Fractional Diffusion Equation in Cylindrical Symmetry: A New Derivation

Mohsen A. Zahran

Theoretical Physics Research Group, Physics Department, Faculty of Science, Mansoura University, P. O. Box 35516, Mansoura, Egypt

Reprint requests to M. A. Z.; E-mail: m.zahran1@mans.edu.eg

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Based on the so-called cylindrical brush structure as a fractal model, we derive the generalized fractional diffusion equation in cylindrical symmetry. Moreover, we derive the fractional calculus and also present the usefulness of fractional ideas in diffusion processes that take place in brush polymer, rheology, and complex systems.

Key words: Fractional Diffusion in Cylindrical Symmetry; Anomalous Diffusion; Brush Structure.

1. Introduction

Diffusion is one of the basic nonequilibrium processes that is of great interest in physicas and many other field. Normal diffusion and its simulation obey Gaussian statistics and can be characterized by mean-square displacement that is asymptotic linear in time, i. e., $< r(t)^2 >\sim t$, where r is the distance the walker has travelled in the time t from the starting point. In many physical systems presented in the literature, however, there is a large number of observations and experiments where this linear time behaviour of the mean-square displacement does not hold. These deviations from linearity are the hallmarks of what is termed anomalous diffusion[1, 2]:

$$\langle r(t)^2 \rangle \sim t^{\gamma}, \quad 0 < \gamma \le 1, \tag{1}$$

where γ is defined as the anomalous diffusion exponent. Diffusion faster than normal, $\gamma > 1$, is called superdiffusion, while it is called subdiffusion when the mean-square displacement grows sublinearly with time, $\gamma < 1$. Examples of these phenomena are numerous, for instance in amorphous semiconductors [3], transport of fluids in porous media [4], two-dimensional rotating flows [5], and diffusion of water in biological tissues [6]. On the basis of the above-mentioned studies, many researchers [1, 2, 7] proposed every kind of forms of anomalous diffusion in disordered fractal media from different points of view. From both physical and mathematical point of view, anomalous processes have posed new questions requiring different descriptions compared to normal diffusion. For example, the standard diffusion paradigm breaks down in the above cases because it rests on restrictive assumptions including locality, Gaussianty, lack of long-rang correlations, and linearity. Also it was realized that anomalous diffusion processes do not belong to the domain of attraction of the central limit theorem but rather to the generalized one which is due to Levy, Gnedenko, Khintchin and Kolmogorov. Anomalous diffusion finds its dynamical origin in nonlocality or memory effect either in space or in time. Also it is, in many cases, related to intermittency, i. e., a phenomenon occuring when the chaotic motion of a trajectory is mixed with regular behaviour. Such behaviour can appear due to the trapping of trajectories near the regular islands in the Hamiltonian case and near the regions containing marginally stable periodic orbits in dissipative systems [8, 9]. There are many powerful methods to study the anomalous diffusion in the presence or the absence of an external velocity or force field such as, continuous time random walk (CTRW) theory [10, 11], fractional Brownian motion [12], generalized master equation [13], and generalized thermostatistics [14]. In particular, the CTRW theory has become a standard tool to model diffusion in anomalous dynamical systems, i. e., diffusion is modeled by a sequences of jumps interrupted by periods of waiting. However, one may remark that it is not straightforward to incorporate force fields and boundary conditions in this formalism.

An alternative approach to processes which display strange kinetics is based on the fractional equations, i. e., differential fractional operators have been intro-

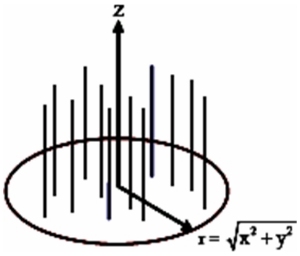

Fig. 1. The brush structure.

