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Beyond monofractional kinetics

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ABSTRACT

We discuss generalized integro-differential diffusion equations whose integral kernels are not of a simple power law form, and thus these equations themselves do not belong to the family of fractional diffusion equations exhibiting a monoscaling behavior. They instead generate a broad class of anomalous nonscaling patterns, which correspond either to crossovers between different power laws, or to a non-power-law behavior as exemplified by the logarithmic growth of the width of the distribution. We consider normal and modified forms of these generalized diffusion equations and provide a brief discussion of three generic types of integral kernels for each form, namely, distributed order, truncated power law and truncated distributed order kernels. For each of the cases considered we prove the non-negativity of the solution of the corresponding generalized diffusion equation and calculate the mean squared displacement.

1. Introduction

Fractional differential equations and their generalizations have attracted much attention in the scientific community for the description of anomalous diffusion and relaxation processes in complex environments [35]. The famed power-law dependence $\langle x^2(t)\rangle \simeq t^\alpha$ of the mean squared displacement (MSD) on time can be captured by fractional diffusion equations with fractional time and/or space derivatives instead of integer order ones. Depending on the anomalous diffusion exponent we distinguish subdiffusion for $0 < \alpha < 1$, normal diffusion for $\alpha = 1$, and superdiffusion for $\alpha > 1$. The case with $\alpha = 2$ corresponds to ballistic motion. Such deviations of the MSD from the linear time dependence are observed in different phenomena, such as subdiffusion of charge carrier motion in amorphous semiconductors [48], anomalous diffusion in biological cells [34,36], anomalous diffusion dynamics in the Earth surface and subsurface hydrology [47,50], superdiffusion in weakly chaotic systems [56], turbulence [39], sound wave propagation in conducting media [59], as well as random search processes [24], to name but a few.

The continuous time random walk (CTRW) model of Scher and Montroll [48] is one of the most popular stochastic models yielding anomalous diffusion for either a long-tailed waiting time probability distribution function (PDF) or a long-tailed jump length PDF. The corresponding time and space fractional diffusion equations can be obtained from the master equation of the CTRW in the diffusion limit [1,33,35,54,55].

In what follows we will be dealing with time fractional operators, only. The time fractional diffusion equation can be either in normal form, that is, the fractional derivative in the Caputo sense stands on the left hand side in the equation, or in its equivalent modified form, where the fractional derivative in the Riemann–Liouville sense stands on the right hand side of the equation. These two forms are equivalent and describe a monofractal or self affine process [53]. However, many natural systems do not exhibit a monoscaling behavior. As important examples of such nonscaling situations we can refer to truncated Lévy flights in the superdiffusive case [28], and to Sinai-like superslow diffusion in the subdiffusive case [15]. The distributed order fractional diffusion equations suggested first in [7] allow one to go beyond the "simple" fractional kinetics. The distributed order derivative introduced originally by Caputo for ordinary differential equations [3–5] is nothing else but a linear operator defined as a weighted sum of different fractional derivatives or an integral of such over their order. Distributed order diffusion equations can be also represented in two

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different forms, referred to as natural and modified forms, which are not equivalent [53]. The cases with different weighting functions, their physical meaning, the corresponding CTRW models and various techniques for finding the solutions have been discussed in a range of works [7–11,17,25–27,29,31,32,43]. We also note that such equations find more and more interest among mathematicians who proved rigorously several results obtained previously in physics literature, and developed the corresponding formalism [18–20,61,62].

In the present paper we consider generalized integrodifferential diffusion equations in normal and modified forms. In the natural form an integrodifferential operator acting on the temporal variable of the probability density function substitutes the first time derivative of the ordinary diffusion equation. The modified form of the equation inherits the first time derivative of the diffusion equation, but contains an additional operator acting on the temporal variable of the right hand side. We note that this last form is essentially a standard form of (the continuous limit of) the generalized master equation as appearing in the Nakajima–Zwanzig formalism [40]. We demonstrate that the distributed order diffusion equations are their particular cases corresponding to certain forms of the integral kernels. We further consider another generic case of the kernels, namely, truncated power law and truncated double power law kernels, a particular case of the truncated distributed order kernel. For all these cases we prove the positivity of the solutions of the corresponding generalized diffusion equations by employing the properties of completely monotone and Bernstein functions. Moreover, we calculate the MSD for all cases showing different nonscaling behavior. We note that generalized diffusion equations in normal form were introduced in [42], and similar equations with memory kernels have been suggested in different contexts, such as fractional diffusion and generalized Langevin equations [60], tempered diffusion processes [22,58], generalized Langevin equation with tempered memory kernel [23], as well as in comb-like models for slow and ultraslow diffusion [44].

This paper is organized as follows. In Section 2 we consider generalized distributed order diffusion equations in the normal form, based on the three particular cases mentioned above. The generalized diffusion equation in the modified form, together with the corresponding particular cases is introduced in Section 3. In Section 4 we briefly discuss the generalized wave equation. A summary is provided in Section 5. For the convenience of the reader, in Appendix A we present a list of properties of the completely monotone and Bernstein functions.

