Cattaneo–type subdiffusion equation

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The ordinary subdiffusion equation, with fractional time derivatives of at most first order, describes a process in which the propagation velocity of diffusing molecules is unlimited. To avoid this non-physical property the Cattaneo diffusion equation has been proposed. Compared to the ordinary subdiffusion equation, the Cattaneo equation contains an additional time derivative of order greater than one and less than or equal to two. The fractional order of the additional derivative depends on the subdiffusion exponent. We study a Cattaneo-type subdiffusion equation (CTSE) that differs from the ordinary subdiffusion equation by an additional integro–differential operator (AO) which may be independent of subdiffusion parameters. The AO describes processes affecting ordinary subdiffusion. The equation is derived combining the modified diffusive flux equation with the continuity equation. It can also be obtained within the continuous time random walk model with the waiting time distribution for the molecule to jump controlled by the kernel of AO. As examples, the CTSEs with the additional Caputo fractional time derivative of the order independent of the subdiffusion exponent and with the AO generated by a slowly varying function are considered. We discuss whether the ordinary subdiffusion equation and CTSE provide qualitative differences in the description of subdiffusion.

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I. INTRODUCTION

Subdiffusion occurs in media in which particle random walk is very hindered. The examples are transport of molecules in viscoelastic chromatin network [1], porous media [2], living cells [3], transport of sugars in agarose gel [4], and antibiotics in bacterial biofilm [5, 6]. Subdiffusion is often defined as an anomalous diffusion process in which the temporal evolution of mean square displacement (MSD) of a particle is $\sigma^2(t) = 2Dt^\alpha/\Gamma(1+\alpha)$, where $\alpha \in (0,1)$ is the subdiffusion parameter (exponent), D is a subdiffusion coefficient given in units of $\mathrm{m}^2/\mathrm{s}^\alpha$. Frequently, ordinary subdiffusion is described by a fractional differential equation [7–15] with the Riemann-Liouville fractional time derivative of $1-\alpha$ order or an equation with the Caputo fractional time derivative of the order α.

For the parabolic normal diffusion equation and subdiffusion equation with a time derivative of at most first order the Green's function $P(x,t)$, which is the probability density of finding the molecule at position x at time t, is greater than zero for any x and $t > 0$. It means that the propagation velocity of some particles is arbitrarily high. To avoid this non–physical property, the Cattaneo normal diffusion equation has been proposed; the equation was originally used to describe heat propagation [16]. The Cattaneo normal diffusion equation involves a second-order time derivative controlled by the parameter τ. The derivation of the equation is based on the assumption that the flux of diffusing molecules is delayed by time τ with respect to the concentration gradient. While the Cattaneo hyperbolic normal diffusion equation is well defined, the Cattaneo subdiffusion equation can take various non-equivalent forms, see for example Refs. [17–25]. It contains a time derivative of the order greater than one and less than or equal to two; the fractional order of this derivative depends on α. The Cattaneo equation with the Caputo and/or the Riemann–Liouville fractional derivatives have been used to describe subdiffusion and

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subdiffusion with reactions [26–31], in particular neutron transport inside the core of a nuclear reactor [32], heat transport in porous media [33], and in a system with glass spheres in a tank filled with air [34]. Cattaneo equations with fractional derivatives other than those mentioned above have also been considered. The examples are the equations with Caputo–Fabrizio fractional time derivative [35], with tempered Caputo derivative [36], and with Hilfer fractional derivative with respect to another function [37].

We consider a Cattaneo-type subdiffusion equation (CTSE) which is defined here as an equation that differs from the ordinary subdiffusion one by an additional operator acting on the time variable. The operator is generated by the constitutive equation describing the relation between the probability density flux and the gradient of Green's function. Combining this equation with the continuity equation the CTSE is obtained. The equation can also be derived within the continuous time random walk model, in which the distribution of the waiting time for a molecule to jump is controlled by the additional operator. The Cattaneo-type subdiffusion equation takes into account a process, called the additional Cattaneo–type process (ACTP), that change ordinary subdiffusion. An example is diffusion of antibiotics in bacterial biofilms. In a dense biofilm subdiffusion of antibiotic molecules may occur. However, bacteria can activate defense mechanisms against the effects of antibiotics. Some of them additionally slow down subdiffusion or temporarily trap antibiotic molecules [38, 39].

In the case of passive subdiffusion, the solutions to the Cattaneo equation and the ordinary subdiffusion one are usually not much different from each other. Then, the latter equation, which appears to be easier to solve, is used to describe diffusion. However, there are processes that both equations provide qualitatively different results even for small τ. Examples of this are diffusive and subdiffusive impedance [40–43]. When considering subdiffusion described by a Cattaneo-type equation, the question arises whether such an equation gives a significant difference compared to the use of the ordinary subdiffusion equation. Therefore, we consider functions describing how the ACTP affects ordinary subdiffusion.

The general subdiffusion equation controlled by a memory kernel (MK) (equivalent to Eqs. (13)–(15) presented later), which is the basis for deriving the Cattaneo-type equation, has been considered to derive various types of anomalous diffusion equations. Examples are equations generated by distributed order MK [44–48], power–law MK [45], and truncated power law MK [44]. The equation with MK has been used to derive multi-fractional diffusion equations [27, 46–48]. Generalized diffusion equations with MK can also be derived by means of the subordination method [49].

