Available online at www.sciencedirect.com
ScienceDirect
Applied Mathematics and Computation 187 (2007) 295–305
APPLIED MATHEMATICS AND COMPUTATION
www.elsevier.com/locate/amc

Some aspects of fractional diffusion equations of single and distributed order

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Dedicated to Professor H.M. Srivastava on the occasion of his 65th birthday

Abstract

The time fractional diffusion equation is obtained from the standard diffusion equation by replacing the first-order time derivative with a fractional derivative of order $\beta \in (0,1)$. The fundamental solution for the Cauchy problem is interpreted as a probability density of a self-similar non-Markovian stochastic process related to a phenomenon of sub-diffusion (the variance grows in time sub-linearly). A further generalization is obtained by considering a continuous or discrete distribution of fractional time derivatives of order less than one. Then the fundamental solution is still a probability density of a non-Markovian process that, however, is no longer self-similar but exhibits a corresponding distribution of time-scales.

MSC 2000: 26A33; 45K05; 60G18; 60J60

Keywords: Anomalous diffusion; Fractional derivatives; Integral transforms; Mellin-Barnes integrals; Stochastic processes; Asymptotic power laws

1. Introduction

The main physical purpose for adopting and investigating diffusion equations of fractional order is to describe phenomena of *anomalous diffusion* usually met in transport processes through complex and/or disordered systems including fractal media. In this respect, in recent years interesting reviews, see e.g. [29,31,40], have appeared, to which (and references therein) we refer the interested reader. All the related models of

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0096-3003/$ - see front matter
doi:10.1016/j.amc.2006.08.126

random walk turn out to be beyond the classical Brownian motion, which is known to provide the microscopic foundation of the standard diffusion, see e.g. [19,37]. The diffusion-like equations containing fractional derivatives in time and/or in space are usually adopted to model phenomena of anomalous transport in physics, so a detailed study of their solutions is required.

Our attention in this paper will be focused on the time fractional diffusion equations of a single or distributed order less than 1, which are known to be models for sub-diffusive processes. Specifically, we have worked out how to express their fundamental solutions in terms of series expansions obtained from their representations with Mellin–Barnes integrals.

In Section 2 we shall recall the main results for the fundamental solution of the time fractional diffusion equation of a single order, which are obtained by applying two different strategies in inverting its Fourier–Laplace transform. Both techniques yield the same power series representations of the required solution: it turns out to be self similar (through a definite space–time scaling relationship), and expressed in terms of a special function of the Wright type. Then, in Section 3, we shall apply the second strategy for obtaining the fundamental solution in the general case of a distributed order. We have provided a representation in terms of a Laplace-type integral of a Wright function, that can be expanded in a series containing powers of the space variable and certain functions of time, responsible for the time-scale distribution. Finally, in Section 4, the main conclusions are drawn. For convenience and self-consistency we provide an Appendix devoted to our notations of fractional calculus.

2. The time fractional diffusion equation of single order

The standard *diffusion equation* in re-scaled non-dimensional variables has the form

$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t), \quad x \in \mathbf{R}, \;\; t \in \mathbf{R}_0^+, \tag{2.1}$$

with $u(x,t)$ as the field variable. We assume the initial condition

$$u(x,0^+) = u_0(x), \tag{2.2}$$

where $u_0(x)$ denotes a given ordinary or generalized function defined on $\mathbf{R}$, that is Fourier transformable in ordinary or generalized sense, respectively. We assume to work in a suitable space of generalized functions where it is possible to deal freely with delta functions, integral transforms of Fourier, Laplace and Mellin type, and fractional integrals and derivatives.

It is well known that the fundamental solution (or *Green function*) of Eq. (2.1) i.e. the solution subjected to the initial condition $u(x,0) = u_0(x) = \delta(x)$, and to the decay to zero conditions for $|x| \to \infty$, is the Gaussian *probability density function* (pdf)

$$u(x,t) = \frac{1}{2\sqrt{\pi}}t^{-1/2}\mathrm{e}^{-x^2/(4t)}, \tag{2.3}$$

that evolves in time with second moment growing linearly with time,

$$\mu_2(t) := \int_{-\infty}^{+\infty} x^2 u(x,t)\,\mathrm{d}x = 2t, \tag{2.4}$$

consistently with a law of *normal diffusion*.[1] We note the *scaling property* of the Green function, expressed by the equation

$$u(x,t) = t^{-1/2}U(x/t^{1/2}), \quad \text{with} \quad U(x) := u(x,1). \tag{2.5}$$

[1] The centred second moment provides the variance usually denoted by $\sigma^2(t)$. It is a measure for the spatial spread of $u(x,t)$ with time of a random walking particle starting at the origin $x = 0$, pertinent to the solution of the diffusion Eq. (2.1) with initial condition $u(x,0) = \delta(x)$. The asymptotic behaviour of the variance as $t \to \infty$ is relevant to distinguish *normal diffusion* ($\sigma^2(t)/t \to c > 0$) from anomalous processes of *sub-diffusion* ($\sigma^2(t)/t \to 0$) and of *super-diffusion* ($\sigma^2(t)/t \to +\infty$).

