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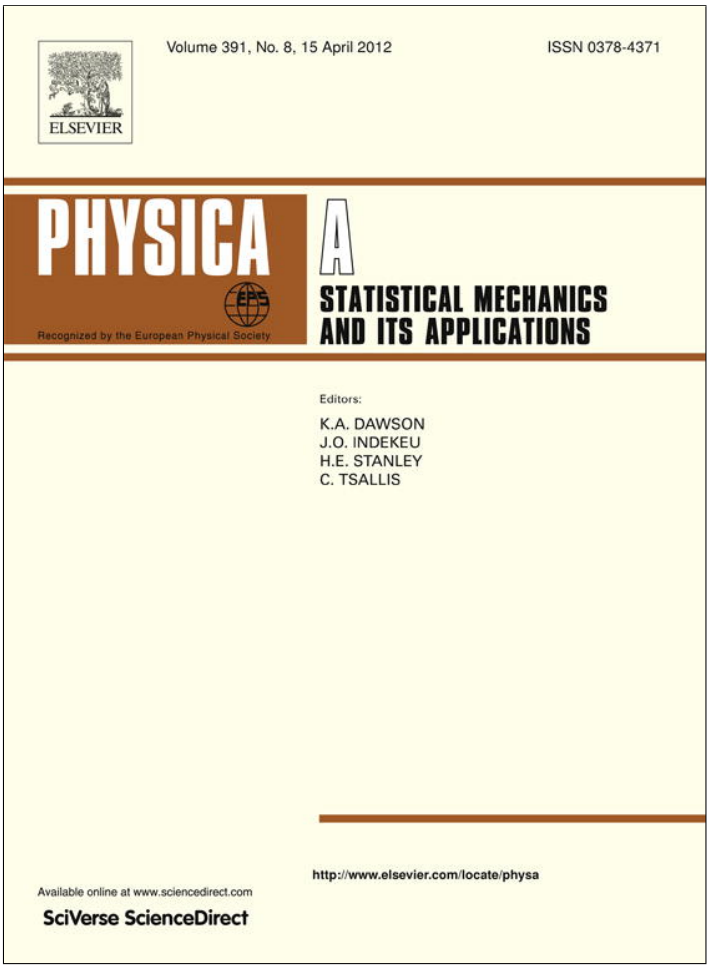

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Generalized space–time fractional diffusion equation with composite fractional time derivative

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ABSTRACT

We investigate the solution of space–time fractional diffusion equations with a generalized Riemann–Liouville time fractional derivative and Riesz–Feller space fractional derivative. The Laplace and Fourier transform methods are applied to solve the proposed fractional diffusion equation. The results are represented by using the Mittag-Leffler functions and the Fox H-function. Special cases of the initial and boundary conditions are considered. Numerical scheme and Grünwald–Letnikov approximation are also used to solve the space–time fractional diffusion equation. The fractional moments of the fundamental solution of the considered space–time fractional diffusion equation are obtained. Many known results are special cases of those obtained in this paper. We investigate also the solution of a space–time fractional diffusion equations with a singular term of the form $\delta(x)\cdot\frac{t^{-\beta}}{\Gamma(1-\beta)}(\beta>0)$.

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1. Introduction

Fractional differential equations are a useful tool for modelling of various anomalous diffusion in complex systems exhibiting pronounced deviations from Brownian diffusion, which is normally described by the standard diffusion equation

$$\frac{\partial}{\partial t}u(x,t)=K_1\frac{\partial^2}{\partial x^2}u(x,t), \tag{1}$$

where K_1 is the diffusion coefficient ($[K_1]=\mathrm{m}^2/\mathrm{s}$). For natural boundary conditions, its Green's function is the famous Gaussian

$$u(x,t)=\frac{1}{\sqrt{4\pi K_1 t}}\exp\left(-\frac{x^2}{4K_1 t}\right) \tag{2}$$

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in one dimension, such that the mean squared displacement assumes the linear form $\langle x(t)^2\rangle = 2K_1 t$. Instead one often observes the power-law behaviour [1]

$$\langle \Delta x(t)^2\rangle = \frac{2K_\gamma t^\gamma}{\Gamma(1+\gamma)}, \tag{3}$$

where K_γ is the generalized diffusion coefficient of dimension $[K_\gamma] = \mathrm{m}^2/\mathrm{s}^\gamma$. The anomalous diffusion exponent γ distinguishes subdiffusion ($0 < \gamma < 1$) and superdiffusion ($1 < \gamma$). There also exist processes, the so-called Lévy flights, whose second moment diverges. Instead, fractional moments of the superdiffusive form $\langle |x|^\delta\rangle^{2/\delta} \propto t^{2/\alpha}$ ($0 < \delta < \alpha \leq 2$) may be defined, see below.

Examples for subdiffusion include tracer dispersion in subsurface hydrology [2], charge carrier motion in amorphous semiconductors [3], diffusion on fractals [4], or the passive motion of lipid granules or telomeres in living cells [5]. Lévy flights occur, for example, in optimized search processes [6].

Similarly, one frequently observes deviations from the exponential relaxation pattern governed by the Debye equation,

$$\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = -\frac{\phi(t)}{\tau}, \tag{4}$$

where $\phi(t)$ is the Debye relaxation function [7,8]. The associated relaxation law $\phi(t) = \phi_0 \exp(-t/\tau)$ is replaced by generalized patterns, such as the stretched exponential $\phi(t) = \phi_0 \exp(-[t/\tau]^\beta)$ (with $0 < \beta < 1$) or the asymptotic power-law $\phi(t) = \phi_0/(1+[t/\tau])^\beta$. A natural extension of the exponential relaxation law is the Mittag-Leffler behaviour

$$\phi(t) = \phi_0 E_\gamma\left(-[t/\tau]^\gamma\right) = \phi_0 \sum_{n=0}^{\infty} \frac{(-[t/\tau]^\gamma)^n}{\Gamma(1+\gamma n)}, \tag{5}$$

whose short-time behaviour $\phi(t) \sim \phi_0 \exp\left(-[t/\tau]^\gamma/\Gamma(1+\gamma)\right)$ matches the stretched exponential pattern, and whose long-time behaviour $\phi(t) \sim \phi_0[\tau/t]^\gamma/\Gamma(1-\gamma)$ is of inverse power-law form [7,8]. Such patterns were, for instance, observed for different types of protein motion [9].

Anomalous diffusion and relaxation behaviours of the above type are often described in terms of fractional order equations and generalized kinetic and stochastic equations [1,8,10–15]. For example, fractional Brownian motion (FBM) [16,17] is a very useful approach to anomalous diffusion. It represents a random process driven by Gaussian noise with correlations $\langle \xi(0)\xi(t)\rangle \simeq \alpha(\alpha-1)t^{\alpha-2}$, the so-called fractional Gaussian noise. FBM is closely related with the generalized Langevin equation (GLE) for a particle driven by fractional Gaussian noise. By the fluctuation dissipation relation [18], the fractional Gaussian noise is compensated by a time-nonlocal noise term with memory integral including a power-law memory kernel. The GLE for this specific choice of the driving noise is also called fractional Langevin equation [10].

An alternative approach to anomalous diffusion is the continuous time random walk (CTRW) theory with independent, random jump increments and waiting times between successive jumps [3,19,20] that generalizes the results of the standard random walk concept. Subdiffusive CTRW describe anomalous diffusion characterized by a distribution of jump lengths with finite variance $\langle \delta x^2\rangle$ and broad distribution of waiting times τ of the form $\psi(\tau) \simeq (\tau*)^\mu/\tau^{1+\mu}$ with $0 < \mu < 1$. Thus, the characteristic waiting time $\int_0^\infty \tau\psi(\tau)\mathrm{d}\tau$ diverges, and the distribution $\psi(\tau)$ is scale-free. For this process the probability density $f(x,t)$ in Fourier–Laplace space fulfils [1,20]

$$\tilde{F}(\kappa, s) = \frac{1/s}{1+K_\mu s^{-\mu}\kappa^2}. \tag{6}$$

The associated equation for this process is the fractional diffusion equation [1,11,21,22] (see the discussion in the next section).

Lévy flights are another special type of CTRW. They are characterized by a finite characteristic waiting times, but have a long-tailed distribution of jump lengths of the form $\lambda(x) \simeq |x|^{-1-\alpha}$ with $0 < \alpha < 2$. Thus, the second moment $\int_{-\infty}^{\infty} |x|^2 \lambda(x)\mathrm{d}x$ diverges [1]. For the Lévy flight the Fourier transform of the probability density $f(x,t)$ is

$$F(\kappa, t) = \exp\left(-K_\alpha t|\kappa|^\alpha\right). \tag{7}$$

A Lévy flight corresponds to a space fractional diffusion equation with Riesz–Weyl derivative [1] (see the discussion in the next section).

In what follows, we propose and analyse a general fractional diffusion equation combining effects of subdiffusion and Lévy flights. The composite fractional operator used for the generalization of the time derivative combines the Riemann–Liouville and Caputo notation, leading to a very flexible framework for the description of complex processes. Composite fractional operators were originally introduced by Hilfer based on fractional time evolutions [8]. In the relaxation dynamics of glassy materials they were shown to provide an excellent description of experimental data over more than ten orders of magnitude, with less parameters than traditional fit functions such as that of Havriliak–Negami [7].

