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LETTER TO THE EDITOR

Fractional diffusion in inhomogeneous media

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Abstract
Starting from the continuous time random walk (CTRW) scheme with the space-dependent waiting-time probability density function (PDF) we obtain the time-fractional diffusion equation with varying in space fractional order of time derivative. As an example, we study the evolution of a composite system consisting of two separate regions with different subdiffusion exponents and demonstrate the effects of non-trivial drift and subdiffusion whose laws are changed in the course of time.

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1. Recently, kinetic equations with partial fractional derivatives were recognized as a useful tool for the description of anomalous diffusion and relaxation phenomena. Examples include systems exhibiting Hamiltonian chaos, disordered medium, underground water pollution, dynamics of protein molecules, motions under the influence of optical tweezers, reactions in complex systems and more, see reviews on fractional kinetics [1–8] and references therein. In particular, the kinetic equation with time-fractional derivative is used for the description of subdiffusion processes, i.e., those for which the mean-squared displacement (MSD) grows in time slower than linearly [2]. Also, it describes slow relaxation processes which are characterized by stretched exponential or power-law response function [4]. Up to now, only the simplest forms of fractional kinetic equations have been considered. On the other hand, it became clear that further theoretical investigations are required in order to incorporate adequate tools for the description of more complicated (and more realistic) random processes, which are described by a set of characteristic exponents, and are therefore of multi-fractional type. Such processes are believed to provide useful models for a host of non-homogeneous and non-stationary processes, thus generalizing more simple fractal processes and exhibiting fractional order behaviour that may vary with time, space and/or control parameters [9]. An adequate kinetic description of these processes requires the use of generalized fractional kinetics based on the concept of *variable order fractional operators*. This calculus was proposed in [10, 11] and very recently was introduced in engineering [12] and in physics [13]. In the present letter we introduce a new type of fractional diffusion equation, namely, the time-fractional diffusion equation with time-fractional derivative whose order depends on space, and we demonstrate by taking a particular example, the non-trivial drift and diffusion properties of such systems.

2. The time-fractional diffusion equation follows as continuous limit from a corresponding generalized master equation for continuous time random walk (CTRW). To obtain a valid form of time-fractional diffusion equation for an inhomogeneous medium, let us first consider an elementary derivation of the generalized master equation, as a balance equation between gain and loss of particles. Although several derivations of such an equation are available [14–17], we give here a heuristic derivation which is especially suited for the situation at hand. In what follows we concentrate on a one-dimensional situation. Generalization to higher dimensions is obvious.

The generalized master equation follows from the two balance conditions guaranteeing the probability conservation: a local one (giving the balance between the probability gain and loss at one site) and the one for transitions between the two sites (representing the continuity). In a non-biased CTRW a particle arriving to a site i at some time t stays there for a sojourn time τ, given by the probability density function (PDF) $\psi_i(\tau)$. The probability for a particle which arrived at the site at time t' to leave it at time between $t > t'$ and $t + \mathrm{d}t$ is given by $\psi_i(t - t')\,\mathrm{d}t$. Leaving a site, it makes a random step in either direction with probability 1/2. A balance equation at each site reads

$$\frac{\mathrm{d}}{\mathrm{d}t} p_i(t) = J_i^+(t) - J_i^-(t), \tag{1}$$

where $J_i^\pm$ are gain and loss fluxes for the site i. Moreover, the particle arriving at the site i at time t' arrives either from the left or from the right. Probability conservation for transitions between sites for a non-biased CTRW then reads

$$J_i^+(t) = \tfrac{1}{2} J_{i-1}^-(t) + \tfrac{1}{2} J_{i+1}^-(t), \tag{2}$$

which allows us to express the balance equation on a site through the loss fluxes only:

$$\frac{\mathrm{d}}{\mathrm{d}t} p_i(t) = \frac{1}{2} J_{i-1}^-(t) + \frac{1}{2} J_{i+1}^-(t) - J_i^-(t). \tag{3}$$

