Composite subdiffusion equation that describes transient subdiffusion

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(Received 25 May 2022; accepted 27 September 2022; published 13 October 2022)

A composite 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 α and D_α to subdiffusion with parameters β and D_β. The parameters are defined by the time evolution of the mean square displacement of diffusing particle $\sigma^2(t) = 2D_i t^i/\Gamma(1+i)$, $i = \alpha, \beta$. The function g controls the process at intermediate times. The composite subdiffusion equation is more general than the ordinary fractional subdiffusion equation with constant parameters; it has potentially wide application in modeling diffusion processes with changing parameters.

DOI: 10.1103/PhysRevE.106.044119

I. INTRODUCTION

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 ψ 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) α in a one-dimensional homogeneous system can be described by an ordinary subdiffusion equation with a fractional time derivative of the order $\alpha \in (0, 1)$,

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

where the Caputo fractional derivative is defined here as

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

where D_α is a generalized diffusion coefficient measured in the units of m^2/s^α, C is a concentration of diffusing particles, and f' denotes the first-order derivative of function f. Equation (1) can be transformed to its equivalent form with the fractional Riemann-Liouville time derivative of the order $1-\alpha$; see, for example, Ref. [2].

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

$$\sigma^2(t) = \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)}. \tag{3}$$

Equation (1) describes the subdiffusion process with constant parameters α and D_α. 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]. The examples are subdiffusion equations with parameters α and D_α dependent on the spatial variable [25,26], transitions from anomalous to Gaussian diffusion [27,28], and subdiffusion equations with linear combination of fractional time derivatives with different parameters α [29–31]. The CTRW model describing anomalous diffusion with changing subdiffusion parameters [32] and the ordinary CTRW model with a waiting time distribution that is a linear combination of two exponential distributions with different timescales [27] have been used to model anomalous diffusion with evolving parameters. Modification of a timescale in a diffusion model can lead to changes in diffusion parameters as well as in the type of diffusion [33,34]. A timescale changing can be made by means of a subordinated method [4,35–38]. Within this method, retarding and accelerating anomalous diffusions have been obtained [39,40]. Examples of processes that lead to a rescaling of diffusion are diffusing diffusivities where the diffusion coefficient evolves over time [37], passages through the layered media [41], and anomalous diffusion in an expanding medium [42]. We mention that a distributed order of fractional derivative in a subdiffusion equation can lead to delayed or accelerated subdiffusion [43–47].

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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 α and D_α, and after a long time (formally $t \to \infty$) the parameters are β and D_β. 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, and it is symbolically written as $(\alpha, D_\alpha) \to (\beta, D_\beta)$.

II. COMPOSITE SUBDIFFUSION EQUATION

Recently, the composite subdiffusion process characterized by parameters α, D_α, and by the function g has been considered in [34,48,49] (the process has been called g subdiffusion in the above cited papers). 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 fulfils the conditions $g(0) = 0$, $g(\infty) = \infty$, and $g'(t) > 0$ for $t > 0$, and the values of the function g are given in a time unit. Composite subdiffusion is described by the following equation:

$$\frac{{}^C\partial_g^\alpha C(x,t)}{\partial t^\alpha} = D_\alpha \frac{\partial^2 C(x,t)}{\partial x^2}, \tag{4}$$

where

$$\frac{{}^C d_g^\alpha f(t)}{dt^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (g(t) - g(u))^{-\alpha} f'(u) du \tag{5}$$

is the g-Caputo fractional derivative of the order $\alpha \in (0, 1)$ with respect to the function g [50]. 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 composite subdiffusion. We mention that equations with fractional time derivatives with respect to other functions have already been used to describe other diffusion processes [51,52].

