response of rough electrodes by de Levie and Vogt [19]. Their result follows from the empirical observation that the effective AC impedance $Z_{el}(\omega)$ of a rough electrode (per unit of macroscopic electrode area) in contact with an electrolyte solution can be represented as

$$Z_{el}(\omega) = R_s + \text{constant}(i\omega C)^{-\alpha} \tag{4.7}$$

where ω is the frequency, R_s the series resistance per unit apparent electrode area, C the capacitance and $0 < \alpha < 1$ is an exponent describing the electrode–electrolyte interfacial roughness ($\alpha = 1$ for flat interfaces). They calculated the apparent current density $I(t)$ following a small-amplitude voltage step of amplitude V, which can be obtained from the impedance by the relation

$$I(t) = VL^{-1}\{1/sZ_{el}(s)\} \tag{4.8}$$

where L^{-1} denotes an inverse Laplace transform, and $Z_{el}(s)$ is obtained from $Z_{el}(\omega)$ by replacing $i\omega$ by s. Combining (4.7) and (4.8), they find

$$\frac{I(t)}{I(0)} = L^{-1}\left(\frac{1}{s^{1-\alpha}(a+s^{\alpha})}\right) \tag{4.9}$$

where $I(0) = V/R_s$ and $a = \text{constant}/(R_s C^{\alpha})$. Equation (4.9) is essentially our result (4.4), with $I(t)/I(0) \equiv P(k,t)$ and $\alpha = 2/d_w$. The possible connection between our fractional calculus approach for diffusion and the AC response of such rough electrodes remains an intriguing question for future studies.

In order to explore the applicability of fractional calculus in other cases, we consider subsequently the standard diffusion equation on fractals and derive the fractional equations for that case. This will lead us to a more general form of (3.2) and to a better understanding of the physics described by fractional equations.

5. Standard diffusion equation on fractals

O'Shaughnessy and Procaccia [10] have proposed a diffusion equation on fractals for the spherically symmetric case of the form

$$\frac{\partial P_{\mathrm{OP}}(r,t)}{\partial t}=\frac{1}{r^{d_f-1}}\frac{\partial}{\partial r}\left(r^{d_f-1}D(r)\frac{\partial P_{\mathrm{OP}}(r,t)}{\partial r}\right) \tag{5.1}$$

with a position dependent diffusion coefficient $D(r)=\langle r^2(t)\rangle/2t=D_0 r^{-\theta}$, $\theta=d_{\mathrm{w}}-2$, and the constitutive equation $j(r,t)=-D(r)\partial P_{\mathrm{OP}}(r,t)/\partial r$. The solution of (5.1) can be obtained exactly [10]

$$P_{\mathrm{OP}}(r,t)=\frac{A}{t^{d_s/2}}\exp[-\mathrm{constant}(r/R)^{d_{\mathrm{w}}}] \tag{5.2}$$

where $A>0$ and $d_s=2d_f/d_{\mathrm{w}}$ is the spectral or fracton dimension [20]. As we mentioned in the introduction, this standard approach leads, according to equation (5.2), to $u'=d_{\mathrm{w}}$ in contrast with the stretched Gaussian form (1.2) with $u=d_{\mathrm{w}}/(d_{\mathrm{w}}-1)$. It may be remarked that (5.1) describes in general a Markovian process in an inhomogeneous medium whose diffusion coefficient varies in space (see for instance van Kampen's book [21]).

From (5.1), the corresponding fractional equation can be obtained by looking for a relation between $j(r,t)$ and a time derivative of $P_{\mathrm{OP}}(r,t)$. For simplicity, we consider the one-dimensional version of (5.1) in what follows, i.e. $d_f=1$. Denoting the Laplace transform of $P_{\mathrm{OP}}(r,t)$ by $P_{\mathrm{OP}}(r,s)$, (5.1) becomes

$$sP_{\mathrm{OP}}(r,s)=D_0\frac{\mathrm{d}}{\mathrm{d}r}\left(r^{-\theta}\frac{\mathrm{d}P_{\mathrm{OP}}(r,s)}{\mathrm{d}r}\right). \tag{5.3}$$

To solve (5.3), let us define $\xi=(2/\sqrt{D_0 d_{\mathrm{w}}^2})(s^{1/d_{\mathrm{w}}}r)^{d_{\mathrm{w}}/2}$ and $P_{\mathrm{OP}}(r,s)=\xi^{\gamma}z(\xi)$, where $\gamma=1-1/d_{\mathrm{w}}$. Then, (5.3) leads to the modified Bessel equation

$$\xi^2\frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2}+\xi\frac{\mathrm{d}z}{\mathrm{d}\xi}-(\xi^2+\gamma^2)z=0$$

whose solution (satisfying the summability condition for $r\to\infty$) is given by $z(\xi)=CK_{\gamma}(\xi)$, where K_{γ} is the modified Bessel function of second kind.