The function $U(x)$ depending on the single variable x turns out to be an even function $U(x) = U(|x|)$ and is called the *reduced Green function*. The variable $X := x/t^{1/2}$ is known as the similarity variable. It is known that the Cauchy problem {(2.1),(2.2)} is equivalent to the integro-differential equation

$$u(x,t) = u_0(x) + \int_0^t \left[\frac{\partial^2}{\partial x^2} u(x,\tau)\right] d\tau, \tag{2.6}$$

where the initial condition is incorporated. Now, by using the tools of the fractional calculus we can generalize the above Cauchy problem in order to obtain the so-called *time fractional diffusion equation* in the two distinct (but mathematically equivalent) forms available in the literature, where the initial condition is understood as (2.2). For the essentials of fractional calculus we refer the interested reader to the Appendix.

If β denotes a real number such that $0 < \beta < 1$ the two forms are as follows:

$$\frac{\partial}{\partial t} u(x,t) = {}_tD^{1-\beta} \frac{\partial^2}{\partial x^2} u(x,t), \quad x \in \mathbf{R}, \ t \in \mathbf{R}_0^+; \qquad u(x,0^+) = u_0(x), \tag{2.7}$$

where ${}_tD^{1-\beta} = {}_tD^1 \, {}_tJ^\beta$ denotes the *Riemann–Liouville* (R–L) time-fractional derivative of order $1-\beta$, see (A.4) with $m = 1$, and

$${}_tD_*{}^\beta u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), \quad x \in \mathbf{R}, \ t \in \mathbf{R}_0^+; \qquad u(x,0^+) = u_0(x), \tag{2.8}$$

where ${}_tD_*^\beta = {}_tJ^{1-\beta} \, {}_tD^1$ denotes the time-fractional derivative of order β intended in the *Caputo* sense, see (A.5) with $m = 1$. In analogy with the standard diffusion equation we can provide an integro-differential form that incorporates the initial condition (2.2): for this purpose we replace in (2.6) the ordinary integral with the Riemann–Liouville fractional integral of order β, ${}_tJ^\beta$, namely

$$u(x,t) = u_0(x) + {}_tJ^\beta \left[\frac{\partial^2}{\partial x^2} u(x,t)\right]. \tag{2.9}$$

Then, the above equations read explicitly:

$$\frac{\partial}{\partial t} u(x,t) = \frac{1}{\Gamma(\beta)} \frac{\partial}{\partial t} \left\{ \int_0^t \left[\frac{\partial^2}{\partial x^2} u(x,\tau)\right] \frac{d\tau}{(t-\tau)^{1-\beta}} \right\}, \quad u(x,0^+) = u_0(x), \tag{2.7$'$}$$

$$\frac{1}{\Gamma(1-\beta)} \int_0^t \left[\frac{\partial}{\partial \tau} u(x,\tau)\right] \frac{d\tau}{(t-\tau)^\beta} = \frac{\partial^2}{\partial x^2} u(x,t), \quad u(x,0^+) = u_0(x), \tag{2.8$'$}$$

$$u(x,t) = u_0(x) + \frac{1}{\Gamma(\beta)} \int_0^t \left[\frac{\partial^2}{\partial x^2} u(x,\tau)\right] \frac{d\tau}{(t-\tau)^{1-\beta}}. \tag{2.9$'$}$$

The two Cauchy problems (2.7) and (2.8) and the integro-differential equation (2.9) are equivalent [2]: for example, we derive (2.7) from (2.9) simply differentiating both sides of (2.9), whereas we derive (2.9) from (2.8) by fractional integration of order β. In fact, in view of the semigroup property (A.2) of the fractional integral, we note that

$${}_tJ^\beta \, {}_tD_*^\beta u(x,t) = {}_tJ^\beta \, {}_tJ^{1-\beta} \, {}_tD^1 u(x,t) = {}_tJ^1 \, {}_tD^1 u(x,t) = u(x,t) - u_0(x). \tag{2.10}$$

In the limit $\beta = 1$ we recover the well-known diffusion Eq. (2.1).