The composite subdiffusion equation can be solved by means of the g-Laplace transform method. The g-Laplace transform is defined as [53]

$$\mathcal{L}_g[f(t)](s) = \int_0^\infty e^{-sg(t)} f(t) g'(t) dt. \tag{6}$$

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:

$$\mathcal{L}_g[f(t)](s) = \mathcal{L}[f(g^{-1}(t))](s). \tag{7}$$

Equation (7) provides the rule

$$\mathcal{L}_g[f(t)](s) = \mathcal{L}[h(t)](s) \Leftrightarrow f(t) = h(g(t)). \tag{8}$$

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 [48]

$$\mathcal{L}_g^{-1}\left[\frac{1}{s^{1+\nu}}\right](t) = \frac{g^\nu(t)}{\Gamma(1+\nu)}, \; \nu > -1, \tag{9}$$

$$\mathcal{L}_g^{-1}[s^\nu e^{-as^\mu}](t) \equiv f_{\nu,\mu}(g(t); a) = \frac{1}{g^{1+\nu}(t)} \sum_{k=0}^\infty \frac{1}{k!\Gamma(-\nu-\mu k)} \left(-\frac{a}{g^\mu(t)}\right)^k, \tag{10}$$

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

The calculations for solving Eq. (4) 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 [53]

$$\mathcal{L}_g\left[\frac{{}^C d_g^\alpha f(t)}{dt^\alpha}\right](s) = s^\alpha \mathcal{L}_g[f(t)](s) - s^{\alpha-1} f(0), \tag{11}$$

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

$$s^\alpha \mathcal{L}_g[C(x,t)](s) - s^{\alpha-1} C(x,0) = D_\alpha \frac{\partial^2 \mathcal{L}_g[C(x,t)](s)}{\partial x^2}. \tag{12}$$

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 the Green's function is the following solution to Eq. (12) for the initial condition $P(x,0|x_0) = \delta(x - x_0)$, where δ denotes the δ-Dirac function, and the boundary conditions $\mathcal{L}_g[P(\pm\infty, t|x_0)](s) = 0$,

$$\mathcal{L}_g[P(x,t|x_0)](s) = \frac{1}{2\sqrt{D_\alpha} s^{1-\alpha/2}} e^{-\frac{|x-x_0|}{\sqrt{D_\alpha}} s^{\alpha/2}}. \tag{13}$$

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

$$P(x,t|x_0) = \frac{1}{2\sqrt{D_\alpha}} f_{-1+\alpha/2,\alpha/2}\left(g(t); \frac{|x-x_0|}{\sqrt{D_\alpha}}\right). \tag{14}$$

Equations (9) and (13) provide

$$\sigma^2(t) = \frac{2D_\alpha}{\Gamma(1+\alpha)} g^\alpha(t). \tag{15}$$

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

$$P(x,t|x_0) = \frac{1}{2\sqrt{D_\alpha}} f_{-1+\alpha/2,\alpha/2}\left(t; \frac{|x-x_0|}{\sqrt{D_\alpha}}\right). \tag{16}$$

We mention that $f_{-1+\alpha/2,\alpha/2}$ is called the Mainardi function [54].

III. TRANSIENT SUBDIFFUSION

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

$$\sigma^2(t) = \begin{cases} \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha, & t \to 0, \\ \frac{2D_\beta}{\Gamma(1+\beta)} t^\beta, & t \to \infty. \end{cases} \tag{17}$$

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

$$g(t) = \begin{cases} t, & t \to 0, \\ At^{\beta/\alpha}, & t \to \infty, \end{cases} \tag{18}$$

where

$$A = \left(\frac{D_\beta \Gamma(1+\alpha)}{D_\alpha \Gamma(1+\beta)} \right)^{\frac{1}{\alpha}}. \tag{19}$$