Our analysis of these phenomena, carried out by means of fractional calculus and integral transforms (Laplace, Fourier), leads to certain special functions in one variable of Mittag-Leffler (M-L) and Wright types. These useful special functions are investigated systematically as relevant cases of the general class of functions which are popularly known as the Fox

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H-functions, after Charles Fox, who initiated a detailed study of these functions as symmetrical Fourier kernels [23]. Mathematical aspects of the boundary-value problems for the time-fractional diffusion equation and their applications in physics have been treated in papers by Engler [24], Fujita [25], Gorenflo et al. [26], Mainardi [27], Metzler and Klafter [28], Mainardi et al. [29], Mainardi and Pagnini [30], Prüss [31], Podlubny [32], Schneider and Wyss [21], Wyss [33], Hilfer [8], Sandev et al. [34], etc. On the other hand, the space-fractional diffusion equation obtained by replacing the second order space-derivative in the diffusion equation by an inverse Riesz potential of order $\beta > 0$ has been also considered (see Ref. [35] and references therein). A further generalization of the classical diffusion equation is the so-called space–time fractional diffusion equation (see Ref. [29] and references therein), where the first order time derivative is replaced with a Caputo-time fractional derivative of order $0 < \beta < 2$ and second-order space derivative with a Riesz–Feller space-fractional derivative of order $0 < \alpha < 2$ (given as a pseudo-differential operator with the Fourier symbol $-|\kappa|^{\alpha}$; $\kappa \in \mathbb{R}$). Mainardi et al. [29] expressed the fundamental solutions of the Cauchy problem for the space–time fractional diffusion equation in terms of the proper Fox H-function, based on their Mellin–Barnes integral representations. The Cauchy problem for nonlinear conservation laws supplied with a space-fractional diffusion term of homogeneous Fourier symbol $(-|\kappa|^{\alpha})$ was analysed by Biler et al. [36] using entropy estimates. Later, Droniou et al. [37] generalized this result by deriving a maximum principle based on the non-negativity of the kernel of the corresponding semi-group. A similar problem was investigated by Achleitner et al. [38], where the space-fractional derivative is of Riesz–Feller type with a non-homogeneous symbol. We note that both space and time fractional operators correspond to the diffusion limit of continuous time random walk models with long-tailed waiting time and/or jump length distributions [35,39–41]. The link between the CTRW's and space–time fractional diffusion equations has been very actively investigated by Scalas et al. [42], Fulger et al. [43], Germano et al. [44], Metzler et al. [41,45], Meerschaert et al. [46], and so on.

The paper is organized as follows. In Section 2, definitions of fractional differential and integral operators are given, and we explain the physical motivation of the problems considered in this paper. The exact solution of the generalized space–time fractional diffusion equations in the infinite domain in terms of M-L and H-functions is obtained in Section 3. The Fourier–Laplace transform method is used to solve the equation analytically. Some special cases are considered. The asymptotic behaviours of the solution are derived, and fractional moments of the fundamental solution are obtained. In Section 4, a numerical method for the solution of generalized fractional differential equations in terms of Grünwald–Letnikov derivatives is discussed for the first time. The numerical solution of the space–time fractional diffusion equation is presented and compared with the asymptotic solution of Section 3. In Section 5, a fractional diffusion equation with a singular term is considered and both exact and asymptotic results are obtained. The conclusions are presented in Section 5.

2. Preliminaries

The Riemann–Liouville (R–L) fractional integral of order $\mu > 0$ with lower limit a is defined by [8,47]

$$\left(I_{a+}^{\mu} f\right)(t) = \frac{1}{\Gamma(\mu)} \int_a^t \frac{f(\tau)}{(t-\tau)^{1-\mu}} \mathrm{d}\tau, \quad t > a,\ \Re(\mu) > 0. \tag{8}$$

For $\mu = 0$, $\left(I_{a+}^{0} f\right)(t) = f(t)$. From the other side, the R–L fractional derivative of order $\mu > 0$ with lower limit a is defined by [8,47]

$$\left(D_{a+}^{\mu} f\right)(t) = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n} \left(I_{a+}^{n-\mu} f\right)(t), \quad \Re(\mu) > 0,\ n = [\Re(\mu)] + 1, \tag{9}$$

where $[\Re(\mu)]$ denotes the integer part of the real number $\Re(\mu)$.

The generalized R–L time fractional derivative of order $0 < \mu < 1$ and type $0 \le \nu \le 1$ (named as the Hilfer fractional derivative [34,48,49] or composite fractional derivative) $D_{0+}^{\mu,\nu}$ is defined by [8]

$$\left(D_{a+}^{\mu,\nu} f\right)(t) = \left(I_{a+}^{\nu(1-\mu)} \frac{\mathrm{d}}{\mathrm{d}t} \left(I_{a+}^{(1-\nu)(1-\mu)} f\right)\right)(t), \quad (0 \le \nu \le 1,\ 0 < \mu < 1). \tag{10}$$

Note that in case when $\nu = 0$ the generalized R–L fractional derivative (10) would correspond to the classical R–L fractional derivative

$$\left({}_{RL}D_{0+}^{\mu} f\right)(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left(I_{0+}^{(1-\mu)} f\right)(t), \tag{11}$$

and in case when $\nu = 1$ it would correspond to the Caputo fractional derivative [50]

$$\left({}_{C}D_{0+}^{\mu} f\right)(t) = \left(I_{0+}^{(1-\mu)} \frac{\mathrm{d}}{\mathrm{d}t} f\right)(t). \tag{12}$$

For the Hilfer-generalized R–L derivative the following formula holds true [49]

$$\left(D_{a+}^{\mu,\nu} \left[(t-a)^{\lambda-1}\right]\right)(x) = \frac{\Gamma(\lambda)}{\Gamma(\lambda-\mu)} (x-a)^{\lambda-\mu-1}, \quad (x > a,\ \Re(\lambda) > 0)\,. \tag{13}$$

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It can be shown also that for a given function with a zero initial condition the following formula is valid [49]

$$D_{0+}^{\mu,\nu}\left({}_{C}D_{0+}^{(1-\nu)(1-\mu)}f\right)(t)=\left({}_{C}D_{0+}^{1-\nu(1-\mu)}f\right)(t). \tag{14}$$

In Ref. [8] it is found for $0<\mu<1$ that the Laplace transform $\mathcal{L}[g(t)](s)=\int_0^\infty g(t)\mathrm{e}^{-st}\mathrm{d}t$ of the generalized R–L fractional derivative (10) is given by

$$\mathcal{L}\left[D_{0+}^{\mu,\nu}f(t)\right]=s^{\mu}\mathcal{L}\left[f(t)\right]-s^{\nu(\mu-1)}\left(I_{0+}^{(1-\nu)(1-\mu)}f\right)(0+), \tag{15}$$

where the initial-value term $\left(I_{0+}^{(1-\nu)(1-\mu)}f\right)(0+)$ is evaluated in the limit as $t\to 0+$ in the space of summable Lebesgue integrable functions

$$L(0,\infty)=\left\{f:\|f\|_1=\int_0^\infty |f(t)|\mathrm{d}t<\infty\right\}. \tag{16}$$

The space fractional derivative $\frac{\partial^\alpha}{\partial|x|^\alpha}$ is the so-called Riesz–Feller space fractional derivative of order α $(0<\alpha\leq 2)$, which is given as a pseudo-differential operator with the Fourier symbol $-|\kappa|^\alpha$, $\kappa\in\mathbb{R}$ [39]

$$\frac{\mathrm{d}^\alpha}{\mathrm{d}|x|^\alpha}f(x)=\mathcal{F}^{-1}\left[-|\kappa|^\alpha F(\kappa)\right](x). \tag{17}$$

Note that

$$F(\kappa)=\mathcal{F}\left[f(x)\right](\kappa)=\int_{-\infty}^{\infty}f(x)\mathrm{e}^{-\imath\kappa x}\mathrm{d}x \tag{18}$$

is the Fourier transform of the function $f(x)$.

The motivation of studying fractional equations of form (23) and (57) is, from one side, the Hilfer generalized R–L time fractional derivative (10), which combine both the derivatives, Caputo and R–L. It is known, from the continuous time random walk (CTRW) theory, that the probability density $f(x,t)$, in case where the characteristic waiting time diverges and the jump length variance is finite, can be obtained from the following two equivalent representations of the fractional diffusion equation [1]

$${}_{RL}D_{0+}^{\mu}f(x,t)-\delta(x)\cdot\frac{t^{-\mu}}{\Gamma(1-\mu)}=K_\mu\frac{\partial^2}{\partial x^2}f(x,t) \tag{19a}$$

$${}_{C}D_{0+}^{\mu}f(x,t)=K_\mu\frac{\partial^2}{\partial x^2}f(x,t) \tag{19b}$$

in the R–L and Caputo sense, respectively, where K_μ is the generalized diffusion constant of physical dimension $[K_\mu]=\mathrm{m}^2/\mathrm{s}^\mu$, and μ is the anomalous diffusion exponent. This can be seen from the Laplace transform of the classical R–L (11) and Caputo (12) fractional derivatives, from where it follows that by considering proper initial conditions the R–L and Caputo derivatives are equivalent since

$$\left({}_{C}D_{0+}^{\mu}f\right)(t)=\left({}_{RL}D_{0+}^{\mu}f\right)(t)-f(0+)\cdot\frac{t^{-\mu}}{\Gamma(1-\mu)}, \tag{20}$$

where $0<\mu<1$. The foregoing equations describe anomalous diffusive processes, due to the non-linear dependence of the variance of the process on the time variable [1], i.e.

$$\langle x^2(t)\rangle\simeq K_\mu t^\mu. \tag{21}$$

The divergence of the characteristic waiting time underlying the time-fractional forms of the Caputo or R–L operators causes weak ergodicity breaking in the sense that for such processes the long-time average of physical quantities is no longer equivalent to the corresponding ensemble averages [51]. In the recent years CTRW models with nonidentical trapping time probability density function over the lattice points are investigated [52,53]. It was shown that even models with finite characteristic waiting time for all lattice points are typically nonergodic [52,53].

