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Letter

Stochastic interpretation of *g*-subdiffusion process

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Recently, we considered the *g*-subdiffusion equation with a fractional Caputo time derivative with respect to another function *g*, T. Kosztołowicz *et al.* [Phys. Rev. E **104**, 014118 (2021)]. This equation offers different possibilities for modeling diffusion such as a process in which a type of diffusion evolves continuously over time. However, the equation has not been derived from a stochastic model and the stochastic interpretation of *g* subdiffusion is still unknown. In this Letter, we show the stochastic foundations of this process. We derive the equation by means of a modified continuous time random walk model. An interpretation of the *g*-subdiffusion process is also discussed.

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Introduction. Subdiffusion occurs in media in which the movement of diffusing molecules is very difficult due to the complex internal structure of the medium. A useful tool used in normal and anomalous diffusion modeling is the continuous time random walk (CTRW) model [1–15], and the citation list on this issue can be significantly extended. Within this model, a distribution of time between particle jumps ψ has a heavy tail for subdiffusion, $\psi(t)\sim 1/t^{1+\alpha}, 0<\alpha<1$ [6–17]. This model provides the "ordinary" subdiffusion equation with the fractional order Riemann-Liouville or Caputo derivative [10–16,18–24]. Recently, a more general subdiffusion equation with the Caputo derivative with respect to another function g has been considered [25] (see also Ref. [26]); we call it the g-subdiffusion equation which describes the g-subdiffusion process. As shown in Ref. [25], this equation describes a process in which a type of diffusion can change over time. As we discuss later, the g-subdiffusion equation can be used to describe a process in which ordinary subdiffusion is additionally slowed down. Such a process may occur, among others, in the diffusion of drugs in a system consisting of packed gel beads immersed in water [27] and in the diffusion of antibiotics in a bacterial biofilm [28]. Unfortunately, g subdiffusion does not yet have a stochastic interpretation. We show how to derive the g-subdiffusion equation by means of a modified CTRW model and we discuss the interpretation of this process.

"Ordinary" subdiffusion equation. The fractional subdiffusion equation with an "ordinary" Caputo derivative of the order $\alpha\in(0,1)$ is [24]

$$\frac{{}^C\partial^\alpha P(x,t)}{\partial t^\alpha}=D\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{1}$$

where the Caputo fractional derivative is defined for $0<\alpha<1$ as

$$\frac{{}^C d^\alpha}{dt^\alpha}f(t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-u)^{-\alpha}f'(u)du, \tag{2}$$

α is a subdiffusion parameter, and D is a generalized diffusion coefficient measured in the units of m^2/s^α. To solve the equation the Laplace transform $\mathcal{L}$ can be used,

$$\mathcal{L}[f(t)](s)=\int_0^\infty e^{-st}f(t)dt. \tag{3}$$

Due to the relation

$$\mathcal{L}\left[\frac{{}^C d^\alpha f(t)}{dt^\alpha}\right](s)=s^\alpha\mathcal{L}[f(t)](s)-s^{\alpha-1}f(0), \tag{4}$$

where $0<\alpha\leqslant 1$, we get

$$s^\alpha\mathcal{L}[P(x,t)](s)-s^{\alpha-1}P(x,0)=D\frac{\partial^2\mathcal{L}[P(x,t)](s)}{\partial x^2}. \tag{5}$$

g-subdiffusion equation. In this Letter, functions describing g subdiffusion are denoted by a tilde. The g-subdiffusion equation reads

$$\frac{{}^C\partial_g^\alpha \tilde{P}(x,t)}{\partial t^\alpha}=D\frac{\partial^2\tilde{P}(x,t)}{\partial x^2}, \tag{6}$$

where $0<\alpha<1$, the Caputo derivative with respect to another function g is defined as [29]

$$\frac{{}^C d_g^\alpha f(t)}{dt^\alpha}=\frac{1}{\Gamma(1-\alpha)}\int_0^t [g(t)-g(u)]^{-\alpha}f'(u)du, \tag{7}$$

the function g fulfills the conditions $g(0)=0$, $g(\infty)=\infty$, and $g'(t)>0$ for $t>0$, and its values are given in a time unit. When $g(t)=t$, the g-Caputo fractional derivative takes a form of the ordinary Caputo derivative. To solve Eq. (6) the g-Laplace transform can be used, and this transform is defined

