

How Does the Diffusion Equation on Fractals Look Like?

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Abstract

Different forms of diffusion equations on fractals proposed in the literature are reviewed and critically discussed. Variants of the known fractional diffusion equations are suggested here and worked out analytically. On the basis of these results we conclude that the quest: “what is the form of the diffusion equation on fractals”, is still open, but we are possibly close to get a satisfactory answer.

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1 Introduction

Diffusion processes are ubiquitous in Nature. They describe a special type of motion in which a material entity, i.e. an atom, molecule or a larger atomic aggregate immersed in a fluid or conducting system, executes an apparently random motion which, for all instances, turns out to be completely unpredictable. Despite this undeterministic behavior, diffusion obeys precise and well known laws. These were formulated more than one century ago by Einstein [1], Smoluchowsky [2] and other pioneers such as Bachelier [3], who studied this problem even earlier to model the random behavior of stock prices.

The diffusion law establishes that, upon averaging over all possible trajectories, a diffusing particle (also called Brownian particle) moves a distance R after time t , from its starting point \vec{r}_0 at $t = 0$, given by

$$R^2 \equiv \langle (\vec{r} - \vec{r}_0)^2 \rangle = 2dD_0t \quad (1)$$

where D_0 (having dimensions of Length²/Time) is the diffusion coefficient and d is the dimensionality of the space in which this transport process is embedded. Eq. (1) reflects the absence of correlations between the intermediate collision events responsible for the ‘chaotic’ motion of the diffusing particle, and also correlations between different trajectories, which can be seen as totally independent.

In what follows, we will assume for simplicity that diffusion takes place within an isotropic medium. It is well known that in this case, the probability $P(r, t)$ that the Brownian particle is located at a distance r at time t , if it started at the origin $\vec{r}_0 = 0$ at $t = 0$, is a Gaussian (see e.g. [4]),

$$P(r, t) = \frac{A_d}{t^{d/2}} \exp\left(-\frac{r^2}{4t}\right) \quad (2)$$

where A_d is obtained from the normalization condition $\int_0^\infty dr r^{d-1} P(r, t) = 1$, $A_d^{-1} = 2^{d-1}\Gamma(d/2)$, the latter is the gamma function (see e.g. [5]), and we have assumed without loss of generality that $D_0 = 1$ ¹. The probability distribution

¹Notice that Eq. (2) is valid when $r < t$, since for $r > t$ one has $P(r, t) = 0$. In what follows we will always refer to the case $r < t$.

function (PDF) $P(r, t)$ is the solution of a second-order partial differential equation known as the standard diffusion equation (SDE), which for a d -dimensional isotropic medium (see e.g. [4]) reads,

$$\frac{\partial P(r, t)}{\partial t} = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} \left(r^{d-1} \frac{\partial P(r, t)}{\partial r} \right). \quad (3)$$

Here, we are interested in studying how such an equation should be modified in order to correctly describe the effects of geometrical constraints on diffusion such as those typical of fractal structures, a problem which has attracted a great deal of attention in recent years (see e.g. [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22]). Despite all these efforts, this problem has not been solved so far in a complete fashion, and the aim of this work is to review some of the attempts which have been performed in solving this quest, by presenting a critical discussion of their partial success and failure.

In Sec. 2 we briefly review the main aspects of the SDE. Sec. 3 summarizes the classical version of the SDE on fractals which admits a simple exact solution. In Sec. 4 we motivate the need for a generalization of the SDE on fractals, suggesting that this can be achieved within the framework of fractional derivatives. This approach leads us to the fractional diffusion equation (FDE) on self-similar structures. In Sec. 5 we suggest a simple (yet not definitive) solution to our problem by introducing a modification of the standard diffusion equation on fractals in a formal fashion. Finally, we summarize our conclusions in Sec. 6.

2 Diffusion Equation in an Isotropic Medium

For convenience, we will solve Eq. (3) in the Laplace domain and denote the Laplace transform of $P(r, t)$ simply as $P(r, s)$, which is given by

$$P(r, s) = \int_0^\infty dt e^{-st} P(r, t). \quad (4)$$

Multiplying Eq. (3) by $\exp(-st)$ and integrating over t one finds,

$$-P(r, t=0) + sP(r, s) = \frac{(d-1)}{r} \frac{\partial P(r, s)}{\partial r} + \frac{\partial^2 P(r, s)}{\partial r^2}$$

which, assuming the initial condition $P(r, t = 0) = \delta(r)$, becomes

$$sP(r, s) = \frac{(d-1)}{r} \frac{\partial P(r, s)}{\partial r} + \frac{\partial^2 P(r, s)}{\partial r^2} \quad \text{for } r > 0. \quad (5)$$

Introducing for convenience the scaled variable $x = rs^{1/2}$, Eq. (5) becomes

$$\frac{d^2 W(x)}{dx^2} + \frac{(d-1)}{x} \frac{dW(x)}{dx} - W(x) = 0 \quad (6)$$

whose solutions in spatial dimensions $d = 1, 2$ and 3 are, respectively: $W_1(x) = \exp(-x)$, $W_2(x) = K_0(x)$ (modified Bessel function of zero order), and $W_3(x) = x^{-1} \exp(-x)$ (see e.g. [5]). In particular, in two-dimensions, W_2 has the asymptotic behaviors, $W_2(x) \sim \sqrt{\pi/2x} e^{-x}$ for $x \rightarrow \infty$, and $W_2(x) \sim -\ln(x/2) + \gamma + \mathcal{O}(x^2)$ for $x \rightarrow 0$, where γ is the Euler constant. These asymptotic behaviors can be detected analytically as illustrated in Appendix A.