The most commonly used function characterizing diffusion is a temporal evolution of the mean square displacement of a diffusing particle. However, MSD alone does not clearly determine the type of diffusion [50, 51]. We also consider the first passage time distribution of a particle through an arbitrarily chosen point $F(t;x)$.

We consider subdiffusion in a one-dimensional homogeneous system with constant parameters. We pay attention to the interpretation of ACTP and assesses how this process affects subdiffusion. In Sec. II the subdiffusion equation generated by the generalized flux equation controlled by a MK β is derived. In Sec. III we consider functions describing subdiffusion. The explicit forms of the functions are given in terms of the Laplace transform. In Sec. IV the function β linear with respect to the parameter τ is considered, this function generates a Cattaneo-type subdiffusion equation. The CTSEs with the additional Caputo fractional time derivative of the order independent of the subdiffusion exponent and with the additional operator generated by a slowly varying function are studied in Secs. V and VI, respectively. Final remarks are in Sec. VII.

II. SUBDIFFUSION EQUATION GENERATED BY GENERALIZED FLUX EQUATION

The subdiffusion equation can be obtained phenomenologically by a combination of the continuity equation

$$\frac{\partial P(x,t)}{\partial t}=-\frac{\partial J(x,t)}{\partial x}. \tag{1}$$

and the constitutive equation that defines the flux J. For ordinary subdiffusion the flux is defined as

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

where $\alpha\in(0,1)$, with the Riemann–Liouville fractional derivative

$$\frac{^{RL}d^{\nu}f(t)}{dt^{\nu}}=\frac{1}{\Gamma(n-\nu)}\frac{d^n}{dt^n}\int_0^t (t-u)^{n-\nu-1}f(u)du, \tag{3}$$

n is a natural number, $n=[\nu]+1$ when $\nu\notin\mathcal{N}$ and $n=\nu\in\mathcal{N}$. Throughout this paper we assume that the initial particle position is $x_0=0$. Combining Eqs. (1) and (2) one gets

$$\frac{\partial P(x,t)}{\partial t}=D\frac{^{RL}\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2}. \tag{4}$$

When deriving a diffusion equation, it is convenient to use the Laplace transform

$$\mathcal{L}[f(t)](s)=\int_0^\infty \mathrm{e}^{-st}f(t)dt\equiv\hat{f}(s). \tag{5}$$

The Laplace transforms of derivatives are

$$\mathcal{L}\left[\frac{^{RL}d_g^{\alpha}f(t)}{dt^{\alpha}}\right](s)=s^{\alpha}\mathcal{L}\left[f(t)\right](s),\ \alpha\in(0,1), \tag{6}$$

$$\mathcal{L}\left[\frac{d^n f(t)}{dt^n}\right] = s^n \mathcal{L}[f(t)](s) - \sum_{i=0}^{n-1} s^{n-1-i} f^{(i)}(0), \quad (7)$$

where $f^{(i)}(t) = d^i f(t)/dt^i$, i and n are natural numbers. The Laplace transforms of Eqs. (1), (2), and (4) are, respectively,

$$s\hat{P}(x,s) - P(x,0) = -\frac{\partial \hat{J}(x,s)}{\partial x}, \quad (8)$$

$$\hat{J}(x,s) = -Ds^{1-\alpha}\frac{\partial \hat{P}(x,s)}{\partial x}, \quad (9)$$

$$s\hat{P}(x,s) - P(x,0) = Ds^{1-\alpha}\frac{\partial^2 \hat{P}(x,s)}{\partial x^2}. \quad (10)$$

The assumption under which the Cattaneo normal diffusion equation was derived is that the flux is delayed with respect to the concentration gradient. However, in the case of subdiffusion, the relation between the flux and the concentration gradient can be assumed in many ways, see Refs. [17, 18]. We assume that

$$\hat{\beta}(s;\tau)\hat{J}(x,s) = -Ds^{1-\alpha}\frac{\partial \hat{P}(x,s)}{\partial x}, \quad (11)$$

β is a memory kernel which depends on the parameter τ. We also assume that for $\tau = 0$ we get ordinary subdiffusion equation, then

$$\hat{\beta}(s,0) = 1. \quad (12)$$

Eqs. (8) and (11) provide

$$\hat{\beta}(s;\tau)\big[s\hat{P}(x,s) - P(x,0)\big] = Ds^{1-\alpha}\frac{\partial^2 \hat{P}(x,s)}{\partial x^2}. \quad (13)$$

For $\hat{\beta}(s;\tau) = 1 + \tau s$ and $\alpha = 1$ we get the well–known Cattaneo normal diffusion equation.

In the time domain Eq. (13) reads

$$\mathcal{B}_{t;\tau}[P(x,t)] = D\frac{{}^{RL}\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2}, \quad (14)$$

where

$$\mathcal{B}_{t;\tau}[f(t)] = \int_0^t \beta(t-t';\tau) f^{(1)}(t')dt'. \quad (15)$$

Constraints on the function β can be derived from additional considerations, see the comment under Eq. (29).