A generalized master equation is a combination of this continuity equation and the equation for $J_i^-(t)$ following from the assumption about the distribution of sojourn times: the particles leaving site i at some time t either were at i from the very beginning (from time $t = 0$) or arrived at i later, at some time $0 < t' < t$:

$$J_i^-(t) = \psi_i(t) p_i(0) + \int_0^t \psi_i(t - t') J_i^+(t')\,\mathrm{d}t'. \tag{4}$$

This equation can be easily solved when noting that $J_i^+(t) = \dot{p}_i(t) + J_i^-(t)$, so that

$$J_i^-(t) = \psi_i(t) p_i(0) + \int_0^t \psi_i(t - t') \left[\frac{\mathrm{d}}{\mathrm{d}t'} p_i(t') + J_i^-(t') \right] \mathrm{d}t', \tag{5}$$

which expresses the loss flux at a site through the probability $p_i(t)$. This integral equation is easily solved via Laplace transformation,

$$\tilde{J}_i^-(s) = \frac{s\tilde{\psi}_i(s)}{1 - \tilde{\psi}_i(s)} \tilde{p}_i(s) \equiv \tilde{\Phi}_i(s) \tilde{p}_i(s), \tag{6}$$

where '$\sim$' denotes the Laplace transform, or, in the time domain,

$$J_i^-(t) = \int_0^t \Phi_i(t-t')p_i(t')\,\mathrm{d}t' \tag{7}$$

with $\Phi_i(t)$ as the inverse Laplace transform of $\tilde{\Phi}_i(s) = s\frac{\tilde{\psi}_i(s)}{1-\tilde{\psi}_i(s)}$. We note that this last equation can be rewritten in the following form having better analytical properties: since the multiplication by s in Laplace space corresponds to taking a time derivative in the time domain, we can put down

$$J_i^-(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t M_i(t-t')p_i(t')\,\mathrm{d}t' \tag{8}$$

with $M_i(t)$ being the inverse Laplace transform of $\tilde{M}_i(s) = \tilde{\psi}_i(s)/(1-\tilde{\psi}_i(s))$. Inserting this last equation into the balance equation (3), one obtains

$$\dot{p}_i(t) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t M_{i-1}(t-t')p_{i-1}(t')\,\mathrm{d}t' + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t M_{i+1}(t-t')p_{i+1}(t')\,\mathrm{d}t' - \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t M_i(t-t')p_i(t')\,\mathrm{d}t'. \tag{9}$$

Assuming that the dependence on i is slow, we can change from a difference to a differential equation. With the lattice constant a and $M_i(t) = M(t,x)$ we get

$$\frac{\partial}{\partial t}p(x,t) = a^2\frac{\partial^2}{\partial x^2}\frac{\partial}{\partial t}\int_0^t M(x,t-t')p(x,t')\,\mathrm{d}t'. \tag{10}$$

For waiting-time distributions being power laws, $\psi_i(t) \cong t^{-1-\beta_i}$, $t\to\infty$, one gets $M(x,t) \propto t^{-1+\beta(x)}$, and the integral operator is the kernel of a Riemann–Liouville derivative of *variable order*,

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial^2}{\partial x^2}\big(K(x)D_t^{1-\beta(x)}p(x,t)\big), \qquad p(x,0) = \delta(x), \tag{11}$$

where

$$D_t^{\mu(x)}p(x,t) \equiv \frac{1}{\Gamma(1-\mu(x))}\frac{\partial}{\partial t}\int_0^t \mathrm{d}\tau\,\frac{p(x,\tau)}{(t-\tau)^{\mu(x)}} \tag{12}$$

is the generalization of the Riemann–Liouville derivative of order μ, $0<\mu\leqslant 1$, which has a Laplace transform,

$$L\big\{D_t^{\mu}p(x,t)\big\} = s^{\mu}\tilde{p}(x,s), \tag{13}$$

and K is a positive function of x, which has a meaning of a diffusion coefficient. Here, the order of differentiation is important: first, the position-dependent time-fractional derivative operator acts on the PDF, and then the second space derivative acts.

