$G$-subdiffusion equation that describes transient subdiffusion

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A $g$–subdiffusion equation with fractional Caputo time derivative with respect to another function $g$ is used to describe a process of a continuous transition from subdiffusion with parameters $\alpha$ and $D_{\alpha}$ to subdiffusion with parameters $\beta$ and $D_{\beta}$. The parameters are defined by the time evolution of the mean square displacement of diffusing particle $\sigma^2(t) = 2D_\iota t^\iota / \Gamma(1 + \iota)$, $\iota = \alpha, \beta$. The function $g$ controls the process at “intermediate” times. The $g$–subdiffusion equation is more general than the “ordinary” fractional subdiffusion equation with constant parameters, it has potentially wide application in modelling diffusion processes with changing parameters.

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Subdiffusion occurs in media, such as gels and bacterial biofilm, where the movement of molecules is very hindered due to a complex structure of a medium [1–14]. Within the Continuous Time Random Walk (CTRW) model subdiffusion is defined as a process in which a time distribution between particle jumps $\psi$ has a heavy tail which makes the average time infinite, $\psi(t) \sim 1/t^{1+\alpha}$ when $t \to \infty$, $0 < \alpha < 1$, and the jump length distribution has finite moments [2–5, 15–19]. The citation list on the above issues can be significantly extended. This model shows that subdiffusion with a constant subdiffusion parameter (exponent) $\alpha$ in a one–dimensional homogeneous system can be described by an “ordinary” subdiffusion equation with a fractional time derivative of the order $\alpha \in (0, 1)$

$$C \partial^{\alpha} C(x, t) \over \partial t^{\alpha} = D_{\alpha} \partial^2 C(x, t) \over \partial x^2,$$

(1)

where the Caputo fractional derivative is defined here as

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

(2)

$D_{\alpha}$ is a generalized diffusion coefficient measured in the units of $m^2/s^\alpha$, $C$ is a concentration of diffusing particles, $f'$ denotes the first–order derivative of function $f$. Eq. [1] can be transformed to its equivalent form with the fractional Riemann–Liouville time derivative of the order $1 - \alpha$, see for example [2].

Subdiffusion parameters are often defined by a time evolution of the mean square displacement $\sigma^2$ of a diffusing particle,

$$\sigma^2(t) = \frac{2D_{\alpha} t^{\alpha}}{\Gamma(1+\alpha)}.$$

(3)

Eq. (1) describes the subdiffusion process with constant parameters $\alpha$ and $D_{\alpha}$. Such a process can occur in a homogeneous system in which the structure does not change with time. However, the structure of a medium may evolve over time continuously changing the parameters. An example is antibiotic subdiffusion in a bacterial biofilm [12–13]. Bacteria have different defense mechanisms against the action of the antibiotic, which can slow down or even significantly accelerate the antibiotic transport [20, 21]. Different models have been used to describe subdiffusion with variable parameters [22–24].

Subdiffusion equations with linear combination of fractional time derivative with different parameters $\alpha$ have been studied in [25–27]. The transmogrifying CTRW model describing anomalous diffusion with changing subdiffusion parameters has been considered in [28]. Modification of a time scale in a diffusion model can lead to changes in diffusion parameters as well as in the type of diffusion [29, 30]. A timescale changing can be made by means of subordinated method [4, 31–34]. Within this method retarding and accelerating anomalous diffusions have been obtained [35, 36]. Examples of processes that lead to a rescaling of diffusion are diffusing diffusivities where the diffusion coefficient evolves over time [33], passages through the layered media [37], and anomalous diffusion in an expanding medium [38]. We mention that distributed order of fractional derivative in subdiffusion equation can lead to delayed or accelerated subdiffusion [39, 40].