III. FUNCTIONS DESCRIBING DIFFUSION

The Green's function is the solution to diffusion equation with the boundary conditions

$$P(\pm\infty,t) = 0, \quad (16)$$

and the initial condition

$$P(x,0) = \delta(x), \quad (17)$$

where δ is the delta–Dirac function. The above initial condition is sufficient to determine the Laplace transform of a time derivative of at most first order. When computing the transform of other operators additional initial conditions may be needed. We assume that the only non-zero initial condition is Eq. (17).

In terms of the Laplace transform the Green's function of Eq. (14) is

$$\hat{P}(x,s) = \frac{\sqrt{\hat{\beta}(s;\tau)}}{2\sqrt{D}s^{1-\alpha/2}} \mathrm{e}^{-\frac{s^{\alpha/2}|x|\sqrt{\hat{\beta}(s;\tau)}}{\sqrt{D}}}. \quad (18)$$

The Green's function Eq. (18) is symmetrical, $P(x,t) = P(-x,t)$, this property is used in deriving further equations. On the basis of the Green's function, other functions characterizing diffusion processes are determined. A frequently used function is the temporal evolution of the mean square displacement σ^2 of diffusing particle,

$$\sigma^2(t) = 2\int_0^\infty x^2 P(x,t)dx. \quad (19)$$

In terms of the Laplace transform we get

$$\hat{\sigma^2}(s) = \frac{2D}{s^{1+\alpha}\hat{\beta}(s;\tau)} \quad (20)$$

Another function that characterizes diffusion is the first passage time distribution F. Assuming $x > 0$, the distribution of time of the first particle passing the point x can be calculated by means of the formula

$$F(t;x) = -\frac{\partial}{\partial t}\int_{-x}^{x} P(x',t)dx'. \quad (21)$$

In terms of the Laplace transform the above equation reads

$$\hat{F}(s;x) = 1 - s\int_{-x}^{x} \hat{P}(x',s)dx'. \quad (22)$$

Putting Eq. (18) to Eq. (22) we get

$$\hat{F}(s;x) = \mathrm{e}^{-\frac{xs^{\alpha/2}\sqrt{\hat{\beta}(s;\tau)}}{\sqrt{D}}}. \quad (23)$$

The probability flux at x is defined as

$$J(x,t) = -\frac{\partial}{\partial t}\int_{-\infty}^{x} P(x',t)dx'. \quad (24)$$

The Laplace transform Eq. (24) is

$$\hat{J}(x,s) = 1 - s\int_{-\infty}^{x} \hat{P}(x',s)dx'. \quad (25)$$

For $x > 0$ we obtain

$$\hat{J}(x,s) = \frac{1}{2}\mathrm{e}^{-\frac{xs^{\alpha/2}\sqrt{\hat{\beta}(s;\tau)}}{\sqrt{D}}}. \quad (26)$$

The equations (23) and (26) provide the relation

$$J(x,t)=\frac{1}{2}F(t;x),\ x>0. \tag{27}$$

For $x<0$ the flux is negative, then $J(x,t)=-F(t;x)/2$.

The equation (14) can also be derived by changing the probability distribution ψ of the waiting time for a molecule to jump within the continuous time random walk model. The model provides the diffusion equation given in terms of the Laplace transform, see Ref. [53],

$$s\hat{P}(x,s)-P(x,0)=\frac{\epsilon^2 s\hat{\psi}(s)}{2[1-\hat{\psi}(s)]}\frac{\partial^2\hat{P}(x,s)}{\partial x^2}, \tag{28}$$

where ϵ is the mean value of a single jump length. Comparing Eqs. (13) and (28) we obtain

$$\hat{\psi}(s)=\frac{1}{1+\lambda s^\alpha\hat{\beta}(s;\tau)}, \tag{29}$$

where $\lambda=\epsilon^2/2D$. The parameter describing subdiffusion is D, ϵ is a scale-dependent parameter. We further assume that ϵ is small, which provides $\lambda\ll 1$. Due to the normalization of ψ, $\hat{\psi}(0)=1$, $\hat{\beta}$ meets the condition $s^\alpha\hat{\beta}(s;\tau)\to 0$ when $s\to 0$.

The question arises whether the Cattaneo subdiffusion equation brings a new quality in comparison with the ordinary subdiffusion equation. We compare the functions F and σ^2 derived for $\tau=0$ and for $\tau\neq 0$. The functions F_R and σ^2_R show the time evolution of the relative change of first passage time distribution and MSD, respectively,

$$F_R(t;x)=\frac{F_{\tau=0}(t;x)-F(t;x)}{F_{\tau=0}(t;x)}, \tag{30}$$

$$\sigma^2_R(t)=\frac{\sigma^2_{\tau=0}(t)-\sigma^2(t)}{\sigma^2_{\tau=0}(t)}, \tag{31}$$

in Eq. (30) x is a parameter. Additionally, we consider the relative change of the Green's function

$$P_R(x,t)=\frac{P_{\tau=0}(x,t)-P(x,t)}{P_{\tau=0}(x,t)}, \tag{32}$$

here x is a random variable, t is a parameter.