In the neighbourhood of $r=0$, one has

$$P_{\mathrm{OP}}(r,s)=C[1+a_1\xi^{2\gamma}+\mathrm{o}(\xi^{2\gamma})]$$

and

$$j(r,s)=-Ca_1 r^{-\theta}\xi^{2\gamma-1}\,\mathrm{d}\xi/\mathrm{d}r+\mathrm{o}(\xi^{2\gamma-1})$$

which are related by $s^{\gamma}P_{\mathrm{OP}}(r,s)\sim j(r,s)$. Thus, the corresponding fractional equation becomes

$$\frac{\partial^{\gamma}P(r,t)}{\partial t^{\gamma}}=-Br^{-\theta}\frac{\partial P(r,t)}{\partial r} \tag{5.4}$$

for $r \to 0$, where $B > 0$ is a constant.

For $r \to \infty$,

$$K_\gamma(\xi) = \mathrm{e}^{-\xi} \left(\frac{\pi}{2\xi}\right)^{1/2} [1 + \mathrm{O}(1/\xi)]$$

and

$$P_{\mathrm{OP}}(r, s) \sim (s^{1/d_w} r)^{\theta/4} \exp[-\mathrm{constant}(s^{1/d_w} r)^{d_w/2}]. \tag{5.5}$$

From the constitutive equation and (5.5) we find $j(r, s) \sim s^{1/2} r^{-\theta/2} P_{\mathrm{OP}}(r, s)$, which leads to the fractional equation

$$\frac{\partial^{1/2} P(r, t)}{\partial t^{1/2}} = -B' r^{-\theta/2} \frac{\partial P(r, t)}{\partial r} \tag{5.6}$$

for $r \to \infty$, where $B' > 0$ is a constant. For simplicity, we have omitted in (5.6) a term $\sim P(r, t)/r^{1+(\theta/2)}$, which is required to obtain the prefactor $(s^{1/d_w} r)^{\theta/4}$ in (5.5). Such terms will not be considered here because they do not modify the form of the exponential factor of $P(r, t)$, for $r/R \to \infty$. It is precisely such an exponential factor to which we draw our attention in the present work.

As we can see from these results, the standard equation (5.1) ($d_f = 1$) corresponds to different fractional equations (5.4) and (5.6), depending on the range of r under consideration. For $r \to 0$, the fractional equation is anomalous, i.e. $\gamma = 1 - 1/d_w > \frac{1}{2}$ for $d_w > 2$, while for $r \to \infty$ it becomes similar to the regular equation (2.4), $\gamma = \frac{1}{2}$. In both cases, however, there exists an extra position-dependent factor $r^{-\theta'}$, with $\theta' = \theta$ (equation (5.4)) and $\theta' = \theta/2$ (equation (5.6)). From (5.4) and (5.6), we are thus led to consider the more general fractional equation

$$\frac{\partial^{\gamma'} P(r, t)}{\partial t^{\gamma'}} = -A' r^{-\theta'} \frac{\partial P(r, t)}{\partial r} \tag{5.7}$$

which includes (2.4), (3.2), (5.4) and (5.6) as particular cases. To see how (5.7) actually works, we study in the next section the solutions of (5.7) in detail.

6. Asymptotic fractional diffusion equation

Let us consider an isotropic and homogeneous random fractal structure embedded in a d-dimensional Euclidean system. We wish to find out to what extent the fractional equation

$$\frac{\partial^{\gamma'} P(r, t)}{\partial t^{\gamma'}} = -A r^{-\theta'} \frac{\partial P(r, t)}{\partial r} \tag{6.1}$$

in the spherically symmetric case, can describe the essential features of the average function $P(r, t)$ for diffusion on fractals. Equation (6.1) is obtained from the constitutive equation

$$j(r, t) = -A r^{-\theta'} \frac{\partial P(r, t)}{\partial r}$$

where $\theta' \geqslant 0$ in general and $A > 0$ is a constant. We adopt the convention that by integrating over r, the differential element of volume is given by

$$\mathrm{d}V(r) = \Lambda r^{d_f-1}\,\mathrm{d}r$$

where d_f is the fractal dimension of the structure and Λ is a constant. The normalization condition for the probability is then written as $\Lambda\int_0^\infty \mathrm{d}r\, r^{d_f-1}P(r,t) = 1$.