We consider subdiffusion in a one–dimensional homogeneous system, diffusive properties of a medium may change over time. At the initial moment the subdiffusion parameters are $\alpha$ and $D_{\alpha}$, and after long time (formally

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$t \to \infty$) the parameters are $\beta$ and $D_\beta$. In these cases subdiffusion is described by the “ordinary” subdiffusion equation. In the “intermediate” time interval there is a continuous transient subdiffusion process in which the subdiffusion parameters are not defined by Eq. (3). We call the process transient subdiffusion, it is symbolically written as $(\alpha, D_\alpha) \to (\beta, D_\beta)$.

Recently, the $g$–subdiffusion process characterized by parameters $\alpha, D_\alpha$, and by the function $g$ has been considered in [20–24]. This process is related to “ordinary” subdiffusion with the same parameters in which the time variable has been rescaled by a deterministic function $g$ which fulfills the conditions $g(0) = 0$, $g(\infty) = \infty$, and $g'(t) > 0$ for $t > 0$, the values of the function $g$ are given in a time unit. $G$–subdiffusion is described by the following $g$–subdiffusion equation

$$\frac{C}{\alpha} \partial_t^\alpha C(x, t) = D_\alpha \partial_x^2 C(x, t),$$

(4)

where

$$\frac{C}{\alpha} \partial_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (g(t) - g(u))^{-\alpha} f'(u)du$$

(5)

is the $g$–Caputo fractional derivative of the order $\alpha \in (0, 1)$ with respect to the function $g$. When $g(t) \equiv t$, the $g$–Caputo fractional derivative takes the form of the “ordinary” Caputo derivative. We will show that transient subdiffusion can be treated as a special case of $g$–subdiffusion. We mention that the solutions to the $g$–subdiffusion equation well describe the experimental results of drug diffusion in a system containing tightly packed beads impregnated with the drug at the initial moment.

The $g$–subdiffusion equation can be solved by means of the $g$–Laplace transform method. The $g$-Laplace transform is defined as

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

(6)

The $g$–Laplace transform is related to the “ordinary” Laplace transform $\mathcal{L}[f(t)](s) = \int_0^\infty e^{-st} f(t)dt$ as follows

$$\mathcal{L}_g[f(t)](s) = \mathcal{L}[f(g^{-1}(t))](s).$$

(7)

Eq. (7) provides the rule

$$\mathcal{L}_g[f(t)](s) = \mathcal{L}[h(t)](s) \iff f(t) = h(g(t)).$$

(8)

The above formula is helpful in calculating the inverse $g$–Laplace transform if the inverse “ordinary” Laplace transform is known. The examples of inverse $g$–Laplace transforms are

$$\mathcal{L}_g^{-1} \left[ \frac{1}{s^{k+\nu}} \right] (t) = \frac{g^\nu(t)}{\Gamma(1+\nu)}, \quad \nu > -1,$$

(9)

$$\mathcal{L}_g^{-1} [s^\nu e^{-a s^\nu}] (t) = f_{\nu, \mu}(g(t); a)$$

(10)

$$= \frac{1}{g^{1+\nu}(t)} \sum_{k=0}^{\infty} \frac{1}{k! \Gamma(-\nu - \mu k)} \left( -\frac{a}{g^\nu(t)} \right)^k.$$

$a, \mu > 0$. The function $f_{\nu, \mu}$ is a special case of the Wright function and the H-Fox function.

The calculations for solving Eq. (3) by means of the $g$–Laplace transform method are similar to those for solving Eq. (1) using the “ordinary” Laplace transform. Due to the relation

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

(11)

where $0 < \alpha \leq 1$, the $g$–Laplace transform of Eq. (4) reads

$$s^\alpha \mathcal{L}_g[C(x, t)](s) - s^{\alpha-1} C(x, 0) = D_\alpha \partial_x^2 \mathcal{L}_g[C(x, t)](s).$$

(12)