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 controls the process in intermediate times, fulfils the conditions $a(0) = 1$, $a(\infty) = 0$, and a generates an increasing function g in the time domain. Since $g(t) \to At^{\beta/\alpha}$ when $t \to \infty$, Eq. (20) provides the additional condition

$$t \to \infty, \;\; a(t)t \to 0. \tag{21}$$

The function a can be assumed as

$$a(t) = \frac{1}{1 + \xi(t)}, \tag{22}$$

where ξ fulfils the conditions $\xi(0) = 0$ and $\xi(\infty) = \infty$. In the following we consider the process in which

$$\xi(t) = Bt^\nu, \tag{23}$$

where B is a parameter measured in the units of $1/\mathrm{s}^{1/\nu}$. The conditions $g(t), g'(t) > 0$ for $t > 0$ are met for any α and β, $\alpha, \beta \in (0, 1)$, when $\nu > 1$. From Eqs. (20), (22), and (23) we get

$$g(t) = \frac{t + ABt^{\frac{\beta}{\alpha}+\nu}}{1 + Bt^\nu}, \tag{24}$$

$\nu > 1$. In this case the Green's function reads

$$P(x, t|x_0) = \frac{1}{2\sqrt{D_\alpha}} f_{-1+\alpha/2,\alpha/2}\left(\frac{t + ABt^{\frac{\beta}{\alpha}+\nu}}{1 + Bt^\nu}; \frac{|x - x_0|}{\sqrt{D_\alpha}} \right), \tag{25}$$

with $\nu > 1$ and A given by Eq. (19).

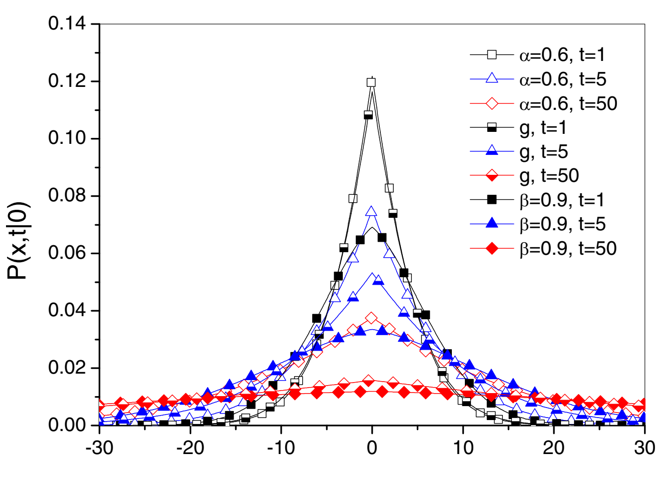

FIG. 1. The Green's functions of the composite subdiffusion equation Eq. (25) that describes the transition (0.6, 10) → (0.9, 20) (half-full symbols) for $\nu = 1.2$. The Green's functions of ordinary subdiffusion equation Eq. (16) are calculated for $\alpha = 0.6$ and $D_\alpha = 10$ (empty symbols) and for $\beta = 0.9$ and $D_\beta = 20$ (full symbols). Time values are given in the legend, and all quantities are given in arbitrarily chosen units.

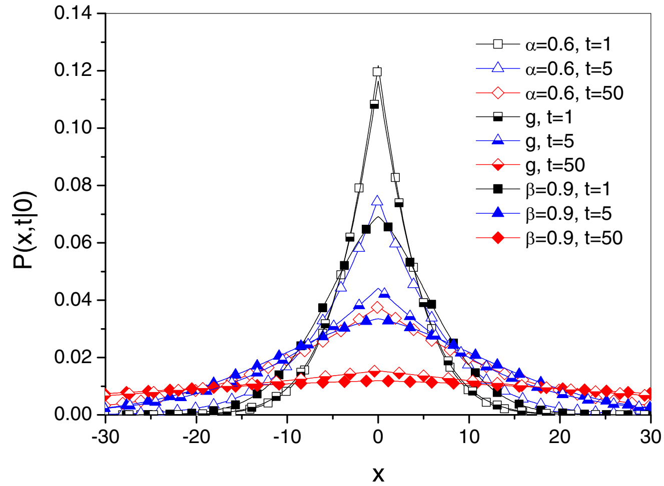

FIG. 2. The description is similar to that for Fig. 1 but for $\nu = 3.0$.