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as [30]

$$\mathcal{L}_g[\tilde{f}(t)](s) = \int_0^\infty e^{-sg(t)}\tilde{f}(t)g'(t)dt. \quad (8)$$

Due to the property [30]

$$\mathcal{L}_g\left[\frac{{}^C d_g^\alpha}{dt^\alpha}\tilde{f}(t)\right](s) = s^\alpha \mathcal{L}_g[\tilde{f}(t)](s) - s^{\alpha-1}\tilde{f}(0), \quad (9)$$

the procedure of solving Eq. (6) is similar to the procedure of solving an ordinary subdiffusion equation by means of the ordinary Laplace transform method. In terms of the g-Laplace transform the g-subdiffusion equation is

$$s^\alpha \mathcal{L}_g[\tilde{P}(x,t)](s) - s^{\alpha-1}\tilde{P}(x,0) = D\frac{\partial^2 \mathcal{L}_g[\tilde{P}(x,t)](s)}{\partial x^2}. \quad (10)$$

Using the g-Laplace transform to Eq. (6) yields Eq. (10) in the same form as Eq. (5).

Model of a particle random walk. To derive the subdiffusion equation we use a simple model of a particle random walk along a one-dimensional homogeneous lattice. Usually, in the CTRW model both a particle jump length and waiting time for a particle jump are random variables. In our considerations, we assume that the jump length distribution λ has the form $\lambda(x) = \frac{1}{2}[\delta(x-\epsilon) + \delta(x+\epsilon)]$, where δ is the delta Dirac function. Only the choice of a particle jump direction is random, where its length ϵ is a parameter. We start with the particle random walk model in which the particle positions and time are discrete. Next, we move to continuous variables. A random walk with discrete time n is described by the equation $P_{n+1}(m) = \frac{1}{2}P_n(m+1) + \frac{1}{2}P_n(m-1)$, where $P_n(m)$ is a probability that a diffusing particle is at the position m after the nth step. Let the initial particle position be $m = 0$. Moving from discrete m to continuous x spatial variable we assume $x = m\epsilon$ and $P_n(x) = P_n(m)/\epsilon$, where ϵ is a distance between discrete sites. The above equations and the relation $[P_n(x+\epsilon) + P_n(x-\epsilon) - 2P_n(x)]/\epsilon^2 = \partial^2 P_n(x)/\partial x^2$, $\epsilon \to 0$, provide the following equation in the limit of small ϵ,

$$P_{n+1}(x) - P_n(x) = \epsilon^2 \frac{\partial^2 P_n(x)}{\partial x^2}. \quad (11)$$

To move from discrete to continuous time we use the formula [1]

$$P(x,t) = \sum_{n=0}^\infty Q_n(t)P_n(x), \quad (12)$$

where $Q_n(t)$ is the probability that a diffusing particle takes n steps in the time interval $(0,t)$. The function Q_n is determined differently for ordinary subdiffusion and g subdiffusion. In the following, we find the rule for determining the functions Q_n and the explicit form of the functions ψ for both processes. These functions, together with Eqs. (11) and (12), provide ordinary subdiffusion and g-subdiffusion equations.

The case of ordinary subdiffusion. In this case the function Q_n is a convolution of n distributions ψ of a waiting time for a particle to jump and a function U which is the probability that a particle does not change its position after the nth step,

$$Q_n(t) = (\underbrace{\psi * \psi * \cdots * \psi}_{n\ \text{times}} * U)(t), \quad (13)$$

where the convolution is defined as

$$(f*h)(t) = \int_0^t f(u)h(t-u)du. \quad (14)$$

The ordinary Laplace transform has the following property that makes the transform useful in determining the function Q_n,

$$\mathcal{L}[(f*h)(t)](s) = \mathcal{L}[f(t)](s)\mathcal{L}[h(t)](s). \quad (15)$$

From Eqs. (12), (13), and (15) we have

$$\mathcal{L}[P(x,t)](s) = \mathcal{L}[U(t)](s)\sum_{n=0}^\infty \mathcal{L}^n[\psi(t)](s)P_n(x). \quad (16)$$