Using the normalization of $P(r, t)$ in Eq. (4), one finds $\int_0^\infty dr r^{d-1} P(r, s) = 1/s$, and writing $P(r, s) = A(r, s)W(x)$, where $A(r, s)$ is a normalization factor, we obtain

$$\begin{aligned} P(r, s) &= \frac{1}{\sqrt{s}} e^{-rs^{1/2}} & (d = 1) \\ &= K_0(rs^{1/2}) & (d = 2) \\ &= \frac{1}{r} e^{-rs^{1/2}} & (d = 3). \end{aligned} \quad (7)$$

It is instructive to recover $P(r, t)$ by considering the inverse Laplace transform of $P(r, s)$, which can be written as (see e.g. [10])

$$P(r, t) = \frac{i}{2\pi} \int_0^\infty d\rho e^{-\rho t} [P(r, \rho e^{i\pi}) - P(r, \rho e^{-i\pi})]. \quad (8)$$

The application to the case $d = 3$ is discussed in Appendix B.

3 Standard Diffusion Equation on Fractals

Let us consider next the conducting medium to be a homogeneous fractal, i.e. characterized by a fractal dimension $d_f < d$. Assuming for simplicity the fractal

structure to be self-similar on all length scales, the standard behavior Eq. (1) is modified on all time scales, yielding (see e.g. [6, 17])

$$R^2 \equiv \langle (\vec{r} - \vec{r}_0)^2 \rangle = a^2 (t/t_0)^{2/d_w} \quad (9)$$

where the exponent $d_w > 2$ is the diffusion exponent (or fractal dimension of the associated random walk, which becomes $d_w = 2$ on homogeneous media as in Eq. (1)). In Eq. (9), a has the dimension of length and t_0 is a characteristic time.

On random fractals, i.e. structures which are self-similar in a statistical sense, Eq. (9) holds asymptotically for $t \gg t_0$. Assuming for the sake of simplicity that Eq. (9) holds for all t , one can incorporate this anomalous diffusion result into the standard diffusion equation, Eq. (3), yielding what we call the standard diffusion equation on fractals [7],

$$\frac{\partial P(r, t)}{\partial t} = \frac{1}{r^{d_f-1}} \frac{\partial}{\partial r} \left(r^{d_f-1} r^{-\theta} \frac{\partial P(r, t)}{\partial r} \right), \quad (10)$$

where $\theta = d_w - 2$. Note that Eq. (10) reduces to Eq. (3) when $d_f = d$ and diffusion becomes normal, i.e. $d_w = 2$ and $\theta = 0$.

To discuss the properties of Eq. (10) it is convenient to write it as

$$\frac{\partial P(r, t)}{\partial t} = \frac{(d_f - 1 - \theta)}{r^{1+\theta}} \frac{\partial P(r, t)}{\partial r} + \frac{1}{r^\theta} \frac{\partial^2 P(r, t)}{\partial r^2}, \quad (11)$$

whose exact solution is simply

$$P(r, t) = \frac{A_{d_s}}{t^{d_s/2}} \exp \left(-\frac{r^{d_w}}{d_w^2 t} \right) \quad (12)$$

as can be verified by direct substitution in Eq. (11), where $d_s = 2d_f/d_w$. The normalization factor A_{d_s} can be obtained from the condition $\int_0^\infty dr r^{d_f-1} P(r, t) = 1$, yielding $A_{d_s}^{-1} = d_w^{d_s-1} \Gamma(d_s/2)$. In the fractal literature, d_s is denoted as the spectral or fracton dimension, and obeys $1 \leq d_s \leq d$ (see e.g. [6, 17]). For fractal percolation clusters for instance $d_s \approx 4/3$. Clearly, Eq. (12) reduces to Eq. (2) when $d_w = 2$ and $d_s = d$.

We consider next the Laplace transform of Eq. (11), which can be written as (cf. Sec. 2)

$$sP(r, s) = \frac{(d_f + 1 - d_w)}{r^{1+\theta}} \frac{\partial P(r, s)}{\partial r} + \frac{1}{r^\theta} \frac{\partial^2 P(r, s)}{\partial r^2}, \quad r > 0 \quad (13)$$

Introducing now the variable $x = r s^{1/d_w}$, we obtain from Eq. (13) the differential equation

$$\frac{d^2 W(x)}{dx^2} + \frac{(d_f + 1 - d_w)}{x} \frac{dW(x)}{dx} - x^\theta W(x) = 0 \quad (14)$$

which is the analogous to Eq. (6), and proceed studying the asymptotic forms of $W(x)$ which will turn useful later for constructing generalizations of the present theory.