The plots of the Green's functions Eq. (25) describing the process $(\alpha, D_\alpha) \to (\beta, D_\beta)$ are compared with the Green's functions for ordinary subdiffusion with parameters (α, D_α) and (β, D_β) in Figs. 1–4. We consider accelerated subdiffusion (0.6, 10) → (0.9, 20) (then $A = 2.81$) and delayed subdiffusion (0.9, 20) → (0.6, 10) ($A = 0.50$), both for $B = 0.1$ and $x_0 = 0$, and all quantities are given in arbitrarily chosen units. The plots show that for larger ν composite subdiffusion goes to the final process faster. The convergence to the final process seems to be faster for the (0.6, 10) → (0.9, 20) process than for the (0.9, 20) → (0.6, 10) one.

IV. PROPOSALS FOR A DIFFERENT USE OF THE COMPOSITE SUBDIFFUSION EQUATION

In Sec. III we have considered the subdiffusion process explicitly defined at some initial and final time intervals. We define the process in intermediate times by choosing the function a and using Eq. (20). However, the composite subdiffusion equation can be used to describe a process for which

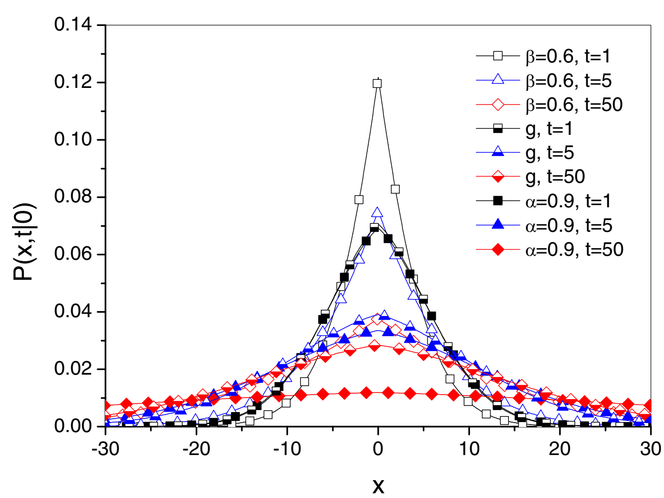

FIG. 3. The Green's functions for the process (0.9, 20) → (0.6, 10). The description is similar to that of Fig. 1 for $\nu = 1.2$.

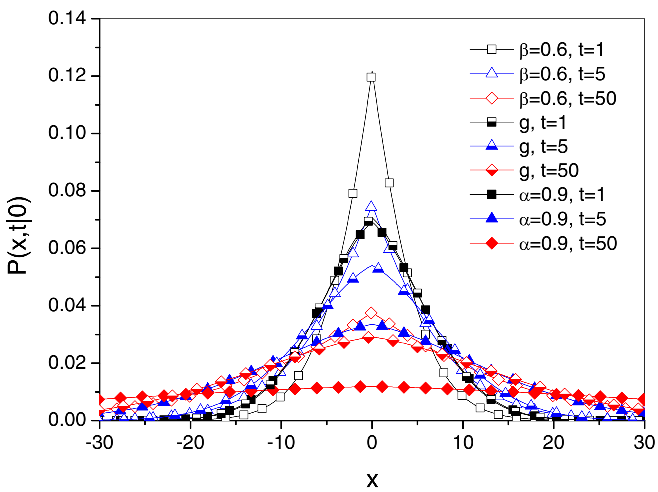

FIG. 4. The description is similar to that for Fig. 3 but for $\nu = 3.0$.