Combining Eqs. (11), (12), and (16) we get

$$\frac{2[1-\mathcal{L}[\psi(t)](s)]}{\epsilon^2\mathcal{L}[\psi(t)](s)}\mathcal{L}[P(x,t)](s) - \frac{2\mathcal{L}[U(t)](s)}{\epsilon^2\mathcal{L}[\psi(t)](s)}P(x,0) = \frac{\partial^2\mathcal{L}[P(x,t)](s)}{\partial x^2}. \quad (17)$$

Comparing Eq. (17) with Eq. (5) we conclude that they are identical only if

$$\frac{1-\mathcal{L}[\psi(t)](s)}{\mathcal{L}[\psi(t)](s)} = \frac{\epsilon^2 s^\alpha}{2D}, \quad \frac{\mathcal{L}[U(t)](s)}{\mathcal{L}[\psi(t)](s)} = \frac{\epsilon^2 s^{\alpha-1}}{2D}.$$

The solutions to the above equations are

$$\mathcal{L}[\psi(t)](s) = \frac{1}{1+\frac{\epsilon^2 s^\alpha}{2D}}, \quad (18)$$

and

$$\mathcal{L}[U(t)](s) = \frac{\epsilon^2 s^{\alpha-1}}{2D\left(1+\frac{\epsilon^2 s^\alpha}{2D}\right)} = \frac{1-\mathcal{L}[\psi(t)](s)}{s}. \quad (19)$$

Due to the relations

$$\mathcal{L}[1](s) = \frac{1}{s}, \quad \mathcal{L}\left[\int_0^t f(u)du\right](s) = \frac{\mathcal{L}[f(t)](s)}{s}, \quad (20)$$

we get

$$U(t) = 1 - \int_0^t \psi(u)du. \quad (21)$$

In order to find the function ψ we use the relation [31]

$$\mathcal{L}^{-1}[s^\nu e^{-as^\beta}](t) = \frac{1}{t^{1+\nu}}\sum_{k=0}^\infty \frac{1}{k!\Gamma(-\nu-\beta k)}\left(-\frac{a}{t^\beta}\right)^k \equiv f_{\nu,\beta}(t;a), \quad (22)$$

where $a, \beta > 0$, and Γ is the Euler's gamma function. The function $f_{\nu,\beta}$ is the Wright function and the special case of Fox's H function. To find the inverse Laplace transform of Eq. (18) first we calculate the inverse Laplace transform of the function $e^{-as^\beta}/(1+\tau s^\alpha)$, where $\tau = \epsilon^2/2D$ and $a, \beta > 0$, using the formula $1/(1+u) = \sum_{n=0}^\infty u^n$ when $|u| < 1$. We get

$$\mathcal{L}\left[\frac{e^{-as^\beta}}{1+\tau s^\alpha}\right](s) = \begin{cases} \frac{1}{\tau}\sum_{n=0}^\infty \left(-\frac{1}{\tau}\right)^n s^{-(n+1)\alpha}e^{-as^\beta}, & s > \frac{1}{\tau^{1/\alpha}}, \\ \sum_{n=0}^\infty (-\tau)^n s^{n\alpha}e^{-as^\beta}, & s < \frac{1}{\tau^{1/\alpha}}. \end{cases} \quad (23)$$

Next, we take the limit of $a \to 0$. From Eqs. (22), (23), and the relations $f_{\nu,\beta}(t;0) = 1/\Gamma(-\nu)t^{1+\nu}$, $1/\Gamma(0) = 0$, we get

$$\psi(t) = \begin{cases} \frac{1}{\tau}\sum_{n=0}^{\infty}\left(-\frac{1}{\tau}\right)^n \frac{t^{(n+1)\alpha-1}}{\Gamma((n+1)\alpha)}, & t < \tau^{1/\alpha}, \\ \sum_{n=0}^{\infty}(-\tau)^{n+1}\frac{t^{-(n+1)\alpha-1}}{\Gamma(-(n+1)\alpha)}, & t > \tau^{1/\alpha}. \end{cases} \tag{24}$$

We have $\psi(t) \approx \alpha\tau/\Gamma(1-\alpha)t^{1+\alpha}$ in the limit of $t \to \infty$. The function ψ was already derived using the relation $\mathcal{L}^{-1}[1/(1+\tau s^\alpha)] = t^{\alpha-1}E_{\alpha,\alpha}(-t^\alpha/\tau)$, where $E_{\alpha,\alpha}(z) = \sum_{n=0}^{\infty} z^n/\Gamma(\alpha(n+1))$ is the two-parameter Mittag-Leffler function (see, for example, Ref. [32]). Then, the function ψ corresponds to Eq. (24) but for the case of $t < \tau^{1/\alpha}$ only.