To do this, we follow the same strategy illustrated in Appendix A. In the limit $x \rightarrow \infty$, we assume the asymptotic form $W_{d_s}^{(\infty)}(x) \sim x^{-\beta} \exp(-ax^\gamma)$, and substituting it into Eq. (14), we find

$$H_{d_s} W_{d_s}^{(\infty)}(x) = \frac{W_{d_s}^{(\infty)}(x)}{x^2} \left[\beta(\beta + d_w - d_f) + a\gamma(d_w - d_f - \gamma + 2\beta)x^\gamma + (a^2\gamma^2 x^{2\gamma} - x^{d_w}) \right], \quad (15)$$

where $H_{d_s} = d^2/dx^2 + [(d_f + 1 - d_w)/x]d/dx - x^{d_w-2}$. Thus, to leading order (cf. Eq. (A2)) the second and third terms in Eq. (15) must vanish and we obtain, $a = \gamma^{-1}$ with

$$\gamma = \frac{d_w}{2} \quad \text{and} \quad \beta = \frac{d_w}{4}(d_s - 1).$$

The limit $x \rightarrow 0$ is described by the ansatz $W_{d_s}^{(0)}(x) \approx 1 - b x^\eta$ leading to

$$H_{d_s} W_{d_s}^{(0)}(x) \cong -b \eta (\eta + d_f - d_w) - x^{d_w-\eta} W_{d_s}^{(0)}(x) \approx 0$$

which can be satisfied if

$$\eta = d_w - d_f$$

generalizing the standard result Eq. (A4). Note that for fractals, $d_w > d_f$, i.e. $\eta > 0$.

Unfortunately, the result Eq. (12) is only partially correct since it describes well the scaling region $r < t^{1/d_w}$ (see e.g. [7, 14, 18]), but fails regarding the asymptotic limit $r > t^{1/d_w}$. Indeed, based on compelling evidence coming from both numerical results and scaling arguments (see e.g. [6, 8, 13, 17]), it is now widely accepted that

$$P(r, t) \sim \frac{1}{t^{d_s/2}} \left(\frac{r}{t^{1/d_w}} \right)^{\alpha_\infty} \exp \left[-\frac{1}{c} \left(\frac{r}{t^{1/d_w}} \right)^u \right] \quad (16)$$

valid in the range $r \gg t^{1/d_w}$, where

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

The correct expression for the exponent α_∞ is still not known accurately (see the different attempts in e.g. [11, 12, 14], and refs. therein). To recover the asymptotic behavior (16), we resort to a different approach based on the concept of fractional derivatives (see e.g. [15, 16, 22]).

4 Fractional Diffusion Equations

4.1 Uniform Systems

We start out with the Laplace transformed Eq. (5), that we now write in the form

$$sP(r, s) = H_d P(r, s) \equiv \left(\frac{(d-1)}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \right) P(r, s) \quad (17)$$

and look for an operator \hat{H}_d such that $\hat{H}_d \times \hat{H}_d = H_d$. The simplest choice has the form

$$\hat{H}_d = \pm \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right), \quad \text{with} \quad \kappa = \frac{d-1}{2}, \quad (18)$$

which coincides with the exact result for $d = 1$ and $d = 3$, as can be easily verified. Now, Eq. (17) can be written in its ‘square-root’ form as (see e.g. [9, 10]),

$$s^{1/2} P(r, s) = \hat{H}_d P(r, s) = -\frac{\partial P(r, s)}{\partial r} - \frac{\kappa}{r} P(r, s) \quad (19)$$

where we have chosen the minus sign since it is the only choice compatible with a bounded solution of $P(r, s)$ for $r \rightarrow \infty$. Eq. (19) is the fractional derivative equivalent to the standard form Eq. (17), where its name comes from the fact that the left-hand side of the equation is related to the Laplace transform of a fractional derivative of order 1/2 (see e.g. [15, 16, 22]).

The solution of Eq. (19) can be obtained at once yielding,

$$P(r, s) = P_0(s) \frac{1}{(rs^{1/2})^\kappa} \exp(-rs^{1/2}) \quad (20)$$

where $P_0^{-1}(s) = s^{1-d/2}\Gamma[(d+1)/2]$ is due to the normalization of $P(r, s)$. The result Eq. (20) coincides with the exact ones Eq. (7) in the cases $d = 1$ and $d = 3$. In $d = 2$, it is only asymptotically correct, and note that because of normalization the prefactor is $2/\sqrt{\pi} = 1.1284$, instead of the exact value $\sqrt{\pi/2} = 1.2533$.