[2] The integro-differential equation (2.9) was investigated via Mellin transforms by Schneider and Wyss [35] in their pioneering 1989 paper. The time fractional diffusion equation in the form (2.8) with the Caputo derivative has been preferred and investigated by several authors. From the earlier contributors let us quote Caputo himself [3], Mainardi, see e.g. [20–22] and Gorenflo et al. [16,17]. In particular, Mainardi has expressed the fundamental solution in terms of a special function (of Wright type) of which he has studied the analytical properties and provided plots also for $1 < \beta < 2$, see also [12,13,25] and references therein. For the form (2.7) with the R–L derivative earlier contributors include the group of Prof. Nonnenmacher, see e.g. [28], and Saichev and Zaslavsky [33].

Let us consider from now on the Eq. (2.8) with $u_0(x) = \delta(x)$: the fundamental solution can be obtained by applying in sequence the Fourier and Laplace transforms to it. We write, for generic functions $v(x)$ and $w(t)$, these transforms as follows:

$$\begin{aligned} &\mathscr{F}\{v(x);\kappa\} = \hat{v}(\kappa) := \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}\kappa x} v(x)\mathrm{d}x, \quad \kappa \in \mathbf{R}, \\ &\mathscr{L}\{w(t);s\} = \tilde{w}(s) := \int_0^{+\infty} \mathrm{e}^{-st} w(t)\mathrm{d}t, \quad s \in \mathbf{C}. \end{aligned} \tag{2.11}$$

Then, in the Fourier–Laplace domain our Cauchy problem [(2.8) with $u(x,0^+) = \delta(x)$], after applying formula (A.6) for the Laplace transform of the fractional derivative and observing $\hat{\delta}(\kappa) \equiv 1$, see e.g. [10], appears in the form $s^\beta \hat{\tilde{u}}(\kappa,s) - s^{\beta-1} = -\kappa^2 \hat{\tilde{u}}(\kappa,s)$, from which we obtain

$$\hat{\tilde{u}}(\kappa,s) = \frac{s^{\beta-1}}{s^\beta + \kappa^2}, \quad 0 < \beta \leqslant 1, \;\; \Re(s) > 0, \;\; \kappa \in \mathbf{R}. \tag{2.12}$$

To determine the Green function $u(x,t)$ in the space–time domain we can follow two alternative strategies related to the order in carrying out the inversions in (2.12).

(S1): invert the Fourier transform getting $\tilde{u}(x,s)$ and then invert the remaining Laplace transform;
(S2): invert the Laplace transform getting $\hat{u}(\kappa,t)$ and then invert the remaining Fourier transform.

Strategy (S1): The strategy (S1) has been applied by Mainardi [20–22] to obtain the Green function in the form

$$u(x,t) = t^{-\beta/2} U(|x|/t^{\beta/2}), \quad -\infty < x < +\infty, \;\; t \geqslant 0, \tag{2.13}$$

where the variable $X := x/t^{\beta/2}$ acts as *similarity variable* and the function $U(x) := u(x,1)$ denotes the *reduced Green function*. Restricting from now on our attention to $x \geqslant 0$, the solution turns out as

$$\begin{aligned} U(x) &= \frac{1}{2} M_{\frac{\beta}{2}}(x) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{(-x)^k}{k!\Gamma[-\beta k/2 + (1-\beta/2)]} \\ &= \frac{1}{2\pi} \sum_{k=0}^{\infty} \frac{(-x)^k}{k!} \Gamma[(\beta(k+1)/2] \sin[(\pi\beta(k+1)/2], \end{aligned} \tag{2.14}$$

where $M_{\frac{\beta}{2}}(x)$ is an entire transcendental function (of order $1/(1-\beta/2)$) of the Wright type, see also [12,13,32].

Strategy (S2): The strategy (S2) has been followed by Gorenflo et al. [11] and by Mainardi et al. [24] to obtain the Green functions of the more general space–time fractional diffusion equations, and requires to invert the Fourier transform by using the machinery of the Mellin convolution and the Mellin–Barnes integrals. Restricting ourselves here to recall the final results, the reduced Green function for the time fractional diffusion equation now appears, for $x \geqslant 0$, in the form:

$$U(x) = \frac{1}{\pi} \int_0^\infty \cos(\kappa x) E_\beta(-\kappa^2) \mathrm{d}\kappa = \frac{1}{2x} \frac{1}{2\pi \mathrm{i}} \int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \frac{\Gamma(1-s)}{\Gamma(1-\beta s/2)} x^s \mathrm{d}s, \tag{2.15}$$

with $0 < \gamma < 1$, where E_β denotes the Mittag–Leffler function, see e.g. [9,23]. By evaluating the Mellin–Barnes integrals using the residue theorem, we arrive at the same power series (2.19).