MSD is known in the entire time domain. Let us assume that

$$\sigma^2(t) = \eta(t), \tag{26}$$

where η fulfils the conditions $\eta(0) = 0$, $\eta(\infty) = \infty$, and $\eta'(t) > 0$ for $t > 0$. We limit our considerations to subdiffusion which is defined here as follows: a diffusion process is subdiffusion if there exist numbers $E > 0$ and $\gamma \in (0, 1)$ such that $\eta(t) < Et^{\gamma}$ for $t > 0$. For ordinary subdiffusion η is a power function, and for slow subdiffusion (ultraslow diffusion) the function contains a combination of logarithm functions. The overviews of the functions η for different diffusion processes are presented in Refs. [55,56]. Comparing Eq. (26) with Eq. (15), we find that the composite subdiffusion equation, Eq. (4), with

$$g(t) = \left[\frac{\Gamma(1+\alpha)\eta(t)}{2D_\alpha}\right]^{1/\alpha}, \tag{27}$$

$\alpha \in (0, 1)$, describes the process which generates Eq. (26). Similar to the model considered in Sec. III, it can be assumed that parameters α and D_α, occurring in the composite subdiffusion equation, characterize the subdiffusion process in some initial time interval.

It is interesting to use the composite subdiffusion equation to describe a subdiffusion process with a time-varying subdiffusion parameter $\tilde{\alpha}(t) \in (0, 1)$. This process can be described by the following equation [57,58]:

$$\frac{^C\partial^{\tilde{\alpha}(t)}C(x,t)}{\partial t^{\tilde{\alpha}(t)}} = D_\alpha \frac{\partial^2 C(x,t)}{\partial x^2}, \tag{28}$$

with the Caputo-type fractional derivative $^C\partial^{\tilde{\alpha}(t)}f(t)/\partial t^{\tilde{\alpha}(t)} = [1/\Gamma(1-\tilde{\alpha}(t))]\int_0^t f'(\tau)(t-\tau)^{-\tilde{\alpha}(t)}d\tau$. However, Eq. (28) is difficult to solve; in practice it can be solved numerically [59]. For the process described by Eq. (28) there is [57]

$$\sigma^2(t) = \frac{2D_\alpha t^{\tilde{\alpha}(t)}}{\Gamma(1+\tilde{\alpha}(t))}. \tag{29}$$

Assuming $\tilde{\alpha}(0) = \alpha$, from Eqs. (26), (27), and (29) we get

$$g(t) = \left(\frac{\Gamma(1+\alpha)}{\Gamma(1+\tilde{\alpha}(t))}\right)^{1/\alpha} t^{\tilde{\alpha}(t)/\alpha}. \tag{30}$$

The composite subdiffusion equation with the function g Eq. (30) describes the subdiffusion process generating the relation (29). Then the Green's function is Eq. (14) with g Eq. (30). The application of the composite subdiffusion equation to modeling processes with a time-varying subdiffusion parameter will be considered in more detail elsewhere.

V. FINAL REMARKS

The aim of this paper is to present the composite subdiffusion equation and its application to describe transient subdiffusion from subdiffusion with parameters α and D_α to subdiffusion with parameters β and D_β. In intermediate times the subdiffusive parameters, defined by Eq. (3), can remain unknown. However, by choosing the function a and using Eq. (20), we define the process in intermediate times. The model uses the composite subdiffusion equation with a Caputo fractional time derivative with respect to another function g, Eq. (4). We have considered a special case of the function g, Eq. (24), which describes accelerating subdiffusion when $\alpha < \beta$ and slowing subdiffusion when $\alpha > \beta$.

We have also shown that the process for which the time evolution of MSD $\sigma^2(t)$ is defined in the entire time domain can be described by the composite subdiffusion equation with the function given by Eq. (27). This equation is solvable by means of the g-Laplace transform method and can be used to model diffusion processes, e.g., in a membrane system, assuming appropriate boundary conditions at the membrane. Of course, $\sigma^2(t)$ do not always define the diffusion process unambiguously. An example of this is the combination of ordinary subdiffusion and superdiffusion, which leads to the relation $\sigma^2(t) \sim t$ characteristic of normal diffusion [60]. In this paper we consider subdiffusion processes, the parameters of which may change over time; normal diffusion is treated here as a special case of subdiffusion for $\alpha = 1$. When the initial process is ordinary subdiffusion, the stochastic interpretation of this process can be found using the modified continuous time random walk model, see Ref. [48]. However, for other processes described by the composite subdiffusion equation, there is no stochastic model so far.

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