duced to replace either the time derivative or the occurring spatial derivatives, or both. It is interesting to note that the fractional equations are suitable for handling external fields and for considering boundary value problems. Also, in many cases, it is possible to map the CTRW formalism to the fractional equations. In previous works [14 – 16], we deduced the fractional Fokker-Planck equation (FFPE) using the comb-like structure as a background model. Moreover, the time fractional diffusion equation which describes the diffusion process through fractal media has been extensively studied [17]. However, the time fractional diffusion in two and three spatial dimensions has not received much attention. Metzler et al. [18] have proposed a generalized diffusion equation composed of an extended Laplacian operator and a fractal time derivative. The solution of their equation has been achieved exactly in terms of the H-function. Recently, some authors [19, 20] have suggested and solved the fractional diffusion equation in cylindrical symmetry (FDECS)

$$p(r,t) = {}_0D_t^{-\gamma}\left(\frac{1}{r}\frac{\partial}{\partial r}rD(r)\frac{\partial}{\partial r}\right)p(r,t), \tag{2}$$

where $p(r,t)$ is the probability density, ${}_0D_t^{-\gamma}$ is the fractional Riemann-Liouville differential operator with order $0 < \gamma < 1$ [17]. Remarkably, the advantage of the Riemann-Liouville operator lies in the straightforward way of including long-range memory effects which are typically found in complex systems. The solution of (2) with the isotropic fractional diffusion equation and constant diffusion coefficient has been obtained in [19]. The solution of (2) subjected to an instantaneous point source has been illustrated via symmetry group in [20]. However to our knowledge, there is no available derivation of (2). This issue is the task of the present work, in other words, the scope of the present paper is restricted to develop an analytical derivation of the FDECS by means of arguments inspired by the brush polymer structure of Cassi and Regina [21]. In this proposed model, the base of the structure is two-dimensional, i. e., $r = \sqrt{x^2+y^2}$ which is the random walk particle diffusive. The trapping process occurs only along the z-direction. The paper is organized as follows: In Section 2, we try to derive the generalized fractional diffusion equation. Section 3 is devoted to the solution of the resulting equation. Some remarks will be given in the final section.

2. The FDECS and the Cylindrical Comb-Like Model

As it is well known, random walks on discrete structure give us a powerful and simple model to understand the microscopical origin of anomalous diffusion. Thus motivated by the brush structure depicted in Fig. 1, one can derive the FDECS. Let us consider the r-component of the current density along the base of the structure

$$J_r = -\delta(z)D(r)\frac{\partial}{\partial r}p(r,z,t), \tag{3}$$

where $D(r)$ is the diffusion coefficient along the backbone and $\delta(z)$ is the delta function, while the z-component of the current along the height of the structure is

$$J_z = -D_0\frac{\partial}{\partial z}p(r,z,t). \tag{4}$$

D_0 along the z-direction is assumed to be constant. From the continuity equation

$$\frac{\partial}{\partial t}p(r,z,t) = -\nabla_{r,z}\cdot J(r,z,t) \tag{5}$$

one gets

$$\begin{aligned}&\frac{\partial}{\partial t}p(r,z,t) = \\ &\left(\delta(z)\frac{1}{r}\frac{\partial}{\partial r}D(r)r\frac{\partial}{\partial r} + D_0\frac{\partial^2}{\partial z^2}\right)p(r,z,t),\end{aligned} \tag{6}$$

which can be rearranged to become the well-known diffusion equation

$$\begin{aligned}&\left[\frac{\partial}{\partial t} - D_0\frac{\partial^2}{\partial z^2}\right]p(r,z,t) = \\ &\delta(z)\left(\frac{1}{r}\frac{\partial}{\partial r}D(r)r\frac{\partial}{\partial r}p(r,z,t)\right).\end{aligned} \tag{7}$$

Therefore, the Green function associated with the homogenous part of (7) and subject to the initial condition $G(z,0) = \delta(z)$ has the following form:

$$G(z,t) = \frac{1}{\sqrt{4\pi D_0 t}}\exp\left(\frac{-z^2}{4D_0 t}\right). \tag{8}$$

One can now obtain the general solution of (7) upon integration over the source term as

$$p(r,z,t) = \int \mathrm{d}t'\mathrm{d}z' G(z-z',t-t')\delta(z) \cdot \left(\frac{1}{r}\frac{\partial}{\partial r}D(r)r\frac{\partial}{\partial r}p(r,z',t')\right). \tag{9}$$

Inserting (8) into (9) and integrating over z' leads to

$$p(r,t) = \frac{\Gamma\left(\frac{1}{2}\right)}{\sqrt{\pi D_0}}\,{}_0D_t^{-1/2}\left(\frac{1}{r}\frac{\partial}{\partial r}D(r)r\frac{\partial}{\partial r}p(r,t)\right), \tag{10}$$

where

$${}_0D_t^{-1/2}p(r,t) = \int_0^t \frac{1}{\Gamma(\gamma)}\frac{p(r,t')}{(t-t')^{1/2}}\mathrm{d}t' \tag{11}$$

is the Riemann-Liouville (R-L) fractional integral operator. Here, it is obvious that the $\frac{1}{2}$-order fractional integration arises due to the trapping of the random walk particle along the z-direction. Also, (10) is linear but nonlocal in time, i. e., $p(r,t)$ at time t depends on the previous history of integration over $t' < t$. In other words, the causality of (10) came from the dependency on past times only. It is worth to mention that, in the case of no trapping along the z-direction, (10) is equivalent to the well-known Richardson's equation for turbulent diffusion for the corresponding choice of $D'(r)$.

