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Behavior of fractional diffusion at the origin

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The present work discusses the fractional diffusion equation based on the Riemann-Liouville fractional time derivatives. It was shown that the normalization conservation constraint leads to the divergency of diffusive agent concentration at the origin. This divergency implies an external source of the diffusive agent at $r\rightarrow 0$. Thus, the Riemann-Liouville fractional time derivative implies a loss of diffusive agent mass, which is compensated for by the source of this agent at the origin. In contrast, the absence of the normalization conservation constraint does not lead to any divergences in the limit $r\rightarrow 0$ and at the same time provides the decay of normalization.

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Today, anomalous diffusion transport is a widely acknowledged phenomenon [1–4]. It is detected by a variety of experimental techniques in different physical systems. Examples of this phenomenon are numerous. It occurs in amorphous semiconductors [5,6], polymers [7–9], composite heterogeneous films [10], porous media [11,12], and many other systems (for references see a recent review [4]). The distinguishing feature of anomalous transport is the power law time dependence for the mean square displacement $\langle x^2\rangle \sim t^{\alpha}$. For $0<\alpha<1$ this process is usually called "subdiffusion" while for $1<\alpha$ it is referred to as "superdiffusion." To describe this phenomenon many authors employ the mathematical technique of fractional time derivatives [4,13–17]. Therefore these processes have also been named fractional diffusion processes after the method [18,19]. In many works the authors replace the integer time derivative of the first order in the diffusion equation by a fractional one on a pure mathematical or heuristic basis [13–17]. However, there are works that prove the validity of the fractional derivatives method for the anomalous diffusion problem based on the continuous time random walk approach and the fractional Fokker-Planck equation [4,20–23]. Nevertheless, the variety of existing mathematical definitions for fractional derivatives (see Ref. [24] and references therein) leads to the possibility to discuss various types of fractional derivatives, depending on the physical situation. Sometimes this leads to many conceptual difficulties in interpretation of the results. At the same time the nonlocal form of a fractional time derivation touches very basic ideas such as irreversibility, locality, and invariance under the time translations [19,25]. Therefore, the physical interpretation of a partial differential equation which involves a fractional time derivative is not a very clear issue today. One possible way to clarify this problem is the consecutive analysis of different ways to introduce a fractional time derivative into a differential equation, investigation of the limiting cases, and comparison between them. The purpose of this work is to discuss two different examples of how to introduce a fractional time derivation into the diffusion equation.

We will be concerned with equations

$$\frac{\partial}{\partial t} f(r,t)=C_{\alpha}\,{}_0D_t^{1-\alpha}[\Delta f(r,t)] \tag{1}$$

and

$${}_0D_t^{\alpha}[f(r,t)]=C_{\alpha}\Delta f(r,t), \tag{2}$$

where $f(r,t)$ denotes the unknown field of the diffusive agent concentration, C_{α} is the fractional diffusion constant with dimension $[\mathrm{m}^2/\mathrm{s}^{\alpha}]$, Δ denotes the differential Laplace operator and ${}_0D_t^{\alpha}$ is the fractional Riemann-Liouville derivative operator of order $0<\alpha<1$ and with the lower limit $t=0$,

$${}_aD_x^{\gamma}[f(x)]=\frac{d}{dx}\,{}_aI_x^{1-\gamma}[f(x)], \tag{3}$$

where

$${}_aI_x^{\varepsilon}[f(x)]=\frac{1}{\Gamma(\varepsilon)}\int_a^x (x-y)^{\varepsilon-1} f(y)dy \tag{4}$$

is the Riemann-Liouville fractional integral operator of order ε with a lower limit a and $\Gamma(\varepsilon)$ is the gamma function.