From the other side, the case of finite characteristic waiting time and diverging jump length variance (Lévy flights) leads to the following space fractional diffusion equation [1,12,39]

$$\frac{\partial}{\partial t}f(x,t)=K_\alpha\frac{\partial^\alpha}{\partial|x|^\alpha}f(x,t), \tag{22}$$

where K_α is the generalized diffusion constant of physical dimension $[K_\alpha]=\mathrm{m}^\alpha/\mathrm{s}$, and α is the Lévy index. We note that the Riesz–Weyl operator in the space-fractional diffusion equation needs modification in the presence of non-natural boundary conditions, due to the highly non-local nature of Lévy flight processes; see the discussion in Ref. [54].

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Similar problems with Caputo or R–L time fractional derivatives and/or Riesz space fractional derivative are considered in Refs. [1,7,8,15,21,27,34,40,45,55–62] and references therein. The solutions of such equations have been represented in terms of M-L function and their generalizations [49,63–66], which for the first time was introduced by Gösta Mittag-Leffler [63], as well as via the Fox H-function [1,34,58,60,67], introduced by Charles Fox [67].

3. Space–time fractional diffusion equation

We study the following generalized space–time fractional diffusion equation:

$$D_{0+}^{\mu,\nu}u(x,t) = K_{\mu,\alpha}\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x,t), \quad t>0, \ -\infty<x<+\infty, \tag{23}$$

with boundary conditions

$$u(\pm\infty,t)=0, \quad t>0 \tag{24}$$

and an initial condition

$$\left(I_{0+}^{(1-\nu)(1-\mu)}u(x,t)\right)(0+)=g(x), \quad -\infty<x<+\infty, \tag{25}$$

where $u(x,t)$ is a field variable, $K_{\mu,\alpha}$ is the generalized diffusion constant of physical dimension $[K_{\mu,\alpha}]=\mathrm{m}^{\alpha}/\mathrm{s}^{\mu}$ (the dimension of $K_{\mu,\alpha}$ can be obtained from definitions (10) and (17) by dimensional analysis), $0<\mu\leq 1$, $0\leq\nu\leq 1$ and $0<\alpha\leq 2$. Note that the numerical value of $K_{\mu,\alpha}$ depends also on ν, but we use simplified notation with indexes μ and α because of the independence of $[K_{\mu,\alpha}]$ on ν.

Let us comment on the importance of application of the Hilfer-composite fractional time derivative. It has been argued that time fractional derivatives are equivalent to infinitesimal generators of generalized time fractional evolutions that arise in the transition from microscopic to macroscopic time scales [7]. In contrast to the first order time derivative, which is an infinitesimal generator of a simple time translation, the fractional derivative of order $0<\alpha\leq 1$ is an infinitesimal generator of a macroscopic time evolution, whose kernel is the one sided stable probability density with stable index α [7]. This transition from first order time derivative to the fractional order time derivative arises in physical problems as shown by Hilfer [8,22,68,69]. The Hilfer-composite time derivative was used by Hilfer to successfully describe the dynamics in glass formers over an extremely large frequency window [7]. From a practical point of view the description in terms of composite-fractional operators increases the versatility of the solution of the dynamic equation in the description of complex data. The fact that with comparatively few parameters excellent fits are possible [7] points at the physical relevance of this approach.

Theorem 1. *The fractional diffusion equation (23) with boundary conditions (24) and an initial condition (25) in case when $0<\mu<1, 0\leq\nu\leq 1,\ 0<\alpha\leq 2$ has a solution of the following form*

$$u(x,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}t^{-(1-\nu)(1-\mu)}E_{\mu,1-(1-\nu)(1-\mu)}\left(-K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\right)\cdot\hat{g}(\kappa)\cdot\mathrm{e}^{-\imath\kappa x}\mathrm{d}\kappa, \tag{26}$$

where $E_{\alpha,\beta}(z)$ is the two parameter M-L function [64],

$$\hat{g}(\kappa)=\mathcal{F}[g(x)]=\int_{-\infty}^{\infty}g(x)\mathrm{e}^{\imath\kappa x}\mathrm{d}x \tag{27}$$

is the Fourier transform of the function $g(x)$ $\left(g(x)=\mathcal{F}^{-1}[\hat{g}(\kappa)]=\frac{1}{2\pi}\int_{-\infty}^{\infty}\hat{g}(\kappa)\mathrm{e}^{-\imath\kappa x}\mathrm{d}\kappa\right)$ and

$$F(x,s)=\mathcal{L}[f(x,t)], \qquad \tilde{F}(\kappa,s)=\mathcal{F}[F(x,s)], \qquad F(\kappa,t)=\mathcal{L}^{-1}[\tilde{F}(\kappa,s)]. \tag{28}$$

Proof. By applying the Laplace transform with respect to the time variable t and Fourier transform with respect to the spatial variable x in Eq. (23) and from the initial condition (25) and boundary conditions (24), we obtain

$$\tilde{U}(\kappa,s)=\frac{s^{-\nu(1-\mu)}}{s^{\mu}+|\kappa|^{\alpha}K_{\mu,\alpha}}\cdot\hat{g}(\kappa), \tag{29}$$

where $\tilde{U}(\kappa,s)=\mathcal{F}\left[U(x,s)\right]$, $U(x,s)=\mathcal{L}\left[u(x,t)\right]$. Applying an inverse Laplace transform to relation (29), by using the following formula [8,32,47]

$$\mathcal{L}[t^{\beta-1}E_{\alpha,\beta}(\pm at^{\alpha})]=\int_{0}^{\infty}\mathrm{e}^{-st}t^{\beta-1}E_{\alpha,\beta}(\pm at^{\alpha})\mathrm{d}t=\frac{s^{\alpha-\beta}}{s^{\alpha}\mp a}, \quad \Re(s)>|a|^{1/\alpha}, \tag{30}$$

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it follows

$$U(\kappa,t)=t^{-(1-\nu)(1-\mu)}E_{\mu,1-(1-\nu)(1-\mu)}\left(-K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\right)\hat{g}(\kappa). \tag{31}$$

Finally, by finding inverse Fourier transform to relation (31) we prove Theorem 1. □

Example 1. The time fractional diffusion equation (23) with boundary conditions (24) and an initial condition $g(x)=\delta(x)$, has a solution of the form

$$u(x,t)=\frac{1}{\alpha|x|}t^{-(1-\nu)(1-\mu)}H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1-(1-\nu)(1-\mu),\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right], \tag{32}$$

where $H_{p,q}^{m,n}\left[z\left|\begin{matrix}(a_p,A_p)\\(b_q,B_q)\end{matrix}\right.\right]$ is the Fox H-function [67,70].

Indeed, by using $\hat{g}(\kappa)=\mathcal{F}\left[\delta(x)\right]=1$, the cosine transform and the properties of the H-function [70], we obtain

$$\begin{aligned}u(x,t)&=\frac{1}{\pi}t^{-(1-\nu)(1-\mu)}\int_0^{\infty}\cos(\kappa x)H_{1,2}^{1,1}\left[K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\left|\begin{matrix}(0,1)\\(0,1),((1-\nu)(1-\mu),\mu)\end{matrix}\right.\right]\mathrm{d}\kappa\\&=\frac{1}{\alpha|x|}t^{-(1-\nu)(1-\mu)}H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1-(1-\nu)(1-\mu),\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right].\end{aligned} \tag{33}$$

Note that if $\alpha=2$, from the definition of the Fox H-function, we obtain [34]

$$u(x,t)=\frac{1}{2|x|}t^{-(1-\nu)(1-\mu)}H_{1,1}^{1,0}\left[\frac{|x|}{\left(K_{\mu,2}t^{\mu}\right)^{1/2}}\left|\begin{matrix}\left(1-(1-\nu)(1-\mu),\frac{\mu}{2}\right)\\(1,1)\end{matrix}\right.\right]. \tag{34}$$

Thus, in the case of the R–L time fractional derivative ($\nu=0$) solution (32) becomes [70]

$$u(x,t)=\frac{1}{\alpha|x|}t^{-(1-\mu)}H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(\mu,\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right]. \tag{35}$$

In the case of the Caputo time fractional derivative ($\nu=1$) solution (32) has the following form

$$u(x,t)=\frac{1}{\alpha|x|}H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1,\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right]. \tag{36}$$

Here we note that solution (36), unlike solution (35), is normalized (see relation (48) from Example 3). Only if we consider a proper singular term with matching power, the solution in the case of a R–L time fractional derivative would be normalized (see the discussion for equivalent formulation (19); see also Example 8 and Remark 3). This non-conservation of the norm is important in certain cases, as described by the Hilfer idea of fractional generators of the dynamics (see for example Ref. [68]).