3. Performing the Laplace transformation of equation (11) and introducing a new function $\tilde{g}(x,s) = K(x)s^{-\beta(x)}\tilde{p}(x,s)$ we get

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\tilde{g}(x,s) - \frac{s^{\beta(x)}}{K(x)}\tilde{g}(x,s) = -\frac{\delta(x)}{s}. \tag{14}$$

This equation is solved with the use of the boundary conditions at infinity, $\tilde{g}(x=\pm\infty,s)=0$, and matching conditions at $x=0$, see below. We present here a simple particular case which allows us to demonstrate non-trivial properties of the solutions of time-fractional diffusion equation with space-dependent time-fractional derivative. Namely, we consider a composite system consisting of two separated regions characterized by different constant diffusion exponents and diffusion coefficients:

$$\beta(x) = \begin{cases} \beta_+, & x > 0 \\ \beta_-, & x < 0, \end{cases} \qquad K(x) = \begin{cases} K_+, & x > 0 \\ K_-, & x < 0. \end{cases} \tag{15}$$

We assume without loss of generality that $\beta_+ > \beta_-$. Then, equation (14) is easily solved separately on the right and left semi-axes, giving

$$\tilde{g}_\pm(x,s) = C_\pm(s)\exp\left(-\frac{|x|s^{\nu_\pm}}{\sqrt{K_\pm}}\right), \qquad \nu_\pm = \frac{\beta_\pm}{2} \tag{16}$$

for $x > 0$ and $x < 0$, respectively. Here, the boundary conditions at infinity have been already used. The first matching condition at $x = 0$ stems from continuity of the PDF, $\tilde{p}(0^+, s) = \tilde{p}(0^-, s)$, which gives

$$\frac{s^{2\nu_+}}{K_+}C_+(s) - \frac{s^{2\nu-}}{K_-}C_-(s) = 0, \tag{17}$$

and the second is obtained after integration equation (14) around $x = 0$,

$$\frac{s^{\nu_+}}{\sqrt{K_+}}C_+(s) - \frac{s^{\nu_-}}{\sqrt{K_-}}C_-(s) = \frac{1}{s}. \tag{18}$$

Equations (17) and (18) allow us to obtain the coefficients $C_\pm(s)$, and instead of equation (16) we get

$$\tilde{p}_\pm(x,s) = \frac{\exp\left(-\frac{|x|s^{\nu_\pm}}{\sqrt{K_\pm}}\right)}{s\left(\sqrt{K_+}s^{-\nu_+} + \sqrt{K_-}s^{-\nu_-}\right)}. \tag{19}$$

Note that the normalization condition, $\int_{-\infty}^{0}\tilde{p}_-(x,s)\,\mathrm{d}x + \int_0^\infty \tilde{p}_+(x,s)\,\mathrm{d}x = s^{-1}$ is fulfilled. Further, the functions $\tilde{p}_\pm(x,s)$ are completely monotonic with respect to s, which can be proved with the use of criteria of complete monotonicity [18], and thus, equation (19), indeed represents the PDF. Now to get the first and the second moments of the PDF, describing drift and diffusion properties respectively, we first obtain their Laplace transforms using equation (19) and then take an inverse Laplace transformation. For the drift, we get

$$\langle x(t)\rangle = \left(\frac{\sqrt{K_+}t^{\nu_+}}{\Gamma(1+\nu_+)} - \frac{\sqrt{K_-}t^{\nu_-}}{\Gamma(1+\nu_-)}\right), \tag{20}$$

whereas for the variance we obtain

$$\mathrm{Var}\{x\} = \langle x^2(t)\rangle - \langle x(t)\rangle^2 = A_+K_+t^{\beta_+} + A\sqrt{K_+K_-}t^{(\beta_++\beta_-)/2} + A_-K_-t^{\beta_-} \tag{21}$$

with

$$\begin{aligned} A_\pm &= \frac{2}{\Gamma(1+\beta_\pm)} - \frac{1}{[\Gamma(1+\beta_\pm/2)]^2}, \\ A &= \frac{2}{\Gamma(1+\beta_+/2)\Gamma(1+\beta_-/2)} - \frac{2}{\Gamma(1+(\beta_++\beta_-)/2)}. \end{aligned} \tag{22}$$

It follows from equations (20)–(22) that the PDF initially concentrated at $x = 0$ evolves as follows: at small times the centre of the PDF shifts to the negative direction, that is, towards the side of smaller β, that is, β_- in our case, and the mean displacement grows as $t^{\beta_-/2}$.