4.2 Homogeneous Fractals

We consider now the fractional diffusion version of Eq. (11), in particular of its Laplace transform Eq. (13). In analogy to Eq. (18), we make the ansatz

$$\hat{H}_{d_s} = -\frac{1}{r^{2\tilde{\theta}}} \left(\frac{\partial}{\partial r} + \frac{\tilde{\kappa}}{r} \right) \quad (21)$$

where its associated fractional diffusion equation reads,

$$s^{1/2}P(r, s) = \hat{H}_{d_s}P(r, s). \quad (22)$$

Then, from Eq. (21) we find

$$\hat{H}_{d_s} \times \hat{H}_{d_s} = \frac{1}{r^{2\tilde{\theta}}} \frac{\partial^2}{\partial r^2} + \frac{2\tilde{\kappa} - \tilde{\theta}}{r^{1+2\tilde{\theta}}} \frac{\partial}{\partial r} + \frac{\tilde{\kappa}(\tilde{\kappa} - 1 - \tilde{\theta})}{r^{2+2\tilde{\theta}}}, \quad (23)$$

where, to be consistent with Eq. (13), the conditions $2\tilde{\theta} = \theta$ and $2\tilde{\kappa} - \tilde{\theta} = \alpha$ must be satisfied, yielding

$$\tilde{\theta} = \frac{\theta}{2} \quad \text{and} \quad \tilde{\kappa} = \frac{d_w}{4}(d_s - 1). \quad (24)$$

Thus, our square-root (fractional derivative) operator Eq. (21) is equivalent to the original one Eq. (13) in two cases. The first one occurs when $\tilde{\kappa} = 0$, i.e. for $d_s = 1$. This result corresponds to topologically one-dimensional fractals, such as paths generated by random walks or self-avoiding random walks (see e.g. [6]), and implies that $d_w = 2d_f$. This is one of the few cases in which we can calculate d_w exactly, at least in the sense that it is completely given by static exponents such as d_f . The other case for which Eq. (21) is equivalent to Eq. (13) corresponds to the limit $\tilde{\kappa} = 1 + \tilde{\theta} = d_w/2$, i.e. $d_s = 3$.

The solution of Eq. (22) can be obtained also easily,

$$P(r, s) = \frac{A_0}{s^{1-d_s/2}} \frac{1}{(r s^{1/d_w})^{\tilde{\kappa}}} \exp\left(-\frac{2}{d_w} r^{d_w/2} s^{1/2}\right) \quad (25)$$

which is equivalent to the asymptotic result discussed in Eq. (15). This is another example of the limitations of the fractional diffusion equation which holds in general only asymptotically, i.e. for $r \rightarrow \infty$. As discussed below, the inverse Laplace transform of Eq. (25) does not behave as in Eq. (12) when $r \rightarrow 0$. This constitutes the main drawback of the fractional diffusion formalism.

4.3 General FDE on Homogeneous Fractals

It is instructive to study a generalization of Eq. (22) which we assume to be of the form

$$s^{1/\gamma} P(r, s) = -\frac{1}{r^{\theta'}} \frac{\partial P(r, s)}{\partial r} - \frac{\kappa}{r^{1+\theta'}} P(r, s) \quad (26)$$

where the exponents γ and θ' are related by $\gamma(1 + \theta') = d_w$, but are otherwise arbitrary obeying $\theta' \geq 0$, $\gamma \leq d_w$ and $\kappa \neq 0$ in general. The solution of Eq. (26) is

$$P(r, s) = \frac{A_0}{s^{1-d_s/2}} \frac{1}{(r s^{1/d_w})^\kappa} \exp\left(-\frac{\gamma}{d_w} (r s^{1/d_w})^{1+\theta'}\right) \quad (27)$$

where the normalization factor is given by

$$A_0^{-1} = \left(\frac{d_w}{\gamma}\right)^{\gamma(d_f - \kappa)/d_w - 1} \Gamma\left(\frac{\gamma}{d_w} (d_f - \kappa)\right).$$

Now we have the elements to discuss the asymptotic behavior $r/t^{1/d_w} \gg 1$ of $P(r, t)$ associated to the inverse Laplace transform of Eq. (27) (see also Appendix C). We do this by evaluating the Laplace transform Eq. (4) using the ansatz

$$P(r, t) \sim \frac{1}{t^{d_s/2}} \left(\frac{r}{t^{1/d_w}}\right)^{\alpha'_\infty} \exp\left[-\frac{1}{c} \left(\frac{r}{t^{1/d_w}}\right)^{u'(\theta')}\right], \quad (28)$$

and applying the saddle-point method (see e.g. the application to this problem discussed in [10]). The results for the exponents α'_∞ and $u'(\theta')$ are

$$\alpha'_\infty = \frac{d_w}{d_w - (1 + \theta')} \left(\frac{(1 + \theta')}{2} (d_s - 1) - \kappa\right) \quad (29)$$

and

$$u'(\theta') = \frac{d_w(1 + \theta')}{d_w - (1 + \theta')}. \quad (30)$$

The latter reduces to our desired result Eq. (16) when $\theta' = 0$, i.e. $u'(0) = u$, and to the standard diffusion equation on fractals Eq. (12), in the limit of large r , when $\theta' = d_w/2 - 1$, i.e. $u' = d_w$. The case $\theta' = 0$ corresponds to the simple exponential decay $P(r, s) \sim \exp(-rs^{1/d_w})$, which is the direct fractal counterpart of the standard results Eq. (7).