IV. CATTANEO–TYPE SUBDIFFUSION EQUATION

Let us assume that

$$\hat{\beta}(s;\tau)=1+\tau\hat{\gamma}(s). \tag{33}$$

Combining Eqs. (13) and (33) we obtain

$$\begin{aligned}(1+\tau\hat{\gamma}(s))\big[s\hat{P}(x,s)-P(x,0)\big]& \\ =Ds^{1-\alpha}\frac{\partial^2\hat{P}(x,s)}{\partial x^2}&.\end{aligned} \tag{34}$$

The inverse Laplace transform of Eq. (34) provides the Cattaneo–type subdiffusion equation

$$\tau\mathcal{D}_t[P(x,t)]+\frac{\partial P(x,t)}{\partial t}=D\frac{{}^{RL}\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{35}$$

where

$$\mathcal{D}_t[f(t)]=\int_0^t\gamma(t-t')f^{(1)}(t')dt'. \tag{36}$$

The function γ is determined by the ACTP. We note that for some γ the operator $\mathcal{D}_t$ can be interpreted as a fractional time derivative.

The Laplace transforms of Green's function and first passage time distribution are

$$\hat{P}(x,s)=\frac{\sqrt{1+\tau\hat{\gamma}(s)}}{2\sqrt{D}s^{1-\alpha/2}}\mathrm{e}^{-\frac{s^{\alpha/2}|x|\sqrt{1+\tau\hat{\gamma}(s)}}{\sqrt{D}}}, \tag{37}$$

$$\hat{F}(s;x)=\mathrm{e}^{-\frac{xs^{\alpha/2}\sqrt{1+\tau\hat{\gamma}(s)}}{\sqrt{D}}}. \tag{38}$$

Assuming $\tau\hat{\gamma}(s)<1$, the above functions can be presented as power series with respect to τ,

$$\hat{P}(x,s)=\frac{1}{2\sqrt{D}s^{1-\alpha/2}}\mathrm{e}^{-\frac{|x|s^{\alpha/2}}{\sqrt{D}}}\sum_{i=0}^\infty\tau^i a_i(x,s)\hat{\gamma}^i(s), \tag{39}$$

$$\hat{F}(s;x)=\mathrm{e}^{-\frac{|x|s^{\alpha/2}}{\sqrt{D}}}\sum_{i=0}^\infty\tau^i b_i(x,s)\hat{\gamma}^i(s). \tag{40}$$

The functions $a_i(x,s)$ and $b_i(x,s)$ are determined applying the following series $\sqrt{1+u}=1+u/2+\sum_{n=2}^\infty(-1)^{n-1}(2n-1)!!u^n/2^n n!$, $|u|<1$, and $\mathrm{e}^{-u}=\sum_{n=0}^\infty(-1)^n u^n/n!$. In the following, we use the approximation of $\hat{P}$ and $\hat{F}$ including four leading terms in the series. For $0\leq i\leq 3$ we have

$$a_0(x,s)=1,\ a_1(x,s)=\frac{1}{2}\Big(1-\frac{|x|s^{\alpha/2}}{\sqrt{D}}\Big), \tag{41}$$

$$a_2(x,s)=\frac{1}{8}\Big(-1-\frac{|x|s^{\alpha/2}}{\sqrt{D}}+\frac{|x|^2s^\alpha}{D}\Big), \tag{42}$$

$$a_3(x,s)=\frac{1}{16}\Big(1+\frac{|x|s^{\alpha/2}}{\sqrt{D}}-\frac{|x|^{3/2}s^{3\alpha/2}}{3D^{3/2}}\Big), \tag{43}$$

$$b_0(x,s)=1,\ b_1(x,s)=-\frac{|x|s^{\alpha/2}}{2\sqrt{D}}, \tag{44}$$

$$b_2(x,s)=\frac{|x|s^{\alpha/2}}{8\sqrt{D}}\Big(1+\frac{|x|s^{\alpha/2}}{\sqrt{D}}\Big), \tag{45}$$

$$b_3(x,s)=\frac{-|x|s^{\alpha/2}}{16\sqrt{D}}\Big(12+\frac{|x|s^{\alpha/2}}{\sqrt{D}}+\frac{|x|^2s^\alpha}{3D}\Big). \tag{46}$$

From Eqs. (20), (29), and (33) we have

$$\hat{\sigma}^2(s)=\frac{2D}{s^{1+\alpha}(1+\tau\hat{\gamma}(s))}, \tag{47}$$

$$\hat{\psi}(s) = \frac{1}{1+\lambda s^\alpha + \lambda\tau s^\alpha \hat{\gamma}(s)}. \tag{48}$$

The series representations of the above functions are

$$\hat{\sigma^2}(s) = \frac{2D}{\Gamma(1+\alpha)s^{1+\alpha}} \sum_{i=0}^{\infty} \tau^i(-\hat{\gamma}(s))^i. \tag{49}$$

$$\hat{\psi}(s) = \sum_{i=0}^{\infty} \tau^i \hat{\gamma}^i(s) \sum_{n=i}^{\infty} \binom{n}{i} (-\lambda)^n s^{n\alpha}. \tag{50}$$