Furthermore, if $\nu=\mu=1$ from relation (32) we obtain the solution of the diffusion equation with space fractional derivative, i.e.

$$u(x,t)=\frac{1}{\alpha|x|}H_{2,2}^{1,1}\left[\frac{|x|}{\left(K_{1,\alpha}t\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right], \tag{37}$$

which is a closed-form representation of a Lévy stable law [1,71]. If in relation (37) we substitute $\alpha=2$, it follows the solution of the classical diffusion equation [72], i.e.

$$u(x,t)=\frac{1}{2|x|}H_{1,1}^{1,0}\left[\frac{|x|}{\sqrt{K_{\mu,\alpha}t}}\left|\begin{matrix}\left(1,\frac{1}{2}\right)\\(1,1)\end{matrix}\right.\right]=\frac{1}{\sqrt{4\pi K_{\mu,\alpha}t}}\cdot\mathrm{e}^{-\frac{x^2}{4K_{\mu,\alpha}t}}. \tag{38}$$

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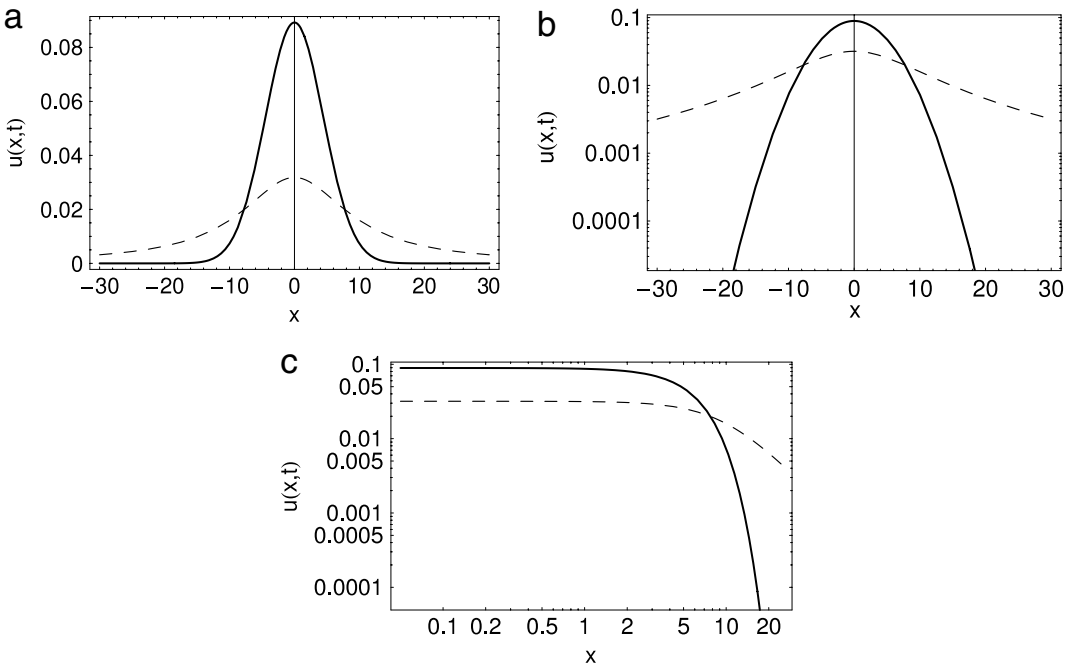

Fig. 1. Graphical representation of solution (37) ($\mu = \nu = 1$, space fractional diffusion equation), $K_{\mu,\alpha} = 1$, $t = 10$, $\alpha = 2$ (solid line), $\alpha = 1$ (dashed line); (a) linear–linear plot; (b) log–linear plot; (c) log–log plot.

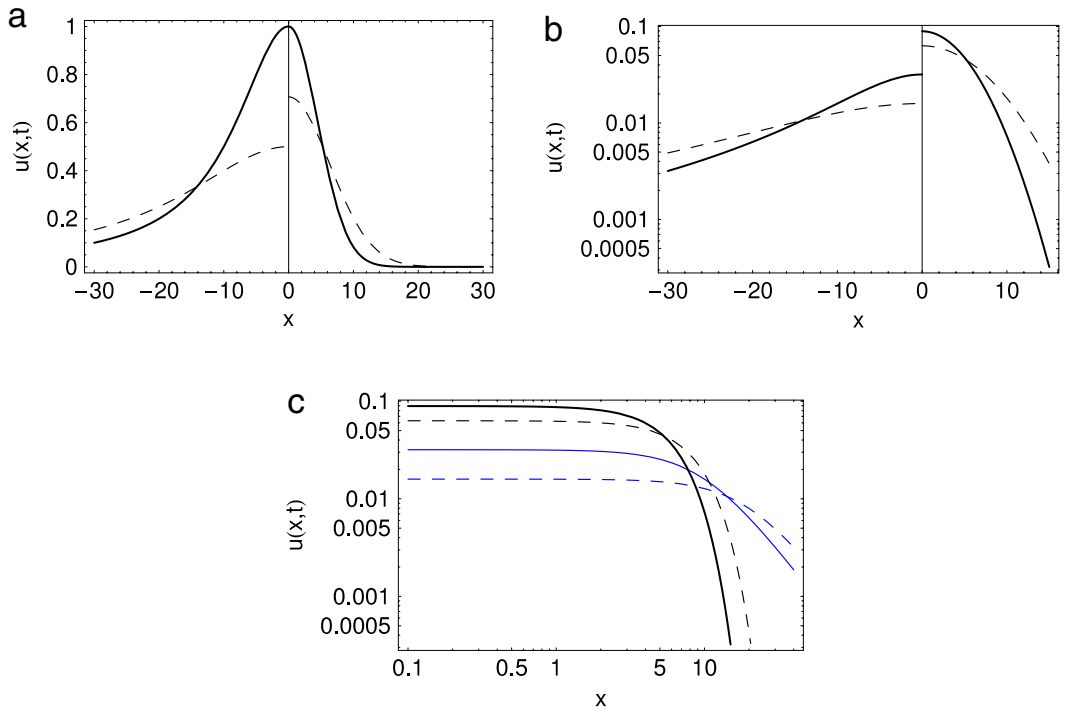

Fig. 2. Graphical representation of solution (37) for $K_{\mu,\alpha} = 1$, (a) (linear–linear plot) $t = 10$ (solid line), $t = 20$ (dashed line); left: $\alpha = 1$ (the solution is divided by a factor $\frac{1}{10\pi}$); right: $\alpha = 2$ (the solution is divided by a factor $\frac{1}{\sqrt{40\pi}}$); (b) (log–linear plot) $t = 10$ (solid line), $t = 20$ (dashed line); left: $\alpha = 1$; right: $\alpha = 2$; (c) (log–log plot) $t = 10$ (solid line), $t = 20$ (dashed line); $\alpha = 1$ (blue line); $\alpha = 2$ (black line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

In this case for $K_{\mu,\alpha} = 1/2$ note that $u(x,t) = \frac{1}{\sqrt{2\pi t}} \cdot \mathrm{e}^{-\frac{x^2}{2t}}$ represents the probability density function of a Wiener process. Solution (32) for different values of parameters is shown in Figs. 1–4.

Remark 1. Let us make few remarks on the fractional diffusion equation (23) with boundary conditions (24) and an initial condition $g(x) = \delta(x)$ in the case when $\alpha = 2$ [34]. This equation for $\nu = 1$ describes diffusion of Montroll–Weiss type.

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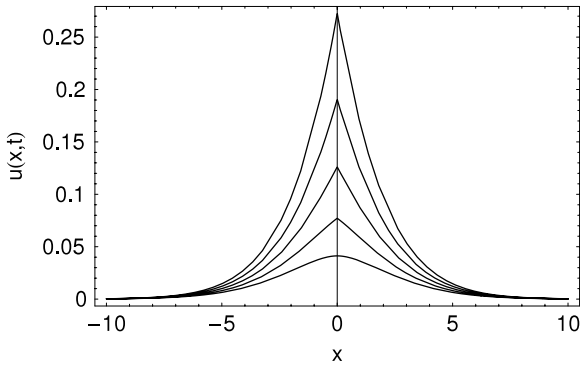

Fig. 3. Graphical representation of solution (34) ($\alpha = 2$, time fractional diffusion equation), $\mu = 1/2, K_{\mu,\alpha} = 1, t = 5, \nu = 0$ (lower line), $\nu = 1/4$, $\nu = 1/2$, $\nu = 3/4$, $\nu = 1$ (upper line).

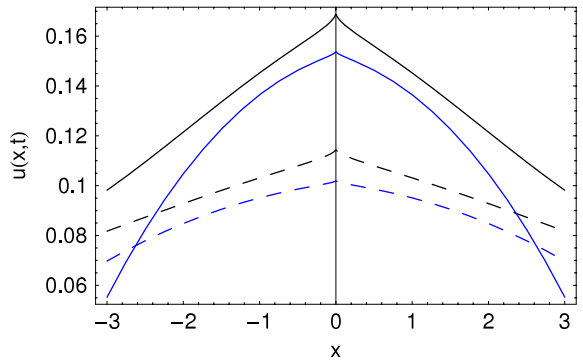

Fig. 4. Graphical representation of solution (36) ($\nu = 1, \alpha = 1.6$, space–time fractional diffusion equation with Caputo time fractional derivative), $K_{\mu,\alpha} = 1, t = 5$ (solid lines), $t = 10$ (dashed lines), $\mu = 0.95$ (black lines), $\mu = 0.9$ (blue lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

It is shown that it can be related to the Montroll–Weiss CTRW, where μ is related to the long time tail exponent [22] (see also Ref. [73]). In this case the solution $u(x, t)$ is a probability density function, i.e. $u(x, t)$ is normalized (see Example 3 and Ref. [34]).

The case $\nu = 0$, which is solved exactly by Hilfer [56], is not related to the Montroll–Weiss CTRW. In this case, a nonlocal initial condition $\left(I_{0+}^{(1-\mu)}u(x, t)\right)(t)|_{t=0+} = \delta(x)$ should be considered [8,56,73]. Contrary to the case $\nu = 1$, the solution $u(x, t)$ for $\nu = 0$ is not normalized, so it does not have probabilistic interpretation [56] (see also Example 3 and Ref. [34]).