However as mentioned above, the FDE fails to describe the behavior of $P(r, t)$ around the origin ($r/t^{1/d_w} \rightarrow 0$), yielding in general a (weak, usually integrable) divergence, as one can see from the explicit inverse transform Eq. (C2). We have tried to modify Eq. (26) in different ways to solve this ‘problem of the origin’, but without reaching satisfactory results (cf. App. D). Other possible forms of the fractional diffusion equation (see e.g. [23]) do not solve this issue either. We discuss a final attempt to combine both the result Eq. (12), valid for $r < t^{1/d_w}$, and the asymptotic one Eq. (16), valid for $r > t^{1/d_w}$.

5 Conjectured Form of the Diffusion Equation on Fractals

In the following, we try to improve on the form of the standard diffusion equation Eq. (10) rather than on its fractional derivative counterpart. We write Eq. (10) in the form,

$$\frac{\partial P(r, t)}{\partial t} = \frac{1}{r^{d_f-1}} \frac{\partial}{\partial r} \left(r^{d_f-1} r^{-\theta} f\left(\frac{r}{t^{1/d_w}}\right) \frac{\partial P(r, t)}{\partial r} \right), \quad (31)$$

where $f(x)$, obeying $f(x) \rightarrow 1$ for $x \rightarrow 0$, is a scaling function whose form for $x \gg 1$ needs to be determined. For our present purposes, we consider next the asymptotic behavior of Eq. (31) by assuming that $P(r, t)$ obeys Eq. (16). In the limit $x \equiv r/t^{1/d_w} \gg 1$, we expect that $f(x) \sim Bx^{\theta_s}$, and determine θ_s so that the resulting $P(r, t)$ is consistent with Eq. (16). To do this, we substitute Eq. (16) into Eq. (31), and make use of the fact that $\partial f(r/t^{1/d_w})/\partial r = \theta_s f(x)/r$. We find,

$$\begin{aligned} - \left(\frac{d_f}{d_w} + \frac{\alpha_\infty}{d_w} \right) + \frac{u}{cd_w} x^u &= x^{-d_w} f(x) (d_f - d_w + \theta_s + \alpha_\infty) \alpha_\infty \\ - x^{u-d_w} f(x) (d_f - d_w + \theta_s + u + 2\alpha_\infty) \frac{u}{c} &+ \frac{u^2}{c^2} x^{2u-d_w} f(x). \end{aligned} \quad (32)$$

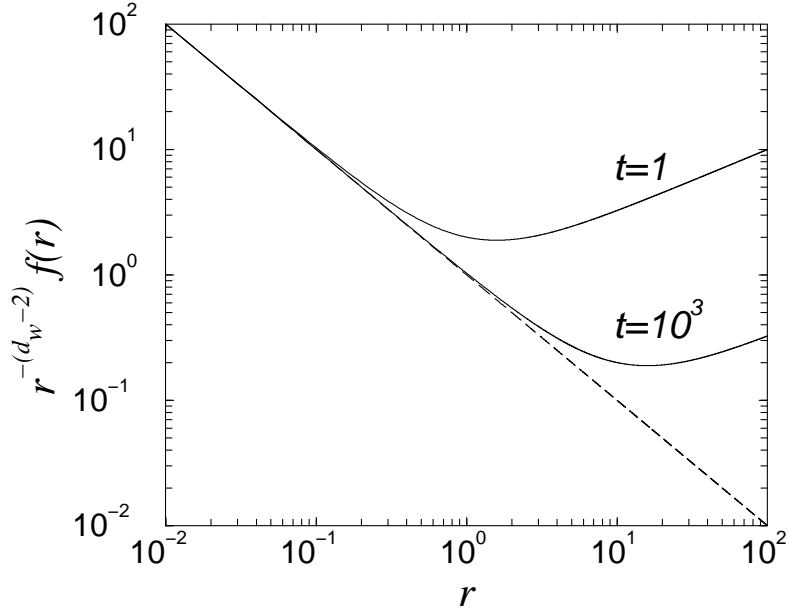


Figure 1: The function $r^{-(d_w-2)}f(r)$ (continuous line) versus r , where the scaling function f has been taken as $f(r) = 1 + (r/t^{1/d_w})^{d_w-u}$, with $B = 1$. We have considered for illustration the cases $t = 1$ (top continuous line) and $t = 10^3$ (bottom continuous line), the unit of length has been taken equal one, and have chosen $d_w = 3$, yielding $u = 3/2$. The dashed line represents the factor $r^{-(d_w-2)}$ corresponding to the standard behavior $f = 1$. Notice that for $t = 1$ only values of $r < 1$ play a role (see discussion in Sec. 1).

To be consistent, f must obey $f(x)x^{u-d_w} \sim B$, i.e.

$$\theta_s = d_w - u,$$

and we obtain,

$$\frac{1}{d_w} = \frac{u}{c}B,$$

which in addition leads to the result $\alpha_\infty = 0$. An illustrative example of a suitable behavior of $f(x)$ is displayed in Fig. 1 for the case $d_w = 3$. Note that the diffusion current, being proportional to $r^{-\theta} f(r/t^{1/d_w}) \partial P(r, t) / \partial r$ (see e.g. [9]), is enhanced at large distances since (in our example) $r^{-\theta} f(r/t^{1/d_w}) \sim r^{1/2}$ for $r > t^{1/d_w}$. This intriguing result remains to be understood, yet the present scheme suggests a formal solution to the problem.