The interpretation of ACTP uses the function ψ. When $\lambda \ll 1$ we have

$$\hat{\psi}(s) \approx \hat{\psi}_{\tau=0}(s)\hat{\psi}_\gamma(s), \tag{51}$$

where

$$\hat{\psi}_{\tau=0}(s) = \frac{1}{1+\lambda s^\alpha}, \tag{52}$$

$$\hat{\psi}_\gamma(s) = \frac{1}{1+\lambda\tau s^\alpha \hat{\gamma}(s)}. \tag{53}$$

In the time domain Eq. (51) reads

$$\psi(t) \approx \int_0^t \psi_{\tau=0}(t-t')\psi_\gamma(t')dt'. \tag{54}$$

The function $\psi_{\tau=0}$ is the distribution of the waiting time for a molecule to jump in a subdiffusive medium characterized by the parameters α and D, ψ_γ is the distribution of the waiting time when an additional mechanism disturbing the jump is turned on.

V. CTSE WITH THE ADDITIONAL CAPUTO FRACTIONAL TIME DERIVATIVE

Let

$$\hat{\gamma}(s) = s^\kappa,\ 0 < \kappa \le 1. \tag{55}$$

In terms of the Laplace transform we get

$$(\tau s^\kappa + 1)\left[s\hat{P}(x,s) - P(x,0)\right] = Ds^{1-\alpha}\frac{\partial^2 \hat{P}(x,s)}{\partial x^2}. \tag{56}$$

Using the relation

$$\mathcal{L}\left[\frac{{}^C\partial^\alpha f(t)}{\partial t^\alpha}\right](s) = s^\alpha \hat{f}(s) - \sum_{i=0}^{n-1} s^{\alpha-1-i} f^{(i)}(0), \tag{57}$$

where

$$\frac{{}^C d^\alpha f(t)}{dt^\alpha} = \frac{1}{\Gamma(n-\alpha)}\int_0^t (t-t')^{n-\alpha-1} f^{(n)}(t')dt' \tag{58}$$

is the Caputo fractional derivative (the natural number n is defined as under Eq. (3)), we get

$$\tau\frac{{}^C\partial^{1+\kappa}P(x,t)}{\partial t^{1+\kappa}} + \frac{\partial P(x,t)}{\partial t} = D\frac{{}^{RL}\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{59}$$

the initial conditions are $P(x,0) = \delta(x)$ and $P^{(1)}(x,0) = 0$.

The following formula plays a key role in calculating the inverse Laplace transforms [52]

$$\mathcal{L}^{-1}\left[s^\nu e^{-as^\beta}\right](t) \equiv f_{\nu,\beta}(t;a) \tag{60}$$
$$= \frac{1}{t^{1+\nu}}\sum_{j=0}^{\infty}\frac{1}{j!\Gamma(-\nu-\beta j)}\left(-\frac{a}{t^\beta}\right)^j,$$

$a, \beta > 0$, $f_{\nu,\beta}$ is a special case of the H–Fox function. From Eqs. (39)–(46) and Eq. (60) we get

$$\begin{aligned}P(x,t) = \frac{1}{2\sqrt{D}}\Bigg[&\xi_{-1+\alpha/2}(|x|,t) + \frac{\tau}{2}\Big(\xi_{-1+\kappa+\alpha/2}(|x|,t) - \frac{|x|}{\sqrt{D}}\xi_{-1+\kappa+\alpha}(|x|,t)\Big) \\ &+ \frac{\tau^2}{8}\Big(-\xi_{-1+2\kappa+\alpha/2}(|x|,t) - \frac{|x|}{\sqrt{D}}\xi_{-1+2\kappa+\alpha}(|x|,t) + \frac{|x|^2}{D}\xi_{-1+2\kappa+3\alpha/2}(|x|,t)\Big) \\ &+ \frac{\tau^3}{16}\Big(\xi_{-1+3\kappa+\alpha/2}(|x|,t) + \frac{|x|}{\sqrt{D}}\xi_{-1+3\kappa+\alpha}(|x|,t) - \frac{|x|^3}{3D^{3/2}}\xi_{-1+3\kappa+2\alpha}(|x|,t)\Big)\Bigg],\end{aligned} \tag{61}$$

$$F(t;x) = \xi_0(|x|,t) - \frac{\tau|x|}{2\sqrt{D}}\xi_{\kappa+\alpha/2}(|x|,t) + \frac{\tau^2|x|}{8\sqrt{D}}\Big(\xi_{2\kappa+\alpha/2}(|x|,t) + \frac{|x|}{\sqrt{D}}\xi_{2\kappa+\alpha}(|x|,t)\Big) \\ - \frac{\tau^3|x|}{16\sqrt{D}}\Big(12\xi_{3\kappa+\alpha/2}(|x|,t) + \frac{|x|}{\sqrt{D}}\xi_{3\kappa+\alpha}(|x|,t) + \frac{|x|^2}{3D}\xi_{3\kappa+3\alpha/2}(|x|,t)\Big), \quad (62)$$

where

$$\xi_\nu(x,t) \equiv f_{\nu,\alpha/2}\left(t;\frac{x}{\sqrt{D}}\right). \quad (63)$$

A special case of this function for $\nu = -1+\alpha/2$ is called the Mainardi function.