The case of g subdiffusion. To get Eq. (10) we use the g-Laplace transform. This transform has the following property [30],

$$\mathcal{L}_g[(f *_g h)(t)](s) = \mathcal{L}_g[f(t)](s)\mathcal{L}_g[h(t)](s), \tag{25}$$

where the g convolution is defined as

$$(f *_g h)(t) = \int_0^t f(u)h[g^{-1}(g(t)-g(u))]g'(u)du. \tag{26}$$

We involve the g convolution in the CTRW model. Then, the procedure for deriving the g-subdiffusion equation using the g-Laplace transform is analogous to the procedure for deriving the ordinary subdiffusion equation using the ordinary Laplace transform. Assuming

$$\tilde{P}(x,t) = \sum_{n=0}^{\infty}\tilde{Q}_n(t)P_n(x) \tag{27}$$

and

$$\tilde{Q}_n(t) = (\underbrace{\tilde{\psi} *_g \tilde{\psi} *_g \cdots *_g \tilde{\psi}}_{n \text{ times}} *_g \tilde{U})(t), \tag{28}$$

from Eqs. (25), (27), and (28) we obtain

$$\mathcal{L}_g[\tilde{P}(x,t)](s) = \sum_{n=0}^{\infty}\mathcal{L}_g[\tilde{U}(t)](s)\mathcal{L}_g^n[\tilde{\psi}(t)](s)P_n(x). \tag{29}$$

From Eqs. (11) and (29) we get

$$\frac{1-\mathcal{L}_g[\tilde{\psi}(t)](s)}{\epsilon^2\mathcal{L}_g[\tilde{\psi}(t)](s)}\mathcal{L}_g[\tilde{P}(x,t)](s) - \frac{\mathcal{L}_g[\tilde{U}(t)](s)}{\epsilon^2\mathcal{L}_g[\tilde{\psi}(t)](s)}\tilde{P}(x,0) = \frac{\partial^2\mathcal{L}[\tilde{P}(x,t)](s)}{\partial x^2}. \tag{30}$$

Equations (30) and (10) are identical only when

$$\mathcal{L}_g[\tilde{\psi}(t)](s) = \frac{1}{1+\frac{\epsilon^2 s^\alpha}{2D}} \tag{31}$$

and

$$\mathcal{L}_g[\tilde{U}(t)](s) = \frac{\epsilon^2 s^{\alpha-1}}{2D\left(1+\frac{\epsilon^2 s^\alpha}{2D}\right)}. \tag{32}$$

Comparing Eqs. (31) and (32) with Eqs. (18) and (19), respectively, we get

$$\mathcal{L}_g[\tilde{\psi}(t)](s) = \mathcal{L}[\psi(t)](s), \tag{33}$$

$$\mathcal{L}_g[\tilde{U}(t)](s) = \mathcal{L}[U(t)](s). \tag{34}$$

From the relation

$$\mathcal{L}_g[\tilde{f}(t)](s) = \mathcal{L}[\tilde{f}(g^{-1}(t))](s), \tag{35}$$

we get the following rule [25],

$$\mathcal{L}_g[\tilde{f}(t)](s) = \mathcal{L}[f(t)](s) \Leftrightarrow \tilde{f}(t) = f(g(t)). \tag{36}$$

Due to Eq. (36), from Eqs. (33) and (34) we obtain

$$\tilde{\psi}(t) = \psi(g(t)), \tag{37}$$

and

$$\tilde{U}(t) = U(g(t)). \tag{38}$$

Equations (24) and (37) provide

$$\tilde{\psi}(t) = \begin{cases} \frac{1}{\tau}\sum_{n=0}^{\infty}\left(-\frac{1}{\tau}\right)^n \frac{g^{(n+1)\alpha-1}(t)}{\Gamma((n+1)\alpha)}, & t < g^{-1}(\tau^{1/\alpha}), \\ \sum_{n=0}^{\infty}(-\tau)^{n+1}\frac{g^{-(n+1)\alpha-1}(t)}{\Gamma(-(n+1)\alpha)}, & t > g^{-1}(\tau^{1/\alpha}). \end{cases} \tag{39}$$

We get $\tilde{\psi}(t) \approx \alpha\tau/\Gamma(1-\alpha)g^{1+\alpha}(t)$ when $t \to \infty$.