6 Concluding Remarks

We have discussed different forms of the diffusion equation on fractal structures. We have shown that so far two different equations seem to be needed for each of the diffusion regimes $r < R$ and $r > R$, where $R \sim t^{1/d_w}$. The former is well described by a standard type of equation (cf. Eq. (10)),

$$\frac{\partial P(r, t)}{\partial t} = \frac{1}{r^{d_f-1}} \frac{\partial}{\partial r} \left(r^{d_f-1} r^{-\theta} \frac{\partial P(r, t)}{\partial r} \right), \quad r < R, \quad (33)$$

where $\theta = d_w - 2$, while the latter by a more elaborated fractional diffusion equation, which in Laplace domain reads (cf. Eq. (26) with $\theta' = 0$),

$$s^{1/d_w} P(r, s) = -\frac{\partial P(r, s)}{\partial r} - \frac{\kappa}{r} P(r, s), \quad r > R. \quad (34)$$

The problem of how to obtain a single equation which is able to interpolate between these two asymptotic regimes is still open, but a possible solution has been indicated (cf. Eq. (31)). Further theoretical work is needed to clarify this intriguing behavior of diffusion on self-similar structures².

²I dedicate this work to Prof. Francesco Mainardi on occasion of his 60th anniversary. I would like to thank him and the University of Bologna for their warm hospitality during the workshop ‘From Waves to Diffusion and Beyond’, Bologna, 20 December 2002.

References

- [1] A. Einstein, *Annalen der Physik* **17**, 132 (1905); *ibid.* **17**, 549 (1905); *ibid.* **17**, 891 (1905).
- [2] M.V. Smoluchowsky, *Annalen der Physik* **21**, 756 (1906).
- [3] L. Bachelier, *Annales Scientifique École Normale Supérieure* **III-17**, 21 (1900).
- [4] L. Reichl, *A Modern Course in Statistical Physics*, (University of Texas Press, Austin, 1980).
- [5] M. Abramowitz and I.A. Stegun, *Pocketbook of Mathematical Functions*, (Verlag Harri Deutsch, Thun, 1984).
- [6] S. Havlin and D. Ben-Avraham, *Advances in Physics* **36**, 695 (1987).
- [7] B. O'Shaughnessy and I. Procaccia, *Physical Review Letters* **54**, 455 (1985); B. O'Shaughnessy and I. Procaccia, *Physical Review A* **32**, 3073 (1985).
- [8] A. Bunde, S. Havlin and H.E. Roman, *Physical Review A* **42**, R6274 (1990).
- [9] M. Giona and H.E. Roman, *Journal of Physics A: Mathematical and General* **25**, 2093 (1992); M. Giona and H.E. Roman, *Physica A* **185**, 87 (1992).
- [10] H.E. Roman and M. Giona, *Journal of Physics A: Mathematical and General* **25**, 2107 (1992).
- [11] H.E. Roman and P. Alemany, *Journal of Physics A: Mathematical and General* **27**, 3407 (1994).
- [12] H.E. Roman, *Physical Review E* **51**, 5422 (1995).
- [13] S. Havlin and A. Bunde, in *Fractals and Disordered Systems*, 2nd ed., eds. A. Bunde and S. Havlin, (Springer Verlag, Berlin, 1996), p. 97.
- [14] H.E. Roman, *Fractals* **5**, 379 (1997).

- [15] F. Mainardi, in *Fractals and Fractional Calculus in Continuum Mechanics*, eds. A. Carpinteri and F. Mainardi, (Springer Verlag, Wien New York, 1997), p. 291.
- [16] R. Hilfer, *Applications of Fractional Calculus in Physics* (World Scientific, Singapore, 2000)
- [17] S. Havlin D. Ben-Avraham, *Diffusion and Reactions in Fractals and Disordered Systems*, (Cambridge University Press, Cambridge, 2000).
- [18] C. Schulzky, C. Essex, M. Davison, A. Franz and K.H. Hoffmann, *Journal of Physics A: Mathematical and General* **33**, 5501 (2000).
- [19] R. Metzler and J. Klafter, *Physics Reports* **339**, 1 (2000).
- [20] M. Davison, C. Essex, C. Schulzky, A. Franz and K.H. Hoffmann, *Journal of Physics A: Mathematical and General* **34**, L289 (2001).
- [21] C. Essex, M. Davison, C. Schulzky, A. Franz and K.H. Hoffmann, *Journal of Physics A: Mathematical and General* **34**, 8397 (2001).
- [22] I.M. Sokolov, J. Klafter and A. Blumen, *Physics Today* **55**, 48 (2002).
- [23] E. Barkai, *Physical Review* **E 63**, 46118 (2001).