Assuming $\tau s^\kappa < 1$ we obtain

$$\hat{\sigma^2}(s) = \frac{2D}{s^{1+\alpha}}\sum_{i=0}^{\infty}(-\tau)^i s^{\kappa i}. \quad (64)$$

It is not possible to calculate the inverse Laplace transform of the series in the above equation term by term. Therefore, we calculate the transform of $\mathrm{e}^{-as^\mu}\hat{\sigma^2}(s)$, $a,\mu > 0$, using Eq. (60), next the limit of the obtained function when $a \to 0^+$ is calculated; the result is independent of the parameter μ. We obtain

$$\sigma^2(t) = 2Dt^\alpha \sum_{i=0}^{\infty}\frac{(-\tau)^i}{\Gamma(1+\alpha-i\kappa)t^{i\kappa}}. \quad (65)$$

In the long time limit the functions Eqs. (62) and (65) generate the following relations

$$F_R(t\to\infty;x) = A_\kappa\frac{\tau}{t^\kappa}, \quad (66)$$

$$\sigma_R^2(t\to\infty) = B_\kappa\frac{\tau}{t^\kappa}, \quad (67)$$

where $A_\kappa = -\Gamma(-\alpha/2)/[2\Gamma(-\kappa-\alpha/2)]$ and $B_\kappa = \Gamma(1+\alpha)/\Gamma(1+\alpha-\kappa)$.

For a sufficiently small s the series expansion of the function $\hat{\psi}$ with respect to τ is

$$\hat{\psi}(s) = \sum_{n=0}^{\infty}\tau^n\sum_{i=n}^{\infty}(-\lambda)^i\binom{i}{n}s^{\alpha i+\kappa n}. \quad (68)$$

Using the same procedure as for calculating Eq. (65), we get

$$\psi(t) = \sum_{n=0}^{\infty}\tau^n\sum_{i=n}^{\infty}\binom{i}{n}\frac{(-\lambda)^i}{\Gamma(-\alpha i-\kappa n)t^{1+\alpha i+\kappa n}}. \quad (69)$$

In the limit of long time we have

$$\psi(t\to\infty) = \frac{-\lambda}{t^{1+\alpha}}\left[\frac{1}{\Gamma(-\alpha)} - \frac{\lambda}{\Gamma(-2\alpha)t^\alpha} + \frac{\tau}{\Gamma(-\alpha-\kappa)t^\kappa}\right]. \quad (70)$$

The equation (69) provides

$$\psi_{\tau=0}(t) = \sum_{i=1}^{\infty}\frac{(-\lambda)^i}{\Gamma(-\alpha i)t^{1+\alpha i}}. \quad (71)$$

Based on Eqs. (53), (55), and (71) we get

$$\psi_\gamma(t) = \sum_{i=1}^{\infty}\frac{(-\lambda\tau)^i}{\Gamma(-(\alpha+\kappa)i)t^{1+(\alpha+\kappa)i}}. \quad (72)$$

For a short time (which corresponds to large s in the Laplace transform) we have $\psi_{\tau=0}(t) \sim 1/t^{1-\alpha}$ and $\psi_\gamma(t) \sim t^\kappa/t^{1-\alpha}$, in the long time limit there is $\psi_{\tau=0}(t) \sim 1/t^{1+\alpha}$ and $\psi_\gamma(t) \sim 1/t^{1+\alpha+\kappa}$. This suggests that for relatively short times the ACTP process is dominant over ordinary subdiffusion, the opposite is true for a long time. The function ψ is a convolution of $\psi_{\tau=0}$ and ψ_γ.

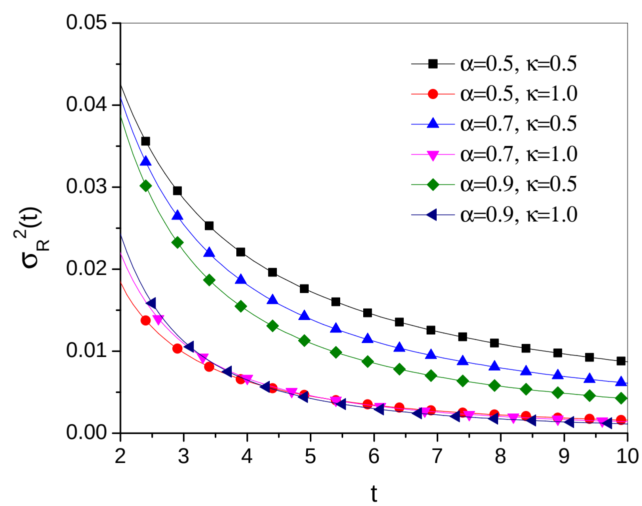

FIG. 1: Time evolution of the relative MSD for the parameters given in the legend, $\tau = 0.1$ and $D = 5$.