The same situation appears for $0 < \mu < 1$ and $0 < \nu < 1$, where the nonlocal initial condition of the form $(I_{0+}^{(1-\nu)(1-\mu)} u(x, t))(t)|_{t=0+} = \delta(x)$ is considered [8,34]. In this case $u(x, t)$ (32) is not normalized (see Example 3 and Ref. [34]) and cannot be related to the Montroll–Weiss CTRW, but it can be used in the description of anomalous relaxation phenomena in dielectrics and viscoelastic phenomena [7,66,74] (see also the discussion in Ref. [34]).

Remark 2. The fractional diffusion equation (23) with boundary conditions (24) and initial condition $g(x) = \delta(x)$ for $0 < \alpha \leq 2$, $0 < \mu \leq 1$ and $\nu = 1$ is the governing equation for the infinitesimal generator of the semigroup for the process $L_\alpha(D_\beta(t))$ (a Lévy α-stable process subordinated to the inverse β-stable subordinator with $0 < \alpha \leq 2$ and $0 < \beta \leq 1$) [75]. This case is numerically studied in detail in Refs. [43,44].

Example 2 (*Asymptotic Expansions*)**.** By using the series expansion of the Fox H-function [70], solution (32) can be expressed by the following series

$$u(x, t) = \frac{K_{\mu,\alpha}^{-1/\alpha} t^{-(1-\nu)(1-\mu)-\mu/\alpha}}{\alpha} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{\sin\left(\frac{1+k}{2}\pi\right)}{\sin\left(\frac{1+k}{\alpha}\pi\right) \Gamma\left(1-(1-\nu)(1-\mu)-\frac{1+k}{\alpha}\mu\right)} \frac{|x|^k}{\left(K_{\mu,\alpha} t^{\mu}\right)^{k/\alpha}}$$
$$+ \frac{|x|^{\alpha-1} t^{-(1-\nu)(1-\mu)-\mu}}{\pi K_{\mu,\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma\left(1-\alpha(1+k)\right) \sin\left[\frac{(1+k)\alpha}{2}\pi\right]}{\Gamma\left(1-(1-\nu)(1-\mu)-\mu-\mu k\right)} \frac{|x|^{\alpha k}}{\left(K_{\mu,\alpha} t^{\mu}\right)^{k}}, \tag{39}$$

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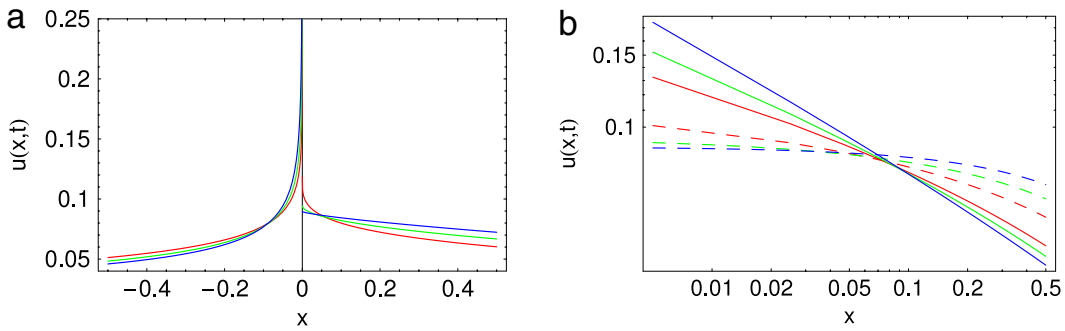

Fig. 5. Graphical representation of asymptotic solution (40), $t = 10$, $K_{\mu,\alpha} = 1$, $\mu = \nu = 1/2$; left: $\alpha = 0.75$ (blue line), $\alpha = 0.85$ (green line), $\alpha = 0.95$ (red line); right: $\alpha = 1.25$ (red line), $\alpha = 1.5$ (green line), $\alpha = 1.75$ (blue line); (a) linear–linear plot; (b) log–log plot, $\alpha < 1$ (solid lines), $\alpha > 1$ (dashed lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

where we employed $\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin(a\pi)}$. Thus, for $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \ll 1$, we obtain

$$u(x,t) \sim \frac{K_{\mu,\alpha}^{-1/\alpha}}{\alpha \sin\left(\frac{\pi}{\alpha}\right)} \cdot \frac{t^{-(1-\nu)(1-\mu)-\mu/\alpha}}{\Gamma\left(1-(1-\nu)(1-\mu)-\frac{\mu}{\alpha}\right)} + |x|^{\alpha-1}\frac{K_{\mu,\alpha}^{-1}}{2\Gamma(\alpha)\cos\left(\frac{\alpha\pi}{2}\right)} \cdot \frac{t^{-(1-\nu)(1-\mu)-\mu}}{\Gamma\left(1-(1-\nu)(1-\mu)-\mu\right)}. \tag{40}$$

Note that the second sum in (39) vanishes in the limit $\mu = 1$. So it is obtained $u(x,t) \sim \frac{K_{1,\alpha}^{-1/\alpha}\Gamma\left(\frac{1}{\alpha}\right)}{\pi\alpha} \cdot t^{-1/\alpha} - |x|^2\frac{K_{1,\alpha}^{-3/\alpha}\Gamma\left(\frac{3}{\alpha}\right)}{2\pi\alpha} \cdot t^{-3/\alpha}$, which for $\alpha = 2$ yields $u(x,t) \sim \frac{1}{\sqrt{4\pi K_{1,2}t}}\left(1 - \frac{|x|^2}{\sqrt{4K_{1,2}t}}\right) \approx \frac{1}{\sqrt{4\pi K_{1,2}t}}e^{-\frac{|x|^2}{\sqrt{4K_{1,2}t}}}$. Graphical representation of asymptotic solution (40) is given in Fig. 5.

From the other side by using the properties and series expansion of the H-function [70] we can find the asymptotic behaviour in case when $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \gg 1$. Thus, it is obtained

$$\begin{aligned} u(x,t) &= \frac{1}{\alpha|x|}t^{-(1-\nu)(1-\mu)}H_{3,3}^{1,2}\left[\frac{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}{|x|}\middle|\begin{matrix}(0,1),\left(0,\frac{1}{\alpha}\right),\left(0,\frac{1}{2}\right)\\ \left(0,\frac{1}{\alpha}\right),\left((1-\nu)(1-\mu),\frac{\mu}{\alpha}\right),\left(0,\frac{1}{2}\right)\end{matrix}\right] \\ &= \frac{1}{\pi\alpha|x|}t^{-(1-\nu)(1-\mu)}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}\Gamma(1+\alpha k)\sin\left(\frac{\alpha k\pi}{2}\right)}{\Gamma\left(1-(1-\nu)(1-\mu)+\mu k\right)}\frac{\left(K_{\mu,\alpha}t^{\mu}\right)^{k}}{|x|^{\alpha k}}, \end{aligned} \tag{41}$$

from where it follows

$$u(x,t) \sim \frac{\Gamma(\alpha)\sin\left(\frac{\alpha\pi}{2}\right)}{\pi\Gamma\left(1+\mu-(1-\nu)(1-\mu)\right)} \cdot |x|^{-\alpha-1}K_{\mu,\alpha}t^{\mu-(1-\nu)(1-\mu)}. \tag{42}$$

For $\mu = 1$ we obtain the known result typical for Lévy distributions $u(x,t) \sim |x|^{-\alpha-1}K_{1,\alpha}t$ [1,71].

The asymptotic behaviour of the solution (34) ($\alpha = 2$, i.e. time-fractional diffusion equation) in case when $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \gg 1$ is given by [34]

$$\begin{aligned} u(x,t) \sim{}& \frac{1}{2\sqrt{(2-\mu)\pi}} \cdot \left(\frac{\mu}{2}\right)^{\frac{(1-\mu)(1-2\nu)}{2-\mu}} \cdot |x|^{\frac{(1-\mu)(1-2\nu)}{2-\mu}} \cdot \left(K_{\mu,2}t^{\mu}\right)^{-\frac{(1-\nu)(1-\mu)+1/2}{2-\mu}} \\ &\times \exp\left[-\frac{2-\mu}{2}\left(\frac{\mu}{2}\right)^{\frac{\mu}{2-\mu}}|x|^{\frac{2}{2-\mu}}\left(K_{\mu,2}t^{\mu}\right)^{-\frac{1}{2-\mu}}\right], \end{aligned} \tag{43}$$

where we used the following asymptotic expansion for large z of the H-function $H_{1,1}^{1,0}(z)$ [21,70]

$$H_{1,1}^{1,0}(z) \sim Bz^{(1-\alpha)/m^*}\exp\left(-m^*C^{1/m^*}z^{1/m^*}\right), \tag{44}$$

where $B = (2\pi)^{(m-p-1)/2}C^{(1-\alpha)/m^*}m^{*-1/2}A_1^{1/2-a_1}B_1^{b_1-1/2}$, $\alpha = a_1 - b_1 + \frac{1}{2}$, $m^* = B_1 - A_1 > 0$ and $C = A_1^{A_1}B_1^{-B_1}$.

If $\nu = 1$, the result (43) is equivalent to that obtained in Refs. [1,76]. For $\alpha = 2$, $\nu = 1$ and $\mu = 1$ from (43) we obtain the solution (38) of the classical diffusion equation.