3. Solution of the FDECS

Remarkably, (10) is an example for a broader class of fractional differential equations such as

$$\frac{\partial^\gamma}{\partial t^\gamma}p(r,t) = \frac{1}{r}\frac{\partial}{\partial r}D'(r)r\frac{\partial}{\partial r}\,p(r,t) + \frac{p(r,0)t^{-\gamma}}{\Gamma(1-\gamma)}, \tag{12}$$

whose solution will be discussed in the present section. For simple case, let us assume that the diffusion coefficient $D'(r)$ in (12) is constant, say D, and there is no geometrical trapping process ($\gamma = 1$). Thus (12) subject to delt initial condition $p(r,o)$ and zero mean admits the classical result of spatial distribution:

$$p(r,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(\frac{-r^2}{4Dt}\right). \tag{13}$$

On the other hand, for the case of diffusion in fractals addressed before in [22], the diffusion cofficient has spatial dependency, i. e. $D(r) = r^{-\theta}$ and normal integer time evolution operator ($\gamma = 1$); then (12) reduces to

$$\frac{\partial}{\partial t}p(r,t) = \frac{1}{r}\frac{\partial}{\partial r}r^{1-\theta}\frac{\partial}{\partial r}p(r,t), \tag{14}$$

and the corresponding solution of (13) becomes

$$p(r,t) \sim t^{-(\theta+1)}\exp\left(\frac{-r^{2+\theta}}{4t}\right). \tag{15}$$

Recently, (12) was considered in [19] associated with the following boundary conditions:

$$\begin{aligned} p(r,0) &= 0 \;\text{ for }\; r < R, \\ p(R,0) = p(R,t) &= C_0, \quad C_0 = \text{Const.}, \\ p(r,0) &= C_0\,H(r-R), \end{aligned} \tag{16}$$

which may be appropriate for the inward diffusion in a cylinder of radius R and unit length. Here $H(r-R)$ is the unit step function. The solution has been achieved via Laplace-Finite Hankal transforms of order zero. More recently, (12) has been studied in [20] and was associated with an instantaneous point source in disordered fractal media. Based on the symmetry group of scaling transformation and the properties of the H-function, the analytical solutions of the concentration distribution are given in [20].

4. Conclusion

It is well known that anomalous diffusion is often associated with a variety of frequency power law scaling phenomena, mostly involved with a nonconserving number of random walks. This model describes physical systems where trapping occurs. To simulate such kind of diffusion process two steps are necessary. First the disordered media or the materials in question have to be modeled, and then the diffusion process itself has to be simulated. In mathematical physics, it is often convenient to have a deterministic equation for the probability distribution of the process, an analogue of the diffusion or Fokker-Planck equations, to be solved under given initial and boundary conditions. For the case of anomalous transport, fractional generalization of such equations may be relevant. Many authors replace the integer time or space derivatives by fractional counterparts on a purely or heuristic basis. However, in the present work and by assuming a cylindrical brush model, in which the random walker diffusive is along the plane $r = \sqrt{x^2+y^2}$ and the trapping processes may occur in z-direction, one can derive the fractional diffusion equation in cylindrical symmetry. This equation would have an integro-differential form instead of first-order derivative with respect to the time equation containing a derivative of fractional order γ. The diffusion along r represents a fractal time process which exhibits an anomalous mean-square displacement of form $\langle r(t)^2 \rangle \sim t^\gamma$, while the diffusion along the z-direction is given by normal mean-square displacement $\langle z(t)^2 \rangle \sim t$. The main point here is the direct connection between the fractional integral operator and the random disappearances or trapping along the fingers of the structure. Also, in this approach, one can easily and straightforward incorporate force fields and boundary conditions into the problems under consideration. There is no doubt that the model presented is a simplified example rather than models of real physical situation. However, we hope that this example helps to clarify general ideas that underlay possible physical applications of fractional time derivatives.

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