2. Generalized diffusion equations in normal form

The generalized diffusion equation in the normal form contains the memory kernel on the left hand side [42],

$$\int_0^t \gamma(t-t')\frac{\partial}{\partial t'}W(x,t')dt' = \frac{\partial^2}{\partial x^2}W(x,t), \tag{1}$$

where $\gamma(t)$ is a non-negative and integrable function. In what follows we will formulate the restrictions on the memory kernel which ensure the non-negativity of the solution of Eq. (1). Throughout the paper we put all dimensional constants equal to 1 for brevity. The physical dimensions of the equations can be easily restored. Here and in what follows the initial condition is assumed to be of the form $W_0(x) = \delta(x)$ without loss of generality.

Note that the generalized diffusion Eq. (1) contains as special cases the standard diffusion equation if we take $\gamma(t) = \delta(t)$, as well as the time fractional diffusion equation in the Caputo form for $\gamma(t) = t^{-\lambda}/\Gamma(1-\lambda)$, $0 < \lambda < 1$, i.e.

$${}_CD_t^{\lambda}W(x,t) = \frac{\partial^2}{\partial x^2}W(x,t), \tag{2}$$

where ${}_CD_t^{\lambda}$ is the Caputo fractional derivative of order λ [37]

$${}_CD_t^{\lambda}f(t) = \frac{1}{\Gamma(1-\lambda)}\int_0^t (t-t')^{-\lambda}\frac{d}{dt'}f(t')dt'. \tag{3}$$

Returning to Eq. (1) and applying the Fourier- and Laplace-transforms[1] in succession one finds the solution in (k, s)-space,

$$W(k,s) = \frac{\hat{\gamma}(s)}{s\hat{\gamma}(s)+k^2}. \tag{4}$$

From here we conclude that the solution is normalized since

$$[W(k,s)]|_{k=0} = \frac{1}{s}. \tag{5}$$

Throughout the paper we will use the subordination approach in order to verify positivity (non-negativity) of the solution of the generalized diffusion equations considered. From Eq. (4) we have

$$W(k,s) = \gamma(s)\int_0^\infty e^{-u\left(s\gamma(s)+k^2\right)}du = \int_0^\infty e^{-uk^2}G(u,s)du, \tag{6}$$

where the function G is given by

$$G(u,s) = \gamma(s)e^{-us\gamma(s)}. \tag{7}$$

Thus, the PDF $W(x, t)$ is given by Meerschaert et al. [29,30]

$$W(x,t) = \int_0^\infty \frac{e^{-\frac{x^2}{4u}}}{\sqrt{4\pi u}}G(u,t)du. \tag{8}$$

The function $G(u, t)$ is the PDF providing the subordination transformation, from time scale t to time scale u. Indeed, at first we note that $G(u, t)$ is normalized with respect to u for any t. From Eq. (7) we find

$$\int_0^\infty G(u,t)\,du = \mathcal{L}_s^{-1}\left[\int_0^\infty \gamma(s)e^{-us\gamma(s)}\,du\right] = \mathcal{L}_s^{-1}\left[\frac{1}{s}\right] = 1. \tag{9}$$

Now, to prove the positivity of $G(u, t)$ it is sufficient to show that its Laplace transform $G(u, s)$ is completely monotone on the positive real axis s. For that we need to show that

(i) the function $\gamma(s)$ is completely monotone, and
(ii) the function $s\gamma(s)$ is a Bernstein function.

If (ii) holds, it follows from Property (5), Appendix A, that the function $e^{-s\gamma(s)}$ is completely monotone since the exponential function is completely monotone and the composition of a completely monotone and a Bernstein function is itself completely monotone. Therefore, $G(u, s)$ will be completely monotone, as a product of two completely monotone functions $e^{-s\gamma(s)}$ and $\gamma(s)$, see Property (1) from Appendix A. In what follows in Section 2 we consider three generic forms of the memory kernel $\gamma(t)$, prove the positivity of the solutions of the corresponding generalized diffusion equations in the normal form and discuss the nonmonoscaling behaviors of the MSDs for each case.

2.1. Distributed order memory kernel

The distributed order fractional diffusion equation in the normal form, which was introduced in [7], is a particular form of the generalized diffusion Eq. (1). Indeed, let us take the memory kernel $\gamma(t)$ as

$$\gamma(t) = \int_0^1 p(\lambda)\frac{t^{-\lambda}}{\Gamma(1-\lambda)}d\lambda, \tag{10}$$

[1] The Laplace transform of a given function $f(t)$ is defined by $f(s) = \mathcal{L}[f(t)] = \int_0^\infty e^{-st}f(t)dt$. The Fourier transform of $f(x)$ is given by $f(k) = \mathcal{F}[f(x)] = \int_{-\infty}^{\infty} f(x)e^{\imath kx}dx$. Therefore, the inverse Fourier transform is defined by $f(x) = \mathcal{F}^{-1}[f(k)] = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(k)e^{-\imath kx}dk$.