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Example 3. The fractional moments

$$\left\langle |x|^{\xi} \right\rangle = 2\int_0^{\infty} x^{\xi} u(x,t)\mathrm{d}x, \quad \xi > 0 \tag{45}$$

of the considered fractional diffusion equation (23) with $g(x) = \delta(x)$ are given by

$$\left\langle |x|^{\xi} \right\rangle = \frac{2}{\alpha} \cdot t^{-(1-\nu)(1-\mu)} \left(K_{\mu,\alpha} t^{\mu}\right)^{\xi/\alpha} \cdot \frac{\Gamma\left(1+\xi\right) \sin\left(\frac{\xi\pi}{2}\right)}{\Gamma\left(1-(1-\nu)(1-\mu)+\frac{\mu\xi}{\alpha}\right) \sin\left(\frac{\xi\pi}{\alpha}\right)}. \tag{46}$$

The case $\mu = 1$ yields [1]

$$\left\langle |x|^{\xi} \right\rangle = \frac{2}{\alpha} \cdot \left(K_{1,\alpha} t\right)^{\xi/\alpha} \cdot \frac{\Gamma\left(1+\xi\right) \Gamma\left(-\frac{\xi}{\alpha}\right)}{\Gamma\left(-\frac{\xi}{2}\right) \Gamma\left(1+\frac{\xi}{2}\right)} = \frac{2}{\alpha} \cdot \left(K_{1,\alpha} t\right)^{\xi/\alpha} \cdot \frac{\Gamma\left(1+\xi\right) \sin\left(\frac{\xi\pi}{2}\right)}{\Gamma\left(1+\frac{\xi}{\alpha}\right) \sin\left(\frac{\xi\pi}{\alpha}\right)}. \tag{47}$$

From (46), for $\xi \to 0$ we obtain

$$\lim_{\xi\to 0} \left\langle |x|^{\xi} \right\rangle = \frac{1}{\Gamma\left(1-(1-\nu)(1-\mu)\right)} \cdot t^{-(1-\nu)(1-\mu)}, \tag{48}$$

thus, the function $u(x,t)$ is not normalized. Note that if $\nu = 0$ it follows $\lim_{\xi\to 0} \left\langle |x|^{\xi} \right\rangle = \frac{1}{\Gamma(\mu)} \cdot t^{-(1-\mu)}$ and if $\nu = 1$, $\lim_{\xi\to 0} \left\langle |x|^{\xi} \right\rangle = 1$.

The case $\xi \to 2$ and $\alpha \to 2$ yields

$$\lim_{\xi\to 2} \left\langle |x|^{\xi} \right\rangle = \frac{2}{\Gamma\left(1+\mu-(1-\nu)(1-\mu)\right)} \cdot K_{\mu,2} t^{\mu-(1-\nu)(1-\mu)}. \tag{49}$$

If $\nu = 0$ it is obtained $\lim_{\xi\to 2} \left\langle |x|^{\xi} \right\rangle = \frac{2}{\Gamma(2\mu)} \cdot K_{\mu,2} t^{-1+\mu}$ and if $\nu = 1$ it is obtained $\lim_{\xi\to 2} \left\langle |x|^{\xi} \right\rangle = \frac{1}{\Gamma(1+\mu)} \cdot K_{\mu,2} t^{\mu}$. For $\mu = 1$ it follows the linear time dependence of the mean square displacement $\left\langle x^2 \right\rangle = 2K_{1,2} t$. This fractional moments may be used, for example, in single molecule spectroscopy [1,77].

4. Numerical scheme for solving the space–time fractional diffusion equation

Several numerical algorithms for solving time fractional differential equations have been developed [78]. Although numerical schemes for solving fractional diffusion equations exist [79,80] the case of generalized fractional derivatives has not been treated so far. We therefore briefly discuss a numerical scheme that was used to numerically solve the space–time fractional diffusion equation of Section 3.

Solving the space–time fractional diffusion equations with a generalized R–L time fractional derivative of order $0 < \mu < 1$ of type $0 \le \nu \le 1$ and with Riesz–Feller space fractional derivative of order $0 < \alpha \le 2$ numerically, is most easily attempted in the Fourier domain, which is also suggested by the analytical calculations in the previous sections. The Fourier transformed equations should then be solved numerically and finally a Fast Fourier Transform (FFT) can be used to transform the found solution to the real space domain. We will treat the equation without the singular source here, as the generalization to a fractional differential equation with a singular source term is straightforward.

By application of Leibnitz rule (71) we invert the order of the fractional derivative and of the Fourier transform. Thus, in Fourier space the fractional diffusion equation (23) with boundary conditions (24) and initial condition (25) reads

$$D_{0+}^{\mu,\nu} \hat{f}(\kappa,t) = -|\kappa|^{\alpha} \hat{f}(\kappa,t), \tag{50}$$

where $\hat{f}(\kappa,t) = \int_{-\infty}^{\infty} \mathrm{e}^{\imath\kappa x} f(x,t)\,\mathrm{d}x$. The initial condition (25) for $g(x) = \delta(x)$ is transformed to

$$I_{0+}^{(1-\nu)(1-\mu)} \hat{f}(\kappa,0) = 1 \tag{51}$$

and the boundary conditions are $\hat{f}(\pm\infty,t) = 0$.

We next perform a shift to obtain homogeneous initial conditions. For that we introduce a function $\hat{h}(\kappa,t)$, defined as $\hat{h}(\kappa,t) = I_{0+}^{(1-\nu)(1-\mu)} \hat{f}(\kappa,t) - 1$. This relation can be inverted by using that ${}_{RL}D_{0+}^{(1-\mu)(1-\nu)} I_{0+}^{(1-\nu)(1-\mu)} \hat{f}(\kappa,t) = \hat{f}(\kappa,t)$ and that the R–L and Caputo fractional derivatives of $\hat{h}(\kappa,t)$ are equivalent since $\hat{h}(\kappa,0+) = 0$. Thus, we find

$$\hat{f}(\kappa,t) = {}_{C}D_{0+}^{(1-\mu)(1-\nu)} \hat{h}(\kappa,t) + \frac{t^{-(1-\nu)(1-\mu)}}{\Gamma(1-(1-\nu)(1-\mu))}, \tag{52}$$

where ${}_{C}D_{0+}^{(1-\mu)(1-\nu)} \hat{h}(\kappa,t)$ denotes the Caputo derivative as before.

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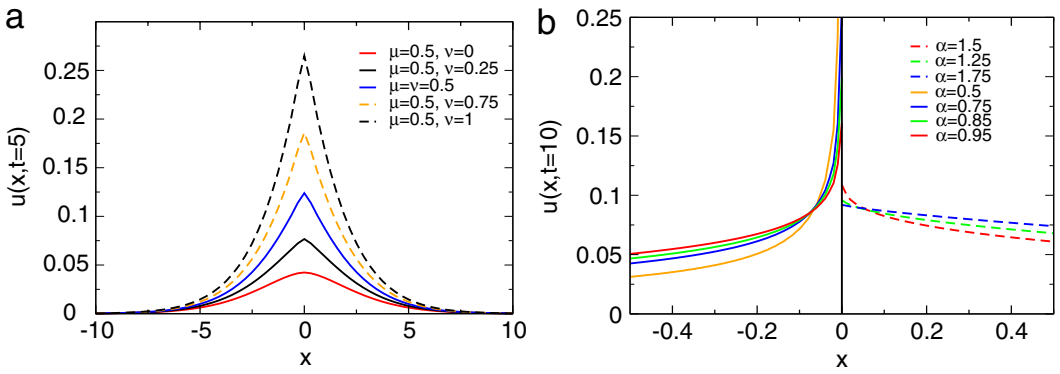

Fig. 6. In (a) the numerical solution of (23) with $g(x) = \delta(x)$ for $t = 5$ with the same parameter values as in Fig. 3 is plotted. It can be clearly seen that the numerical results are in excellent agreement with the exact solutions. In (b) we numerically reproduce the asymptotic results of Fig. 5 for $t = 10$. The asymptotic solutions and the numerical results are in close agreement.

If we next substitute the definition of $\hat{h}(\kappa, t)$ and its inverse (52) in Eq. (50) and use relations (13) and (14) we obtain the following equation for $\hat{h}(\kappa, t)$

$$\left[{}_{C}D_{0+}^{1-\nu(1-\mu)} + |\kappa|^{\alpha}\,{}_{C}D_{0+}^{(1-\nu)(1-\mu)}\right]\hat{h}(\kappa, t) = -|\kappa|^{\alpha}\frac{t^{-(1-\nu)(1-\mu)}}{\Gamma(1-(1-\nu)(1-\mu))} - \frac{t^{-1+\nu(1-\mu)}}{\Gamma(\nu(1-\mu))}. \tag{53}$$

Eq. (53) is solved numerically by approximating the fractional derivatives in the usual way by Grünwald–Letnikov expressions. The Grünwald–Letnikov derivative of order α at time step $t_l = l\Delta t$ of function $h(t)$ is defined as ${}_{GL}D_{t_k}^{\alpha}h(t)$ [32]

$${}_{GL}D_{t_l}^{\alpha}h(t) = (\Delta t)^{-\alpha}\sum_{j=0}^{l}(-1)^j\binom{\alpha}{j}h(t_l - t_j), \tag{54}$$

where the binomial coefficient $\binom{\alpha}{j}$ is defined as $\binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{\Gamma(j+1)\Gamma(\alpha-j+1)}$. This derivative can be shown to be equivalent to the R–L derivative for $\alpha \leq 1$ if $h(t)$ is continuous [32]. The Grünwald–Letnikov derivative is commonly used as a discretization needed for the numerical evaluation of fractional derivatives.