Denoting the Laplace transform of $P(r,t)$ by $P(r,s)$ and proceeding as in the solution of (3.3) we obtain from (6.1)

$$P(r,s) = \frac{C}{s^{1-d_f\gamma'/(1+\theta')}}\exp\left[-\frac{s^{\gamma'}r^{1+\theta'}}{A(1+\theta')}\right] \qquad (6.2)$$

where $C = (1+\theta')/\{\Lambda[A(1+\theta')]^{d_f/(1+\theta')}\Gamma(d_f/(1+\theta'))\}$.

The two parameters γ' and θ' in (6.2) are not independent of each other. A relation between them is obtained by requiring that $\int_0^\infty \mathrm{d}r\, r^{d_f-1}r^2P(r,t) \sim t^{2/d_w}$. This condition yields

$$\frac{\gamma'}{1+\theta'} = \frac{1}{d_w}. \qquad (6.3)$$

In accordance with (6.3), we can write (6.2) as

$$P(r,s) = \frac{C}{s^{1-d_f/d_w}}\exp\left[-\frac{(s^{1/d_w}r)^{1+\theta'}}{A(1+\theta')}\right]. \qquad (6.4)$$

In order to obtain $P(r,t)$, the inverse Laplace transform of (6.4) needs to be evaluated. The asymptotic behaviour of $P(r,t)$, however, can be derived analytically by conventional methods. To this end, we assume the following scaling form for $P(r,t)$,

$$P(r,t) \sim t^{-d_s/2}\exp\left[-\text{constant}\left(\frac{r}{R}\right)^{u'}\right] \qquad (6.5)$$

when $t \to \infty$ and $r/R \gg 1$, and evaluate the Laplace transform of (6.5), $P(r,s)$, by using the steepest descent technique. Comparison with (6.4) yields $1+\theta' = u'd_w/(u'+d_w)$, or equivalently

$$u' = \frac{d_w(1+\theta')}{d_w-(1+\theta')}. \qquad (6.6)$$

This result can be compared with the corresponding functions discussed in sections 3 and 5. For the FBM, for instance, one has $u' = 2$ from (3.1), and, according to (6.6) $\theta' = (d_w-2)/(d_w+2)$, while $\gamma' = 2/(d_w+2)$ from (6.3). We now see how our fractional equation (3.2) has to be modified in order that its asymptotic solution reproduces the FBM result (3.1). Also, comparing the exact solution (5.2) of the standard diffusion equation on fractals (5.1), $u' = d_w$, with (6.6) we find $\theta' = (d_w-2)/2 = \theta/2$ and $\gamma' = \frac{1}{2}$, as obtained in (5.6).

We see that the differential equation (6.1) is quite general and can describe asymptotically the FBM results and the standard diffusion equation on fractals. For a more general application of (6.1) to fractals, one of the two parameters γ' or θ' remains to be determined in the equation. This degree of freedom is at the heart of the approach and means that, in principle, all the fractional equations (6.1) having different parameters γ' and θ' compatible with (6.3) should be taken into account for a complete description of anomalous dynamical processes on fractals.

For many practical applications, however, one is not interested in all the details of the transport process. Our discussion thus turns to the solution of one fractional equation which proves to play a prominent role in this approach. This equation is obtained when $\theta' = 0$, implying $\gamma' = 1/d_w$, which leads to the simplest form of (6.1). In this case, the radial current $j(r,t)$ is related to the radial derivative of $P(r,t)$ (constitutive equation) simply by

$$j(r,t) = -A\frac{\partial P(r,t)}{\partial r} \tag{6.7}$$

as for diffusion in regular systems (equation (2.2)) (first Fick's law), while the anomalies in the diffusion process are taken into account by the fractional time derivative of $P(r,t)$. We thus arrive at the fractional equation

$$\frac{\partial^{1/d_w} P(r,t)}{\partial t^{1/d_w}} = -A\frac{\partial P(r,t)}{\partial r} \tag{6.8}$$

which we denote as the asymptotic fractional diffusion equation on fractals.

Both the anomalous diffusion exponent d_w and the parameter A in (6.8) can be determined from the mean-square displacement $\langle r^2(t)\rangle$, which is assumed as known and obeying $\langle r^2(t)\rangle = \mathrm{B}t^{2/d_w}$. A simple calculation then yields $A = [\Gamma(1 + 2/d_w)/(d_f(1+d_f))]^{1/2}B^{1/2}$.