At the same time the PDF spreads and the variance growth is proportional to t^{β_-}. At a critical time instant defined as

$$t_{\mathrm{cr}} = \left[\sqrt{\frac{K_-}{K_+}}\frac{\Gamma(1+\beta_+/2)}{\Gamma(1+\beta_-/2)}\right]^{2/(\beta_+-\beta_-)}, \tag{23}$$

the mean value $\langle x(t)\rangle$ of the PDF stops moving and then at $t > t_{\mathrm{cr}}$ accelerates to the positive side of greater β, that is, β_+ in our case. The mean displacement grows as $t^{\beta_+/2}$, and the mean-squared displacement at large times evolves as t^{β_+}.

Now, we turn to the analysis of the PDF, see equation (19). Recalling the Laplace-transform pairs,

$$\exp(-s^{\nu})/l_{\nu}(t), \qquad 0 < \nu < 1 \tag{24}$$

and

$$\frac{s^{\mu-\sigma}}{s^{\mu}+\lambda}\bigg/ t^{\sigma-1}E_{\mu,\sigma}(-\lambda t^{\mu}), \qquad \lambda, \mu, \sigma > 0, \tag{25}$$

where $l_\nu(t)$ is the extremely asymmetric Lévy stable PDF with the Lévy index ν [18], and $E_{\mu,\sigma}(z)$ is the generalized Mittag–Leffler function [19], we present the PDF in the convolution form as

$$p_{\pm}(x,t) = \int_0^t \mathrm{d}\tau\, \frac{1}{\zeta^{1/\nu_\pm}} l_\nu\left(\frac{\tau}{\zeta^{1/\nu_\pm}}\right)\frac{(t-\tau)^{-\nu_-}}{\sqrt{K_-}}E_{\nu_+-\nu_-,1-\nu_-}\left(-\sqrt{\frac{K_+}{K_-}}(t-\tau)^{\nu_+-\nu_-}\right) \tag{26}$$

where $\zeta = (\sqrt{K_\pm}/|x|)^{1/\nu_\pm}$, the sign '−' corresponds to the negative semi-axis and the sign and '+' to the positive semi-axis, respectively. Note that $\zeta^{-1/\nu}l(\tau/\zeta^{1/\nu}) = \delta(\tau)$ at $x = 0$, so that equation (26) delivers the same result as can be obtained from equation (19) by setting $x = 0$ and then carrying out an inverse Laplace transform.

We also note that the particular case of the system considered here, namely, the case of the composite normal—subdiffusive system with $\beta_+ = 1$ was considered in the papers [20, 21]. The results obtained there for the drift and the variance at large times correspond to the particular cases of the limits given by equations (20) and (21) at large t, respectively, if one put $\beta_+ = 1$.

4. In summary, based on the CTRW approach for the spatially inhomogeneous system with the power-law waiting-time PDF whose exponent varies in space we obtain the time-fractional diffusion equation with varying in space order of the time derivative of the Riemann–Liouville form in the right-hand side of the equation. For this equation, the order in which derivatives act is important, namely, first the time derivative acts on the PDF and then the second space derivative acts. By taking a simple example of a composite medium consisting of two semi-infinite subdiffusive systems with different subdiffusion exponents, we demonstrate the appearance of the drift which at small times is in the direction of the region with smaller diffusion exponent and at large times is in the direction of larger diffusion exponent. We also show the change of the time dependence for drift and diffusion spreading in the course of time.

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