We link the g convolution with the ordinary convolution. Let $\tilde{f}(t) = f(g(t))$ and $\tilde{h}(t) = h(g(t))$. After simple calculation we get

$$(\tilde{f} *_g \tilde{h})(t) = (f * h)(g(t)). \tag{40}$$

From Eqs. (27), (28), and (40) we have

$$\tilde{P}(x,t) = \sum_{n=0}^{\infty} Q_n(g(t))P_n(x). \tag{41}$$

Comparing Eqs. (41) and (12) we obtain

$$\tilde{P}(x,t) = P(x,g(t)). \tag{42}$$

Interpretation. The g-subdiffusion process is associated to ordinary subdiffusion controlled by the same parameter α. The waiting time for a particle jump in the g-subdiffusion process is controlled by the functions ψ and g. A particle jump that would occur with some probability after time t in an ordinary subdiffusion process will occur with the same probability after time $\tilde{t} = g^{-1}(t)$ in the g-subdiffusion process. If $g(t) < t$, we have $t < \tilde{t}$, and subdiffusion is then slowed down. When $g(t) > t$, subdiffusion is accelerated.

An example of g subdiffusion is the diffusion of molecules in a medium consisting of a matrix in which there are narrow channels. If the channels have a complicated geometric structure and diffusing molecules do not interact with the matrix, then ordinary subdiffusion controlled by the parameter α occurs. If the matrix provides the diffusing molecules with additional energy, subdiffusion can be accelerated. When temporary penetration of a molecule into the matrix is possible, then the molecule "disappears" from the channels and may diffuse further upon returning to a channel. In this case, ordinary subdiffusion is slowed down. Such a process occurs in a vessel filled with alginate beads immersed in water in which a colistin antibiotic diffuses [27]. Other examples of the possible application of the g-subdiffusion equation is the diffusion of drugs [33–36] or fertilizers [37–39] in systems consisting of beads immersed in water. We also suppose that the g-subdiffusion model can be used to describe the diffusion of antibiotics in a biofilm. Biofilms usually have a gel structure. When the antibiotic does not interact with bacteria, ordinary antibiotic subdiffusion in the biofilm is expected. However, bacteria in the biofilm have different defense mechanisms against the action of the antibiotic. These mechanisms may hinder or even facilitate antibiotic subdiffusion (see Ref. [28] and the references cited therein). Thus, the application of the g-subdiffusion equation to describe this process may be effective.

Final remarks. We have shown that the g-subdiffusion equation can be derived by means of the modified CTRW model (we call it the g-CTRW model). In the g-CTRW model we use g convolution and the g-Laplace transform instead of "ordinary" convolution and the "ordinary" Laplace transform, respectively, which are used in the "ordinary" CTRW model.

We note that the condition $\mathcal{L}_g[\tilde{\psi}(t)](0) = 1$ does not guarantee that the function $\tilde{\psi}$ is normalized. Therefore, $\tilde{\psi}$ is not a probability distribution. Thus, it seems that the g-CTRW model is merely a mathematical procedure. However, this model can be interpreted as an ordinary CTRW model in which the timescale is controlled by the function $g(t)$ [see Eqs. (37)–(42)]. The key issue for the g-subdiffusion process is determining the parameter α and the function g. An example of their determination from empirical data is shown in Ref. [27].

In practice, the transformations made in deriving the g-subdiffusion equation within the g-CTRW model are the same as in deriving the ordinary subdiffusion equation using ordinary CTRW. Within the ordinary CTRW, subdiffusion-reaction equations [40] as well as the Green's functions and membrane boundary conditions for a system in which a thin membrane separates different subdiffusive media [41] have been derived. Within the g-CTRW model the same procedures can also be used to derive g-subdiffusion-reaction equations, Green's functions, and boundary conditions at the membrane for the processes described by g-subdiffusion equations.

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