Both Eq. (1) and Eq. (2) intend to describe anomalous diffusion transport. However, from a mathematical point of view they are not equivalent. They may be regarded as two different examples [24] of introducing a fractional derivation through the Riemann-Liouville fractional integral (4). Obviously, the Riemann definition (3), the "right-hand side" definition, may be replaced by the "left-hand side" or Liouville definition ${}_a\overline{D}_x^{\gamma}[f(x)]={}_aI_x^{1-\gamma}[d/dx f(x)]$. Upon applying ${}_0I_t^{1-\alpha}$ to Eq. (1) one sees that Eq. (1) can be represented in the form ${}_0\overline{D}_t^{\alpha}[f(r,t)]=C_{\alpha}\Delta f(r,t)$, which is similar to Eq. (2).

Another important consideration is the initial condition. Equation (1) requires an initial condition in the form $f(r,0)=g(r)$ or, in particular, for the Green function

$$f(r,0)=f_0\delta(r), \tag{5}$$

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where $\delta(r)$ is the Dirac measure at the origin and f_0 is the strength of the initial pulse of concentration at the origin. In contrast, Eq. (2) requires the initial condition for the Green function in the form [19,25]

$$ {}_0I_t^{1-\alpha}[f(r,0)] = f_{0,\alpha}\delta(r), \tag{6}$$

where $f_{0,\alpha}$ is once again a constant.

The exact solutions of both Eq. (1) with initial condition (5) and Eq. (2) with initial condition (6) are known [19,26] and represented through the Fox H functions [27] as

$$f(r,t) = \frac{f_0}{(\pi r^2)^{d/2}} H_{12}^{20}\left(\frac{r^2}{4C_\alpha t^\alpha} \middle| \begin{matrix} (1,\alpha) \\ (d/2,1),(1,1) \end{matrix} \right) \tag{7}$$

for Eq. (1) and

$$f(r,t) = \frac{f_{0,\alpha} t^{\alpha-1}}{(\pi r^2)^{d/2}} H_{12}^{20}\left(\frac{r^2}{4C_\alpha t^\alpha} \middle| \begin{matrix} (\alpha,\alpha) \\ (d/2,1),(1,1) \end{matrix} \right) \tag{8}$$

for Eq. (2). Here d is the Euclidean dimension of the space where the diffusion occurs.

Upon introducing $z = r^2/4C_\alpha t^\alpha$ and using the H-function definition [27] in the case of Eq. (7) one obtains for $d=1$,

$$f(z,t) = \frac{f_0}{\sqrt{4\pi C_\alpha t^\alpha}} \sum_{k=0}^{\infty} \frac{(-z)^k}{k!} \left(\frac{\Gamma(1/2-k)}{\Gamma(1-\alpha(1/2+k))} + \frac{\Gamma(-1/2-k)\sqrt{z}}{\Gamma(1-\alpha(1+k))} \right); \tag{9a}$$

for $d=2$,

$$f(z,t) = \frac{f_0}{4\pi C_\alpha t^\alpha} \times \sum_{k=0}^{\infty} \frac{2\psi(1+k) - \alpha\psi(1-\alpha(1+k)) - \ln(z)}{k!^2 \Gamma(1-\alpha(1+k))} z^k; \tag{9b}$$

and for $d=3$,

$$f(z,t) = \frac{f_0}{(4\pi C_\alpha t^\alpha)^{3/2}} \sum_{k=0}^{\infty} \frac{(-z)^k}{k!} \left(\frac{\Gamma(-1/2-k)}{\Gamma(1-\alpha(3/2+k))} + \frac{\Gamma(1/2-k)}{\Gamma(1-\alpha(1+k))\sqrt{z}} \right), \tag{9c}$$

where $\psi(x)$ is the logarithmic derivative of the gamma function. Solution (8) gives for $d=1$,

$$f(z,t) = \frac{f_{0,\alpha} t^{\alpha/2-1}}{\sqrt{4\pi C_\alpha}} \sum_{k=0}^{\infty} \frac{(-z)^k}{k!} \left(\frac{\Gamma(1/2-k)}{\Gamma(\alpha(1/2-k))} + \frac{\Gamma(-1/2-k)\sqrt{z}}{\Gamma(-\alpha k)} \right) \tag{10a}$$