APPENDIX

A Asymptotic Forms

It is instructive to determine the asymptotic behavior of $W(x)$, in both the $x \rightarrow \infty$ and $x \rightarrow 0$ limits, by appropriately studying Eq. (6). In the former case, we assume the asymptotic form $W_d^{(\infty)}(x) \sim x^{-\beta} \exp(-x)$, and substitute it into Eq. (6), yielding

$$\frac{d^2 W_d^{(\infty)}(x)}{dx^2} + \frac{(d-1)}{x} \frac{dW_d^{(\infty)}(x)}{dx} - W_d^{(\infty)}(x) = \frac{W_d^{(\infty)}(x)}{x} [2\beta - (d-1)] + W_d^{(\infty)}(x) \mathcal{O}(x^{-2}). \quad (\text{A1})$$

To leading order, we expect

$$HW_d^{(\infty)}(x) \approx W_d^{(\infty)}(x)/x^2, \quad (\text{A2})$$

where the operator $H = d^2/dx^2 + [(d-1)/x]d/dx - 1$, yielding the condition $2\beta - (d-1) = 0$, i.e.

$$\beta = \frac{1}{2}(d-1) \quad (\text{A3})$$

thus,

$$W_d(x) \sim x^{-(d-1)/2} e^{-x}, \quad x \rightarrow \infty,$$

in agreement with the exact solutions reported for Eq. (6). The limit $x \rightarrow 0$ can be studied by assuming $W_d^{(0)}(x) \sim a + b x^\eta$. Using this form back into Eq. (6) we find,

$$HW_d^{(0)}(x) = b \eta (\eta + d - 2) x^{\eta-2} - (a + b x^\eta + \dots),$$

yielding the condition $\eta + d - 2 = 0$, i.e.

$$\eta = 2 - d, \quad (\text{A4})$$

in agreement with the exact results of Eq. (6). Note that in two dimensions, the result $\eta = 0$ is related to a logarithmic divergence. Indeed, if in this case we assume $W_2^{(0)}(x) \approx -\ln x$, and insert this into Eq. (6), the power law divergent terms x^{-2} cancel out exactly.

B The Inverse Laplace Transform

As an illustration of how Eq. (8) works, we consider the case $d = 3$, where $P(r, s) = r^{-1} \exp(-rs^{1/2})$. Let us consider first the argument of the integral. It reads,

$$P(r, \rho e^{i\pi}) - P(r, \rho e^{-i\pi}) = -\frac{2i}{r} \sin(r\rho^{1/2}),$$

then

$$\begin{aligned} P(r, t) &= \frac{1}{\pi r} \int_0^\infty d\rho e^{-\rho t} \sin(r\rho^{1/2}) \\ &= \frac{2}{\pi r} \int_0^\infty d\rho \rho e^{-\rho^2 t} \sin(r\rho) \\ &= \frac{2}{\pi r} \frac{\sqrt{\pi}}{4t^{3/2}} r e^{-r^2/4t} \end{aligned} \quad (\text{B1})$$

which can be written (cf. Eq. (2) using $\Gamma(3/2) = \sqrt{\pi}/2$) as

$$P(r, t) = \frac{1}{\sqrt{4\pi}} \frac{1}{t^{3/2}} e^{-r^2/4t}.$$

C The Inverse Laplace Transform of the General FDE Eq. (27)

To obtain the expression for $P(r, t)$ corresponding to Eq. (27), we proceed as in Appendix B. We find,

$$P(r, t) = \frac{A_0}{\pi} \frac{1}{r^\kappa} \int_0^\infty d\rho \frac{e^{-\rho t}}{\rho^\varepsilon} \exp[-C \cos(\pi/\gamma)] \sin[\pi\varepsilon + C \sin(\pi/\gamma)] \quad (\text{C1})$$

where

$$C = \frac{\gamma}{d_w} (r\rho^{1/d_w})^{1+\theta'}$$

and

$$\varepsilon = 1 - \left(\frac{d_s}{2} - \frac{\kappa}{d_w} \right) = 1 - \frac{(d_f - \kappa)}{d_w}.$$

Introducing the variable $x = \rho t$, Eq. (C1) becomes

$$\begin{aligned}
P(r, t) = \frac{A_0}{\pi} \frac{1}{t^{d_s/2}} \left(\frac{r}{t^{1/d_w}} \right)^{-\kappa} \int_0^\infty dx x^{-\varepsilon} \\
\exp \left(-x - \frac{\gamma}{d_w} \left(\frac{r}{t^{1/d_w}} \right)^{1+\theta'} x^{1/\gamma} \cos(\pi/\gamma) \right) \\
\sin \left(\pi\varepsilon + \frac{\gamma}{d_w} \left(\frac{r}{t^{1/d_w}} \right)^{1+\theta'} x^{1/\gamma} \sin(\pi/\gamma) \right). \quad (\text{C2})
\end{aligned}$$