The asymptotic solution of (6.8), for $t \to \infty$ and $r/R \to \infty$, is given by the *stretched* Gaussian

$$P(r,t) \sim P(0,t)\ \exp\left[-\text{constant}\left(\frac{r}{R}\right)^u\right] \tag{6.9}$$

with

$$u = \frac{d_w}{d_w - 1}$$

which corresponds to the lowest value of u' in (6.6)†. Within our approach, (6.8) determines the asymptotic behaviour for the whole family of fractional equations, since the solutions of (6.1) for $\theta' > 0$ decay much faster than (6.9) for $r/R \to \infty$. (For an heuristic derivation of (6.8) we refer to [23]). Thus, our result (6.9) reproduces the accepted stretched Gaussian result (1.2) for diffusion on fractals.

† Equation (6.9) contains an extra factor of the form $f(x) \sim x^\alpha$, where $x = r/R$ and $\alpha = u(d_s - 1)/2$. For more details see [22].

7. Concluding remarks

We have proposed a generalization of the standard diffusion equation for describing transport phenomena in complex media such as random fractal structures. The new equation, obtained within the framework of the fractional calculus, represents a promising tool for studying anomalous transport behaviour in these random media.

The present fractional calculus method constitutes a significant change in the usual approach to the problem. In the formulation of the standard diffusion equation on fractals for instance, one usually starts from the continuity equation (2.1) and modifies the constitutive equation (2.2) in order to satisfy the expected scaling for the mean-square displacement (1.1) [10]. Our approach consists essentially in keeping unaltered the constitutive relation between the (radial) current and particle concentration P, while the anomalies of the diffusion process are described by a non-integer (fractional) temporal derivative of P. This is equivalent to an integro-differential equation for P, which in practice is solved by standard Laplace transformations. The solution of the equation is obtained analytically and reproduces the asymptotic behaviour of the probability density function on random fractals such as the infinite percolation cluster at criticality.

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Appendix. Mathematical background

The fractional derivative of order q (for real q) of a function $f(x)$ with respect to $x - x_0$ is defined as [12],

$$\frac{\mathrm{d}^q f(x)}{\mathrm{d}(x-x_0)^q} = \lim_{N\to\infty} \frac{1}{\Gamma(-q)} \left(\frac{x-x_0}{N}\right)^{-q} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f\left(x - j\frac{(x-x_0)}{N}\right). \quad \text{(A1)}$$

It can be shown that, for $q = n$, (n positive integer), (A1) reduces to the usual derivative of order n. For $q = n$ (n negative integer), it corresponds to the multiple integral of order n.

Definition (A1) corresponds to the integral representation

$$\frac{\mathrm{d}^q f(x)}{\mathrm{d}(x-x_0)^q} = \frac{\mathrm{d}^{n(q)}}{\mathrm{d}x^{n(q)}} \left[\frac{1}{\Gamma(n(q)-q)} \int_{x_0}^{x} \frac{f(y)}{(x-y)^{q+1-n(q)}}\,\mathrm{d}y\right] \quad \text{(A2)}$$

where $n(q)$ is the smallest non-negative integer so that

$$q - n(q) < 0. \quad \text{(A3)}$$

Of course, if $q < 0$, $n(q) = 0$. Definition (A2) can be written formally as

$$\frac{\mathrm{d}^q f(x)}{\mathrm{d}x^q} = \frac{\mathrm{d}^{n(q)}}{\mathrm{d}x^{n(q)}} \left(\frac{\mathrm{d}^{q-n(q)} f}{\mathrm{d}x^{q-n(q)}}\right). \quad \text{(A4)}$$

From (A2) and (A3), we have for $0 < q < 1$, taking $x_0 = 0$ without loss of generality, that

$$\frac{\mathrm{d}^q f(x)}{\mathrm{d}x^q} = \frac{1}{\Gamma(1-q)} \frac{\mathrm{d}}{\mathrm{d}x} \int_0^x \frac{f(y)}{(x-y)^q} \,\mathrm{d}y.$$

The Laplace transform $L[\mathrm{d}^q f(x)/\mathrm{d}x^q]$ of $\mathrm{d}^q f(x)/\mathrm{d}x^q$ can be obtained from (A2) and (A4) by applying the convolution theorem, and

$$L\left[\frac{\mathrm{d}^q f(x)}{\mathrm{d}x^q}\right] = \begin{cases} s^q L[f] & q < 0 \\ s^q L[f] - \displaystyle\sum_{j=0}^{n(q)-1} s^j \frac{\mathrm{d}^{q-1-j} f(0)}{\mathrm{d}x^{q-1-j}} & q > 0. \end{cases}$$

If the initial conditions for the derivatives of $f(x)$, $\mathrm{d}^{q-1-j} f(0)/\mathrm{d}x^{q-1-j} = 0$ ($j = 0, \ldots, n(q) - 1$), then

$$L\left[\frac{\mathrm{d}^q f(x)}{\mathrm{d}x^q}\right] = s^q L[f] \tag{A5}$$

for all q.

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