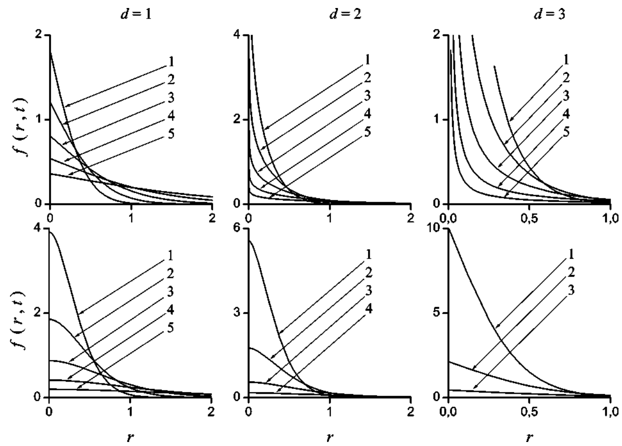

FIG. 1. Schematic picture presenting $f(r,t)$ vs r for the different time moments. The upper row corresponds to Eqs. (9). The bottom row corresponds to Eqs. (10). The solutions for $d=1$ are in the left-hand panels, for $d=2$ in the middle, for $d=3$ on right-hand side. Curves with label 1 are calculated for $t=0.01$, with label 2 for $t=0.1\sqrt{0.1}$, with label 3 for $t=0.1$, with label 4 for $t=\sqrt{0.1}$, and with label 5 for $t=1$. For numerical evaluations $\alpha=0.7$, $C_\alpha=1$, $f_0=1$, and $f_{0,\alpha}=1$ were used.

for $d=2$,

$$f(z,t) = \frac{f_{0,\alpha}}{4\pi C_\alpha t} \sum_{k=0}^{\infty} \frac{2\psi(1+k) - \alpha\psi(-\alpha k) - \ln(z)}{k!^2 \Gamma(-\alpha k)} z^k; \tag{10b}$$

and for $d=3$,

$$f(z,t) = \frac{f_{0,\alpha} t^{-\alpha/2-1}}{(4\pi C_\alpha)^{3/2}} \sum_{k=0}^{\infty} \frac{(-z)^k}{k!} \left(\frac{\Gamma(-1/2-k)}{\Gamma(-\alpha(1/2+k))} + \frac{\Gamma(1/2-k)}{\Gamma(-\alpha k)\sqrt{z}} \right). \tag{10c}$$

Note that both Eq. (7) and Eq. (8) imply axial symmetry of $f(r,t)$ for $d=2$ and spherical symmetry for $d=3$. The key point is that only solution (7) has a probabilistic interpretation for $f(r,t)$ since only for this equation normalization holds constant while for Eq. (8) normalization decays [19,25] as $t^{\alpha-1}$.

Despite the fact that solutions (7) and (8) are already known [19,26] it seems that representations (9) and (10) have not been derived before. Figure 1 presents some examples of Eqs. (9) and Eqs. (10).

It was mentioned perviously [19] that the nonlocal form of the initial condition (6) leads to the divergence of $f(r,t)$ for $t \to 0$. Recent works [25,28,29] discuss this fact in relation to the fractional stationarity concept which establishes, in addition to the conventional constants, a second class of stationary states that obey power law time dependence.