The Green’s function $P(x, t|x_0)$ is interpreted as a probability density of finding a diffusing particle, located initially at $x_0$, at point $x$ at time $t$. The $g$–Laplace transform of Green’s function is the following solution to Eq. (11) for the initial condition $P(x, 0|x_0) = \delta(x-x_0)$, where $\delta$ denotes the delta–Dirac function, and the boundary conditions $\mathcal{L}_g[P(\pm \infty, t|x_0)](s) = 0$,

$$\mathcal{L}_g[P(x, t|x_0)](s) = \frac{1}{2\sqrt{D_\alpha s^{1-\alpha/2}}} e^{-\frac{|x-x_0|^2}{4D_\alpha s^{1-\alpha/2}}}.$$  

(13)

From Eqs. (10) and (13) we obtain

$$P(x, t|x_0) = \frac{1}{2\sqrt{D_\alpha}} f_{-1+\alpha/2, \alpha/2} \left( g(t); \frac{|x-x_0|}{\sqrt{D_\alpha}} \right).$$

(14)

Eqs. (9) and (13) provide

$$\sigma^2(t) = \frac{2D_\alpha}{\Gamma(1+\alpha)} g^\alpha(t).$$

(15)

Putting $g(t) \equiv t$ in Eq. (14) we get the Green’s function for the “ordinary” subdiffusion equation

$$P(x, t|x_0) = \frac{1}{2\sqrt{D_\alpha}} f_{-1+\alpha/2, \alpha/2} \left( t; \frac{|x-x_0|}{\sqrt{D_\alpha}} \right).$$

(16)

We mention that $f_{-1+\alpha/2, \alpha/2}$ is called the Mainardi function.

We assume that at the initial moment the subdiffusion parameters are $\alpha$ and $D_\alpha$, and in the long time limit they are $\beta$ and $D_\beta$, $\alpha \neq \beta$. Then,

$$\sigma^2(t) = \begin{cases} 2D_\beta t^{\beta}, & t \to \infty, \\ 2D_\alpha \frac{t^{\alpha}}{\Gamma(1+\alpha)} \bar{f}^\alpha, & t \to 0, \end{cases} \quad \frac{\alpha}{\beta} < 1.$$  

(17)

Eq. (17) coincides with Eq. (15) if

$$g(t) = \begin{cases} t, & t \to 0, \\ A t^{\beta/\alpha}, & t \to \infty, \end{cases}$$

(18)
where
\[ \alpha = \left( \frac{D_\beta \Gamma(1+\alpha)}{D_\alpha \Gamma(1+\beta)} \right)^{\frac{1}{\beta}}. \tag{19} \]

Guided by Eq. \[18\] we propose
\[ g(t) = a(t)t + (1-a(t))At^{\beta/\alpha}, \tag{20} \]
where a non-negative function \( a \) fulfills the conditions \( a(0) = 1 \), \( a(\infty) = 0 \), and \( a \) generates an increasing function \( g \) in the time domain. Since \( g(t) \rightarrow At^{\beta/\alpha} \) when \( t \rightarrow \infty \), Eq. \[20\] provides the additional condition
\[ t \rightarrow \infty, a(t)t \rightarrow 0. \tag{21} \]

The function \( a \) can be assumed as
\[ a(t) = \frac{1}{1 + \xi(t)}, \tag{22} \]
where \( \xi \) fulfills the conditions \( \xi(0) = 0 \) and \( \xi(\infty) = \infty \). In the following we consider Eq. \[22\] with the power function \( \xi(t) = Bt^\nu \), where \( B \) is a parameter measured in the units of \( 1/s^{1/\nu} \). The condition \[21\] is met for any \( \alpha \) and \( \beta, \alpha, \beta \in (0,1) \), when \( \nu > 1 \). Then, the function \( g \) is
\[ g(t) = \frac{t + ABt^{\beta + \nu}}{1 + Bt^\nu}, \tag{23} \]
where \( \nu > 1 \). In this case the Green’s function reads
\[ P(x, t|x_0) = \frac{1}{2\sqrt{D_\alpha}} \times f_{-1+\alpha/2,\alpha/2} \left( \frac{t + ABt^{\beta + \nu}}{1 + Bt^\nu}, \frac{|x - x_0|}{\sqrt{D_\alpha}} \right), \tag{24} \]
with \( A \) given by Eq. \[19\].