The figures 1–3 show the plots of the relative functions σ_R^2, F_R, and P_R, respectively. Values of variables and parameters are given in arbitrarily chosen units. When ACTP has a large impact on subdiffusion the relative

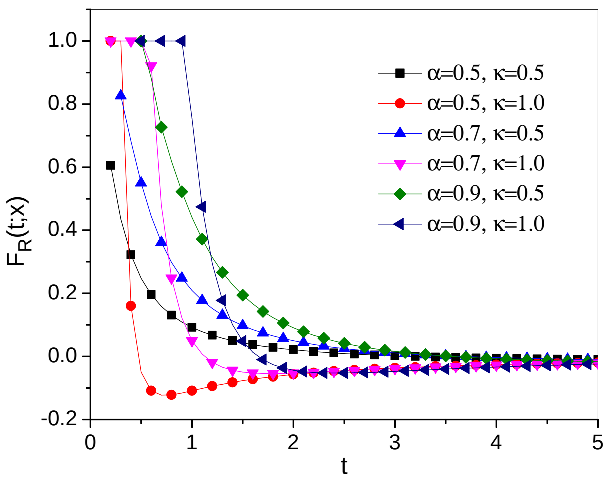

FIG. 2: Time evolution of the relative first passage time for the parameters given in the legend, $x = 10$, $\tau = 0.1$ and $D = 5$.

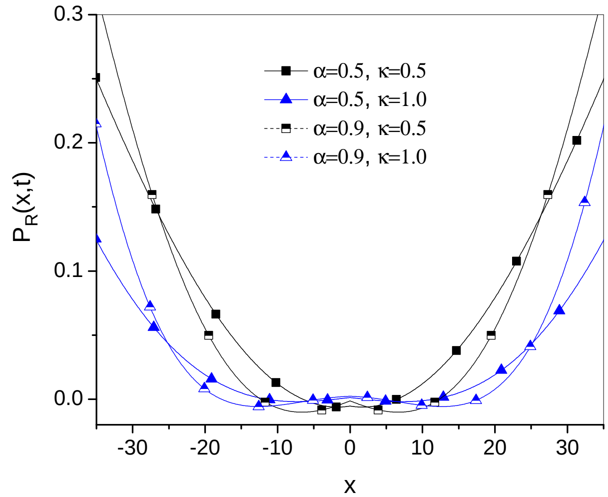

FIG. 3: The relative Green's function P_R for α and κ given in the legend, $t = 20$, $\tau = 0.1$, and $D = 10$.

functions take large values and when the impact is small the functions are close to zero. Figs. 1 and 2 suggest that the ACTP disappears over time, the main influence on the functions is the parameter κ. In Fig. 3 we see that the ACTP increases with moving away from the initial position of a particle. This effect causes that the probability of finding the particle far from its initial position is much lower when the process is described by the Cattaneo-type subdiffusion equation.

VI. CTSE WITH AN ADDITIONAL OPERATOR GENERATED BY A SLOWLY VARYING FUNCTION

A slowly varying function $\mathcal{R}(t)$ at infinity fulfils the relation

$$\frac{\mathcal{R}(at)}{\mathcal{R}(t)} \to 1 \tag{73}$$

when $t \to \infty$ for any $a > 0$. Functions that have finite limits when $t \to \infty$ and logarithmic functions are examples of slowly varying functions.

Let $\hat{\gamma}$ be a slowly varying function. In the following, we use the strong Tauberian theorem to determine the inverse Laplace transform in the long-time limit [54]: *if $\phi(t) \geq 0$, $\phi(t)$ is ultimately monotonic like $t \to \infty$, $\mathcal{R}$ is slowly varying at infinity, and $0 < \rho < \infty$, then each of the relations*

$$\hat{\phi}(s) \approx \frac{\mathcal{R}(1/s)}{s^{\rho}} \tag{74}$$

as $s \to 0$ and

$$\phi(t) \approx \frac{\mathcal{R}(t)}{\Gamma(\rho)t^{1-\rho}} \tag{75}$$

as $t \to \infty$ implies the other.

In the following $\mathcal{R}(1/s) \equiv \hat{\gamma}(s)$ and $\gamma(t)$ denotes the exact inverse Laplace transform of $\hat{\gamma}(s)$ ($R(t)$ in the long time limit and $\gamma(t)$ can be expressed by different formulas).

When $s \to 0$, the Green's function Eq. (37) is approximated as

$$\hat{P}(x,s) = \frac{\sqrt{1+\tau\mathcal{R}(1/s)}}{2\sqrt{D}s^{1-\alpha/2}} \times \left[1 - \frac{s^{\alpha/2}|x|\sqrt{1+\tau\mathcal{R}(1/s)}}{\sqrt{D}}\right]. \tag{76}$$

Using the strong Tauberian theorem we get in the long time limit

$$P(x,t) = \frac{\sqrt{1+\tau\mathcal{R}(t)}}{2\sqrt{D}\Gamma(1-\alpha/2)t^{\alpha/2}} \times \left[1 - \frac{\Gamma(1-\alpha/2)\sqrt{1+\tau\mathcal{R}(t)}|x|}{\sqrt{D}\Gamma(1-\alpha)t^{\alpha/2}}\right]. \tag{77}$$

Putting the above equation to Eq. (21) we get

$$F(t\to\infty;x)=\frac{|x|}{2\sqrt{D}\Gamma(1-\alpha/2)\sqrt{1+\tau\mathcal{R}(t)}t^{\alpha/2}}\times\left[\frac{1+\tau\mathcal{R}(t)}{t}-\tau\mathcal{R}^{(1)}(t)\right]. \quad (78)$$