Let us further discuss the behavior of the fractional diffusion at the origin $r \to 0$ for different dimensions d. From Eqs. (9) for $t>0$ one immediately obtains in the case of $d=1$,

$$\lim_{r\to 0} f(r,t) = \frac{f_0}{2\Gamma(1-\alpha/2)\sqrt{C_\alpha t^\alpha}}; \tag{11a}$$

in the case of $d=2$,

$$\lim_{r\to 0} f(r,t) = \lim_{r\to 0} \frac{f_0 \ln(4C_\alpha t^\alpha/r^2)}{4\pi\Gamma(1-\alpha)C_\alpha t^\alpha} \sim \ln\left(\frac{1}{r}\right); \tag{11b}$$

in the case of $d=3$,

$$\lim_{r\to 0} f(r,t) = \lim_{r\to 0} \frac{f_0}{4\pi r\Gamma(1-\alpha)C_\alpha t^\alpha} \sim \frac{1}{r}, \tag{11c}$$

while Eqs. (10) for $t>0$ give in the case of $d=1$,

$$\lim_{r\to 0} f(r,t) = \frac{f_{0,\alpha} t^{\alpha-1}}{2\Gamma(\alpha/2)\sqrt{C_\alpha t^\alpha}}; \tag{12a}$$

in the case of $d=2$,

$$\lim_{r\to 0} f(r,t) = \frac{\alpha f_{0,\alpha}}{4\pi C_\alpha t}; \tag{12b}$$

in the case of $d=3$

$$\lim_{r\to 0} f(r,t) = -\frac{f_{0,\alpha} t^{\alpha-1}}{4\pi\Gamma(-\alpha/2)(C_\alpha t^\alpha)^{3/2}}. \tag{12c}$$

Thus, the solution of Eq. (1) with initial condition (5) for any $t>0$ is finite for $d=1$, exhibits logarithmic divergence for $d=2$, and diverges as $1/r$ for $d=3$, while the solution of Eq. (2) with initial condition (6) is always finite at the origin $r\to 0$ [see Eqs. (11), Eqs. (12), and Fig. 1].

Let us discuss the heuristic merit of the results derived. The key difference between Eq. (1) and Eq. (2) is the conservation of the normalization for solution (7) and the decay of the normalization for solution (8). This normalization constraint for Eq. (1) was introduced in order to provide the probabilistic interpretation for the diffusive particle concentration $f(r,t)$ of Eq. (7) and to obtain a consistent correspondence between the fractional diffusion and conventional diffusion. However, solution (7) exhibits divergency of $f(r,t)$ at the origin for $d=2$ and $d=3$, while the conventional diffusion equation does not lead to any divergencies for the Green function [30] at the limit $r\to 0$ and $t>0$. In the case of the classical diffusion equation such divergences imply constant sources of the diffusive agent at the origin. Thus, one could conclude that a fractional derivative either ${}_0\bar{D}_t^\alpha$ or ${}_0D_t^\alpha$, implies the loss of diffusive agent mass. However, in the case of Eq. (1) this deficit is compensated for by the ''virtual source'' of diffusion agent at the origin while for Eq. (2) this fact results in decay of normalization. For the fractional time derivatives based on the Riemann-Liouville fractional integral this conclusion is independent of the order α.

The ''virtual sources'' of diffusion agent at the origin for Eq. (1) mean that some mass injected at the origin. However, this injection is not defined by the boundary conditions of the problem. Thus, the presence of such ''virtual sources'' in solutions (7) and (9) is physically meaningless and one needs to resolve this contradiction. A possible way to solve this problem is to use some regularization methods, as has been done for the modified porous medium equation of Barenblatt's type [31]. Such a regularization of Eq. (1) would be the subject of future investigations.

Another interesting observation is that replacement of the ''left-hand side'' definition of the fractional time derivative with the ''right-hand side'' definition affects $\lim_{r\to 0} f(r,t)$, which depends on the space variable r. Thus, in a sense, the divergence of $f(r,t)$ at $r\to 0$ for Eq. (1) could be replaced by a nonlocality of the initial condition (6) at $t\to 0$ for Eq. (2). This time-space relationship is not an unexpected finding. It hints for us to pay attention to the variational formulation of the diffusion type equation in view of the fractional calculus and the fractional stationarity concept [25,28,29]. This problem would be a direction for future investigation.

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