Discretizing Eq. (53) using the above-mentioned discretization leads immediately to the following backward numerical scheme that determines $\hat{h}$ at time step $t_i = i\Delta t$

$$\begin{aligned}\hat{h}(\kappa, t_i) = &-\frac{|\kappa|^{\alpha}(\Delta t)^{\mu}i^{-(1-\nu)(1-\mu)}}{(1+|\kappa|^{\alpha}(\Delta t)^{\mu})\Gamma(1-(1-\nu)(1-\mu))} - \frac{i^{-1+\nu(1-\mu)}}{(1+|\kappa|^{\alpha}(\Delta t)^{\mu})\Gamma(\nu(1-\mu))}\\ &-\frac{\sum_{j=1}^{i}(-1)^j\binom{1-\nu(1-\mu)}{j}\hat{h}(t_i - t_j) + |\kappa|^{\alpha}(\Delta t)^{\mu}\sum_{j=1}^{i}(-1)^j\binom{(1-\nu)(1-\mu)}{j}\hat{h}(t_i - t_j)}{1+|\kappa|^{\alpha}(\Delta t)^{\mu}}.\end{aligned} \tag{55}$$

By applying the Grünwald–Letnikov approximation in relation (52) at time step t_i, we find

$$\hat{f}(\kappa, t_i) = (\Delta t)^{-(1-\mu)(1-\nu)}\sum_{j=0}^{i}(-1)^j\binom{(1-\nu)(1-\mu)}{j}\hat{h}(\kappa, (i-j)\Delta t) + \frac{(i\Delta t)^{-(1-\nu)(1-\mu)}}{\Gamma(1-(1-\nu)(1-\mu))}. \tag{56}$$

Example 4. We illustrate the accuracy of the numerical scheme by first solving Eq. (23) numerically for different values of ν; this shows that the exact solution plotted in Fig. 3 and the numerical solutions are in excellent agreement. We next compare the asymptotic results of Fig. 5(a) with the numerical solution for $\mu = \nu = 1/2$ and varying values of α.

In Fig. 6 we plotted the numerical solutions of (23) for different values of ν and keeping $\mu = 1/2$ fixed and $\alpha = 2$. The perfect agreement between Figs. 6(a) and Fig. 3 illustrates the way numerical solutions can be obtained for time fractional partial differential equations that are in very good agreement with the exact results. In Fig. 6(b) we show that the asymptotic expansion displayed in Fig. 5 is valid for $t = 10$, as the numerical calculations show almost exactly the same behaviour.

We next turn to space–time fractional diffusion equations with a singular term.

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5. Space–time fractional diffusion equation with a singular term

We also study a generalized space–time fractional diffusion equation with a singular term:

$$D_{0+}^{\mu,\nu}u(x,t)=K_{\mu,\alpha}\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x,t)+\delta(x)\frac{t^{-\beta}}{\Gamma(1-\beta)},\quad t>0,\ -\infty<x<+\infty, \tag{57}$$

where $\beta>0$, with boundary conditions (24) and an initial condition (25).

Theorem 2. *The fractional diffusion equation (57) with boundary conditions (24) and an initial condition (25) in case when $0<\mu<1,\ 0\leq\nu\leq 1,\ 0<\alpha\leq 2$ has a solution of the following form*

$$\begin{aligned}u(x,t)=&\frac{1}{2\pi}\int_{-\infty}^{\infty}t^{-(1-\nu)(1-\mu)}E_{\mu,1-(1-\nu)(1-\mu)}\left(-K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\right)\cdot\hat{g}(\kappa)\cdot\mathrm{e}^{-\imath\kappa x}\mathrm{d}\kappa\\&+\frac{t^{-(\beta-\mu)}}{\alpha|x|}\cdot H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1-(\beta-\mu),\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right]\end{aligned} \tag{58}$$

where $\hat{g}(\kappa)=\mathcal{F}[g(x)]$ is the Fourier transform of the function $g(x)$ and

$$F(x,s)=\mathcal{L}[f(x,t)],\qquad\tilde{F}(\kappa,s)=\mathcal{F}[F(x,s)],\qquad F(\kappa,t)=\mathcal{L}^{-1}[\tilde{F}(\kappa,s)]. \tag{59}$$

Proof. The Laplace transform with respect to the time variable t and Fourier transform with respect to the space variable x to Eq. (57) and the initial condition (25) and boundary conditions (24) give

$$\tilde{U}(\kappa,s)=\frac{s^{-\nu(1-\mu)}}{s^{\mu}+|\kappa|^{\alpha}K_{\mu,\alpha}}\cdot\hat{g}(\kappa)+\frac{s^{\beta-1}}{s^{\mu}+|\kappa|^{\alpha}K_{\mu,\alpha}}, \tag{60}$$

where $\tilde{U}(\kappa,s)=\mathcal{F}\left[U(x,s)\right]$, $U(x,s)=\mathcal{L}\left[u(x,t)\right]$. The inverse Laplace transform to relation (60) yields

$$U(\kappa,t)=t^{-(1-\nu)(1-\mu)}E_{\mu,1-(1-\nu)(1-\mu)}\left(-K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\right)\hat{g}(\kappa)+t^{-(\beta-\mu)}E_{\mu,1-(\beta-\mu)}\left(-K_{\mu,\alpha}|\kappa|^{\alpha}t^{\mu}\right). \tag{61}$$

Finally, by finding inverse Fourier transform to relation (61) we prove Theorem 2. □

Example 5. The space–time fractional diffusion equation (57) with boundary conditions (24) and an initial condition $g(x)=\delta(x)$, has a solution of the form

$$\begin{aligned}u(x,t)=&\frac{1}{\alpha|x|}t^{-(1-\nu)(1-\mu)}H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1-(1-\nu)(1-\mu),\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right]\\&+\frac{t^{-(\beta-\mu)}}{\alpha|x|}\cdot H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}}\left|\begin{matrix}\left(1,\frac{1}{\alpha}\right),\left(1-(\beta-\mu),\frac{\mu}{\alpha}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\alpha}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right].\end{aligned} \tag{62}$$

This solution for $\alpha=2$ becomes [34]

$$\begin{aligned}u(x,t)=&\frac{t^{-(1-\nu)(1-\mu)}}{2|x|}\cdot H_{1,1}^{1,0}\left[\frac{|x|}{\sqrt{K_{\mu,\alpha}t^{\mu}}}\left|\begin{matrix}\left(1-(1-\nu)(1-\mu),\frac{\mu}{2}\right)\\(1,1)\end{matrix}\right.\right]\\&+\frac{t^{-(\beta-\mu)}}{2|x|}\cdot H_{1,1}^{1,0}\left[\frac{|x|}{\sqrt{K_{\mu,\alpha}t^{\mu}}}\left|\begin{matrix}\left(1-(\beta-\mu),\frac{\mu}{2}\right)\\(1,1)\end{matrix}\right.\right].\end{aligned} \tag{63}$$

Graphical representation of the solution (63) for various values of the parameters is given in Fig. 7.

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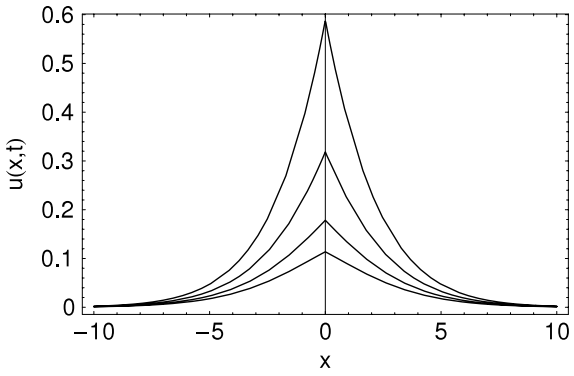

Fig. 7. Graphical representation of solution (63) for $K_{\mu,\alpha}=1$, $t=10$, $\mu=\nu=1/2$, $\beta=0.25$ (upper line), $\beta=0.5$, $\beta=0.75$, $\beta=1$ (lower line).

Example 6 (*Asymptotic Expansions*)**.** The asymptotic behaviour of the solution (62) can be obtained in a same way as it was done in Example 2. Thus, solution (62) can be expressed by the following series

$$u(x,t) = \frac{K_{\mu,\alpha}^{-1/\alpha} t^{-(1-\nu)(1-\mu)-\mu/\alpha}}{\alpha} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{\sin\left(\frac{1+k}{2}\pi\right)}{\sin\left(\frac{1+k}{\alpha}\pi\right)} \left[A(k,t)+B(k,t)\right] \frac{|x|^k}{\left(K_{\mu,\alpha}t^{\mu}\right)^{k/\alpha}}$$
$$+ \frac{|x|^{\alpha-1}}{\pi K_{\mu,\alpha}} \sum_{k=0}^{\infty} (-1)^k \Gamma\left(1-\alpha(1+k)\right) \sin\left[\frac{(1+k)\alpha}{2}\pi\right] \left[C(k,t)+D(k,t)\right] \frac{|x|^{\alpha k}}{\left(K_{\mu,\alpha}t^{\mu}\right)^{k}}, \tag{64}$$

where $A(k,t) = \frac{t^{-(1-\nu)(1-\mu)-\frac{\mu}{\alpha}}}{\Gamma\left(1-(1-\nu)(1-\mu)-\frac{1+k}{\alpha}\mu\right)}$, $B(k,t) = \frac{t^{-(\beta-\mu)-\frac{\mu}{\alpha}}}{\Gamma\left(1-(\beta-\mu)-\frac{1+k}{\alpha}\mu\right)}$, $C(k,t) = \frac{t^{-(1-\nu)(1-\mu)-\mu}}{\Gamma(1-(1-\nu)(1-\mu)-\mu-\mu k)}$, $D(k,t) = \frac{t^{-\beta}}{\Gamma(1-\beta-\mu k)}$.