Note that a related equation reported in [10] has an error. The correct expression is given by Eq. (C2). We can check this by considering the uniform limit, $d_f = d$, $d_w = 2$, corresponding to $\gamma = 2$ and $\theta' = 0$. In addition, we take $\kappa = (d-1)/2$, to be consistent with Eq. (18) and Eq. (19), yielding $\varepsilon = (3-d)/4$. We obtain,

$$\begin{aligned}
P(r, t) = \frac{A_0}{\pi} \frac{1}{t^{d/2}} \left(\frac{r}{t^{1/2}} \right)^{-(d-1)/2} \int_0^\infty dx x^{-(3-d)/4} \times \\
e^{-x} \sin \left(\frac{\pi}{4}(d+1) - \frac{r}{t^{1/2}} x^{1/2} \right), \quad (\text{C3})
\end{aligned}$$

where

$$A_0^{-1} = \Gamma \left(\frac{d+1}{2} \right).$$

For instance, in the case $d = 1$ Eq. (C3) yields, with $A_0 = 1$,

$$\begin{aligned}
P(r, t) &= \frac{1}{\pi} \frac{1}{t^{1/2}} \int_0^\infty dx x^{-1/2} e^{-x} \cos \left(\frac{r}{t^{1/2}} x^{1/2} \right) \\
&= \frac{2}{\pi} \frac{1}{t^{1/2}} \int_0^\infty dy e^{-y^2} \cos \left(\frac{r}{t^{1/2}} y \right) \\
&= \frac{1}{\sqrt{\pi}} \frac{1}{t^{1/2}} e^{-r^2/4t}. \quad (\text{C4})
\end{aligned}$$

While in $d = 3$, the other exact limit of the theory, Eq. (C3) yields, where again $A_0 = 1$,

$$\begin{aligned}
P(r, t) &= \frac{1}{\pi} \frac{1}{t^{3/2}} \left(\frac{r}{t^{1/2}} \right)^{-1} \int_0^\infty dx e^{-x} \sin \left(\frac{r}{t^{1/2}} x^{1/2} \right) \\
&= \frac{2}{\pi} \frac{1}{t^{3/2}} \left(\frac{r}{t^{1/2}} \right)^{-1} \int_0^\infty dy y e^{-y^2} \sin \left(\frac{r}{t^{1/2}} y \right) \\
&= \frac{1}{\sqrt{4\pi}} \frac{1}{t^{3/2}} e^{-r^2/4t}. \quad (\text{C5})
\end{aligned}$$

D An Attempt to Deal with the Problem of the Origin

There exists a simple remedy to eliminate the divergence near $r \rightarrow 0$ due to the ‘source’ term, $\sim 1/r$, typically occurring within the FDE such as Eq. (26). Let us consider the latter in the case $\theta' = 0$, i.e. $\gamma = d_w$. We suggest the form

$$s^{1/d_w} P(r, s) = -\frac{\partial P(r, s)}{\partial r} - \frac{\kappa s^{1/d_w}}{B + r s^{1/d_w}} P(r, s). \quad (\text{D1})$$

One can take $B(d_w) = \cos(\pi/d_w)$, for instance, so that $B(2) = 0$, and Eq. (D1) reduces to Eq. (19) in the standard case. Now, Eq. (D1) yields,

$$P(r, s) = \frac{A_0}{s^{1-d_s/2}} \frac{1}{(B + r s^{1/d_w})^\kappa} \exp(-r s^{1/d_w}). \quad (\text{D2})$$

This result leads to the same asymptotic form of $P(r, t)$ as in Eq. (16), but in contrast to Eq. (C2) it does not display a divergence when $r \rightarrow 0$. This can be seen from the explicit expression of $P(r, t)$ which can be obtained as in Eq. (C2) as,

$$P(r, t) = \frac{A_0}{\pi} \frac{1}{t^{d_s/2}} \int_0^\infty dx x^{-\varepsilon} Y^{-\kappa}(x) \exp\left(-x - \left(\frac{r}{t^{1/d_w}}\right) x^{1/d_w} \cos(\pi/d_w)\right) \sin\left(\pi\varepsilon + \left(\frac{r}{t^{1/d_w}}\right) x^{1/d_w} \sin(\pi/d_w) + \kappa\Phi\right) \quad (\text{D3})$$

where $\varepsilon = 1 - d_s/2$,

$$Y^2(x) = \left(1 + 2\frac{r}{t^{1/d_w}} x^{1/d_w}\right) \cos^2(\pi/d_w) + \left(\frac{r}{t^{1/d_w}}\right)^2 x^{2/d_w} \quad (\text{D4})$$

and

$$\Phi = \arctan\left[\frac{(r/t^{1/d_w})x^{1/d_w}}{1 + (r/t^{1/d_w})x^{1/d_w}} \tan(\pi/d_w)\right].$$

The result Eq. (D3) is still not satisfactory since, as one can realize by numerically performing the integrations in Eq. (D3), $P(r, t)$ displays in general a non-monotonous behavior for $r/t^{1/d_w} < 1$. In particular, it does not behave as $P(r, t) \sim t^{-d_s/2} (1 - r^{d_w}/d_w^2 t)$ when $r \rightarrow 0$. On the basis of this, and other more complex ansatz that we do not discuss here, we conclude that the FDE can be considered useful only in the asymptotic limit $r/t^{1/d_w} \gg 1$.