The plots of Green’s functions Eq. \[24\] describing the process \( (\alpha, D_\alpha) \rightarrow (\beta, D_\beta) \) are compared with the Green’s functions for “ordinary” subdiffusion with parameters \( (\alpha, D_\alpha) \) and \( (\beta, D_\beta) \) in Figs. \[1\] and \[2\]. We consider accelerated subdiffusion \((0.6, 10) \rightarrow (0.9, 20)\) and delayed subdiffusion \((0.9, 20) \rightarrow (0.6, 10)\), both for \( B = 0.1 \) and \( x_0 = 0 \), all quantities are given in arbitrarily chosen units. The plots show that for larger \( \nu \) \( g \)-subdiffusion goes to the final process faster. The convergence to the final process seems to be faster for the \((0.6, 10) \rightarrow (0.9, 20)\) process than for the \((0.9, 20) \rightarrow (0.6, 10)\) one.

In general, the \( g \)-subdiffusion equation can be applied to describe subdiffusion for which the MSD time evolution is other than Eq. \[3\]. Let us assume that
\[ \sigma^2(t) = \eta(t), \tag{25} \]
where \( \eta \) fulfills the conditions \( \eta(0) = 0, \eta(\infty) = \infty, \) and \( \eta'(t) > 0 \) for \( t > 0 \). Comparing Eq. \[25\] with Eq. \[15\] we find that the \( g \)-subdiffusion equation Eq. \[4\] with
\[ g(t) = [\Gamma(1+\alpha)\eta(t)/2D_\alpha]^{1/\alpha}, \] where \( 0 < \alpha < 1 \), describes the process which generates Eq. \[25\]. As a particular case, subdiffusion with time-varying subdiffusion parameter may be defined by the following relation which is a simple generalization of Eq. \[3\] \[29\]
\[ \sigma^2(t) = A\tilde{t}^{\tilde{\alpha}(t)}, \tag{26} \]
with \( 0 < \tilde{\alpha}(t) < 1 \) for \( t > 0 \). It may seem that such a process can be described by the “ordinary” subdiffusion equation...
with the time-varying order of the fractional derivative

\[
\frac{C \partial^{\alpha(t)} C(x, t)}{\partial t^{\alpha(t)}} = D_\alpha \frac{\partial^2 C(x, t)}{\partial x^2}.
\]  

(27)

However, Eq. (27) is difficult to solve, in practice it can be solved numerically [51]. The process which generated Eq. (26) can be described by the \( g \)-subdiffusion equation with \( g(t) = [\Lambda \Gamma(1 + \alpha)/2D_\alpha]^{\alpha/\alpha \Gamma(1/\alpha)} \).

FIG. 3: The Green’s functions for the process \((0.9, 20) \rightarrow (0.6, 10)\). The description is similar to that of Fig. 1 for \( \nu = 1.2 \).

FIG. 4: The description is similar as that for Fig. 3 but for \( \nu = 3.0 \).

The aim of this paper has been to present the \( g \)-subdiffusion model and its application to describe transient subdiffusion from subdiffusion with parameters \( \alpha \) and \( D_\alpha \) to subdiffusion with parameters \( \beta \) and \( D_\beta \). In "intermediate" times the subdiffusive parameters, defined by Eq. (27), can remain unknown. We have considered a special case of the function \( g \), Eq. (27), which describes accelerating subdiffusion when \( \alpha < \beta \) and slowing subdiffusion when \( \alpha > \beta \). The model uses the \( g \)-subdiffusion equation with Caputo fractional time derivative with respect to another function \( g \).

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