The equation (78) provides

$$F_R(t\to\infty;x)=1-\sqrt{1+\tau\mathcal{R}(t)}+\frac{\tau t\mathcal{R}^{(1)}(t)}{\sqrt{1+\tau\mathcal{R}(t)}}. \quad (79)$$

From Eqs. (31), (47), and the strong Tauberian theorem we obtain

$$\sigma^2(t\to\infty)=\frac{2Dt^\alpha}{\Gamma(1+\alpha)(1+\tau\mathcal{R}(t))}, \quad (80)$$

$$\sigma_R^2(t\to\infty)=\frac{\tau\mathcal{R}(t)}{1+\tau\mathcal{R}(t)}. \quad (81)$$

As an example we consider the CTSE with

$$\hat{\gamma}(s)\equiv\mathcal{R}(1/s)=c\log\frac{s^2+as+b}{s^2-as+b}, \quad (82)$$

then

$$\mathcal{R}(t)=c\log\frac{bt^2+at+1}{bt^2-at+1}, \quad (83)$$

where the parameters a and c are given in the units of 1/s, b of 1/s^2. The inverse Laplace transform of $\hat{\gamma}(s)$ is [55]

$$\gamma(t)=4ct^{-1}\sinh(at/2)\cos(t\sqrt{b-a^2/4}). \quad (84)$$

In the limit of long time we get

$$F_R(t\to\infty;x)=A\frac{\tau}{t}, \quad (85)$$

$$\sigma_R^2(t\to\infty)=B\frac{\tau}{t}, \quad (86)$$

where $A=-2ac/[b\alpha(2+\alpha)]$ and $B=2ac/b$.

The process is described by Eq. (35), where the kernel Eq. (84) of the operator $\mathcal{D}_t$ has an oscillatory component. To find the solutions to the equation in the long time limit the strong Tauberian theorem has been used. In this solution, the oscillatory component does not occur. This is because the ACTP decays for long times.

VII. FINAL REMARKS

In our considerations, the constitutive equation relating the flux and the concentration gradient is modified by the integral operator with kernel $\beta(t;\tau)$. In the time domain the equation reads

$$\int_0^t\beta(t-t';\tau)J(x,t')dt'=-D\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial P(x,t)}{\partial x}. \quad (87)$$

Combining the above equation with the continuity equation we get the generalized subdiffusion equation. When $\hat{\beta}(s;\tau)=1+\tau\hat{\gamma}(s)$, $\beta(t;\tau)=\delta(t)+\tau\gamma(t)$ in the time domain, we have the Cattaneo–type subdiffusion equation that differs from the ordinary subdiffusion one by an integro–differential operator with kernel $\gamma(t)$. When $\hat{\gamma}(s)=s^\kappa$ with $0<\kappa<1$, which corresponds to $\gamma(t)\sim 1/t^{1+\kappa}$, the operator is the Caputo fractional time derivative of the order $1+\kappa$. The functions σ_R^2, F_R, and P_R can be interpreted as measures of the influence of ACTP on subdiffusion.

For the process described by the CTSE with additional operator being the Caputo fractional time derivative there is $\sigma_R^2\sim F_R\sim 1/t^\kappa$, $0<\kappa<1$, while for the equation with additional operator generated by a slowly varying function $\hat{\gamma}$ we have $\sigma_R^2\sim F_R\sim 1/t$ when $t\to\infty$. This suggests that the ACTP described by a slowly variable function decays more quickly over time.

The persistent random walk model has been used to derive the Cattaneo subdiffusion equation [56, 57]. The CTSE can be derived within the "ordinary" continuous time random walk model with the waiting time of a molecule to jump ψ Eq. (48). This distribution has a heavy tail modified by ACTP, see Eq. (70). It can be interpreted as a subdiffusion model which includes an "additional" process that affects the kinetics of subdiffusion. The additional process may be independent of the process generating subdiffusion. In our considerations, we have assumed that the parameters κ and α in Eq. (59) are independent of each other. As we have mentioned in Sec. I, an example would be subdiffusion (or normal diffusion when $\alpha=1$) of antibiotics in a bacterial biofilm. The defense mechanisms of bacteria against the action of antibiotics can change the random walk of antibiotic molecules. In our opinion, the Cattaneo-type equation can be used to describe such processes. It may be interesting to use the Cattaneo-type equation in modeling the spread of an epidemic. The first arrival of an infected object to some point may create new source of infection. Since ACTP changes the distribution of F, the use of Eqs. (4) and (59) (with possibly added reaction terms in both equations) in epidemic modeling may give qualitatively different results.

When $\hat{\beta}(s\to 0;\tau)\to 1$, which corresponds to $\hat{\gamma}(s)\to 0$, the effect generated by the function β disappears over time, $F_R(t,x)\to 0$ and $\sigma_R^2(t)\to 0$ when $t\to\infty$. In order to make the additional Cattaneo-type process noticeable also for long time, it can be assumed that the parameter τ increases over time. This case is met when $\mathcal{L}[\tau\gamma(t)](s)$ does not goes to zero when $s\to 0$.

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