Thus for $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \ll 1$, we obtain

$$u(x,t) \sim \frac{K_{\mu,\alpha}^{-1/\alpha}}{\alpha \sin\left(\frac{\pi}{\alpha}\right)} \cdot \frac{t^{-(1-\nu)(1-\mu)-\mu/\alpha}}{\Gamma\left(1-(1-\nu)(1-\mu)-\frac{\mu}{\alpha}\right)} + |x|^{\alpha-1} \frac{K_{\mu,\alpha}^{-1}}{2\Gamma(\alpha)\cos\left(\frac{\alpha\pi}{2}\right)} \cdot \frac{t^{-(1-\nu)(1-\mu)-\mu}}{\Gamma\left(1-(1-\nu)(1-\mu)-\mu\right)}$$
$$+ \frac{K_{\mu,\alpha}^{-1/\alpha}}{\alpha \sin\left(\frac{\pi}{\alpha}\right)} \cdot \frac{t^{-(\beta-\mu)-\mu/\alpha}}{\Gamma\left(1-(\beta-\mu)-\frac{\mu}{\alpha}\right)} + |x|^{\alpha-1} \frac{K_{\mu,\alpha}^{-1}}{2\Gamma(\alpha)\cos\left(\frac{\alpha\pi}{2}\right)} \cdot \frac{t^{-\beta}}{\Gamma\left(1-\beta\right)}. \tag{65}$$

For $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \gg 1$, one can obtain

$$u(x,t) = \frac{1}{\pi\alpha|x|} t^{-(1-\nu)(1-\mu)} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}\Gamma(1+\alpha k)\sin\left(\frac{\alpha k\pi}{2}\right)}{\Gamma\left(1-(1-\nu)(1-\mu)+\mu k\right)} \frac{\left(K_{\mu,\alpha}t^{\mu}\right)^k}{|x|^{\alpha k}}$$
$$+ \frac{1}{\pi\alpha|x|} t^{-(\beta-\mu)} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}\Gamma(1+\alpha k)\sin\left(\frac{\alpha k\pi}{2}\right)}{\Gamma\left(1-(\beta-\mu)+\mu k\right)} \frac{\left(K_{\mu,\alpha}t^{\mu}\right)^k}{|x|^{\alpha k}}, \tag{66}$$

from where

$$u(x,t) \sim \frac{\Gamma(\alpha)\sin\left(\frac{\alpha\pi}{2}\right)}{\pi\Gamma\left(1-(1-\nu)(1-\mu)+\mu\right)} \cdot |x|^{-\alpha-1} K_{\mu,\alpha} t^{\mu-(1-\nu)(1-\mu)} + \frac{\Gamma(\alpha)\sin\left(\frac{\alpha\pi}{2}\right)}{\pi\Gamma\left(1+2\mu-\beta\right)} \cdot |x|^{-\alpha-1} K_{\mu,\alpha} t^{2\mu-\beta}. \tag{67}$$

As a special case $\alpha=2$ in case when $\frac{|x|}{\left(K_{\mu,\alpha}t^{\mu}\right)^{1/\alpha}} \gg 1$; from relation (44) we obtain the asymptotic behaviour of the solution (63) [34]

$$u(x,t) \sim \frac{1}{2\sqrt{(2-\mu)\pi}} \cdot \left(\frac{\mu}{2}\right)^{\frac{(1-\mu)(1-2\nu)}{2-\mu}} \cdot |x|^{\frac{(1-\mu)(1-2\nu)}{2-\mu}} \cdot \left(K_{\mu,2}t^{\mu}\right)^{-\frac{(1-\nu)(1-\mu)+1/2}{2-\mu}}$$
$$\times \exp\left[-\frac{2-\mu}{2}\left(\frac{\mu}{2}\right)^{\frac{\mu}{2-\mu}} |x|^{\frac{2}{2-\mu}} \left(K_{\mu,2}t^{\mu}\right)^{-\frac{1}{2-\mu}}\right]$$
$$+ \frac{1}{2\sqrt{(2-\mu)\pi}} \cdot \left(\frac{\mu}{2}\right)^{\frac{2\beta-\mu-1}{2-\mu}} \cdot |x|^{\frac{2\beta-\mu-1}{2-\mu}} \cdot \left(K_{\mu,2}t^{\mu}\right)^{-\frac{(\beta-\mu)+1/2}{2-\mu}}$$
$$\times \exp\left[-\frac{2-\mu}{2}\left(\frac{\mu}{2}\right)^{\frac{\mu}{2-\mu}} |x|^{\frac{2}{2-\mu}} \left(K_{\mu,2}t^{\mu}\right)^{-\frac{1}{2-\mu}}\right]. \tag{68}$$

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Example 7. Following the procedure in Example 3, the fractional moments (45) of the fractional diffusion equation (57) with $g(x) = \delta(x)$ are given by

$$\left\langle |x|^{\xi} \right\rangle = \frac{2}{\alpha} \cdot t^{-(1-\nu)(1-\mu)} \left(K_{\mu,\alpha} t^{\mu}\right)^{\xi/\alpha} \cdot \frac{\Gamma\left(1+\xi\right) \sin\left(\frac{\xi\pi}{2}\right)}{\Gamma\left(1-(1-\nu)(1-\mu)+\frac{\mu\xi}{\alpha}\right) \sin\left(\frac{\xi\pi}{\alpha}\right)} + \frac{2}{\alpha} \cdot t^{-(\beta-\mu)} \left(K_{\mu,\alpha} t^{\mu}\right)^{\xi/\alpha} \cdot \frac{\Gamma\left(1+\xi\right) \sin\left(\frac{\xi\pi}{2}\right)}{\Gamma\left(1-(\beta-\mu)+\frac{\mu\xi}{\alpha}\right) \sin\left(\frac{\xi\pi}{\alpha}\right)}. \tag{69}$$

Example 8. The space–time fractional diffusion equation (57) with boundary conditions (24) and an initial condition $g(x) = 0$, has a solution of the form

$$u(x,t) = \frac{t^{-(\beta-\mu)}}{\alpha|x|} \cdot H_{3,3}^{2,1}\left[\frac{|x|}{\left(K_{\mu,\alpha} t^{\mu}\right)^{1/\alpha}} \middle| \begin{matrix} \left(1, \frac{1}{\alpha}\right), \left(1-(\beta-\mu), \frac{\mu}{\alpha}\right), \left(1, \frac{1}{2}\right) \\ (1,1), \left(1, \frac{1}{\alpha}\right), \left(1, \frac{1}{2}\right) \end{matrix} \right]. \tag{70}$$

This result follows directly from Theorem 2.

Remark 3. Note that the solution (70) of Eq. (57) for $\beta = \mu$ is equivalent to the solution (36) of Eq. (23) for $\nu = 1$, which is in fact a proof of the statement for the equivalent formulations (19). Thus for $\beta = \mu = 1$ and $\alpha = 2$ we obtain the solution of the classical diffusion equation (38), which for $K_{\mu,\alpha} = 1/2$ is the same as the probability density function of a Wiener process. Furthermore, if the singular term is of form $\delta(x) \frac{t^{-(1-\nu)(1-\mu)-\mu}}{\Gamma(1-(1-\nu)(1-\mu)-\mu)}$, the solution of Eq. (57) with boundary conditions (24) and an initial condition $g(x) = 0$ is the same as the solution (32) of Eq. (23) with boundary conditions (24) and an initial condition $g(x) = \delta(x)$ (see Example 1).

6. Conclusions

We found exact solution of the space–time fractional diffusion equations with a generalized R–L time fractional derivative of order $0 < \mu < 1$ and type $0 \leq \nu \leq 1$ and Riesz–Feller space fractional derivative of order $0 < \alpha \leq 2$. The fundamental solution of the equation is obtained. The solutions of the equations are expressed in terms of the M-L function and H-function. Asymptotic behaviours of the solutions are found. The fractional moments of the fundamental solution of the considered space–time fractional diffusion equation are calculated. Many already known results are recovered. Exact and asymptotic solutions and fractional moments of the space–time fractional diffusion equation with a singular term are obtained as well. A numerical scheme for solving space–time fractional diffusion equations with a generalized composite (Hilfer) time derivative is reported for the first time in the literature and the numerical results are compared with the asymptotic and exact results. It is shown that they are in good agreement.

Given the successful application of the generalized composite (Hilfer) derivative for modelling of highly non-trivial dielectric data by Hilfer [7], we believe that extended fractional equation discussed here will be useful in science and engineering.

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Appendix. Leibnitz rule

Let $f(x,\omega)$ and $\frac{\partial^{\alpha}}{\partial\omega^{\alpha}} f(x,\omega)$ be continuous functions of their variables for all $x, \omega \in \mathbb{R}$. Furthermore, let $\int_{-\infty}^{\infty} |f(x,\omega)| \mathrm{d}x < \infty$ and $\left|\frac{\partial^{\alpha} f}{\partial\omega^{\alpha}}\right| \leq h(x)$, where $h(x)$ is a piecewise continuous such that $\int_{-\infty}^{\infty} h(x)\mathrm{d}x < \infty$. Then

$$\frac{\mathrm{d}^{\alpha}}{\mathrm{d}\omega^{\alpha}} \int_{-\infty}^{\infty} f(x,\omega)\mathrm{d}x = \int_{-\infty}^{\infty} \frac{\partial^{\alpha}}{\partial\omega^{\alpha}} \left[f(x,\omega)\right] \mathrm{d}x. \tag{71}$$

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