Both strategies allow us to prove that the Green function is non-negative and normalized, so it can be interpreted as a spatial probability density evolving in time with the similarity law (2.13). Although the two strategies are equivalent for yielding the required result, the second one appears more general and so more suitable for treating the more complex case of fractional diffusion of distributed order, see the next Section.

Of particular interest is the evolution of the second moment as it can be derived from Eq. (2.12) noting that

$$\widetilde{\mu}_2(s) = -\frac{\partial^2}{\partial \kappa^2} \hat{\tilde{u}}(\kappa = 0, s) = \frac{2}{s^{\beta+1}}, \quad \text{so } \mu_2(t) = 2\frac{t^\beta}{\Gamma(\beta+1)}. \tag{2.16}$$

When $0 < \beta < 1$ the sub-linear growth in time is consistent with an anomalous process of *sub-diffusion*.

3. The time-fractional diffusion equation of distributed order

The fractional diffusion equation (2.8) can be generalized by using the notion of fractional derivative of distributed order in time.[3] We now consider the so-called *time-fractional diffusion equation of distributed order*

$$\int_0^1 b(\beta)[{}_tD_*^\beta u(x,t)]\mathrm{d}\beta = \frac{\partial^2}{\partial x^2}u(x,t), \quad b(\beta) \geqslant 0, \ \int_0^1 b(\beta)\mathrm{d}\beta = 1, \tag{3.1}$$

with $x \in \mathbf{R}$, $t \geqslant 0$, subjected to the initial condition $u(x,0^+) = \delta(x)$. Clearly, some special conditions of regularity and boundary behaviour will be required for the weight function $b(\beta)$, that we call the order-density.

Equations of type (3.1) have recently been discussed in [6–8,36] and in [30]. As usual,we have considered the initial condition $u(x,0^+) = \delta(x)$ in order to keep the probability meaning. Indeed, already in the paper [6], it was shown that the Green function is non-negative and normalized, so allowing interpretation as a density of the probability at time t of a diffusing particle to be in the point x. The main interest of the authors in [6–8,36] was devoted to the second moment of the Green function (the displacement variance) in order to show the subdiffusive character of the related stochastic process by analyzing some interesting cases of the order-density function $b(\beta)$. For a thorough general study of fractional pseudo-differential equations of distributed order let us cite the paper by Umarov and Gorenflo [39]. For a relationship with the Continuous Random Walk models we may refer to the paper by Gorenflo and Mainardi [15].

In this paper, extending the approach by Naber [30], we provide a general representation of the fundamental solution corresponding to a generic order-density $b(\beta)$. By applying in sequence the Fourier and Laplace transforms to Eq. (3.1) in analogy with the single-order case, see Eq. (2.12), we obtain

$$\left[\int_0^1 b(\beta)s^\beta \mathrm{d}\beta\right]\hat{\tilde{u}}(\kappa,s) - \int_0^1 b(\beta)s^{\beta-1}\mathrm{d}\beta = -\kappa^2\hat{\tilde{u}}(\kappa,s),$$

from which

$$\hat{\tilde{u}}(\kappa,s) = \frac{B(s)/s}{B(s)+\kappa^2}, \quad \Re(s) > 0, \ \kappa \in \mathbf{R}, \tag{3.2}$$

where

$$B(s) = \int_0^1 b(\beta)s^\beta \mathrm{d}\beta. \tag{3.3}$$

Before trying to get the solution in the space–time domain it is worth to outline the expression of its second moment as it can be derived from Eq. (3.2) using (2.16). We have, for κ near zero,

$$\hat{\tilde{u}}(\kappa,s) = \frac{1}{s}\left(1 - \frac{\kappa^2}{B(s)} + \cdots\right), \quad \text{so } \widetilde{\mu_2}(s) = -\frac{\partial^2}{\partial\kappa^2}\hat{\tilde{u}}(\kappa=0,s) = \frac{2}{sB(s)}. \tag{3.4}$$

Then, from (3.4) we are allowed to derive the asymptotic behaviours of $\mu_2(t)$ for $t \to 0^+$ and $t \to +\infty$ from the asymptotic behaviours of $B(s)$ for $s \to \infty$ and $s \to 0$, respectively, in virtue of the Tauberian theorems. The expected sub-linear growth with time is shown in the following special cases of $b(\beta)$ treated in [6,7]. The first case is *slow diffusion* (power-law growth) where

$$b(\beta) = b_1\delta(\beta-\beta_1) + b_2\delta(\beta-\beta_2), \quad 0 < \beta_1 < \beta_2 \leqslant 1, \ b_1 > 0, \ b_2 > 0, \ b_1 + b_2 = 1.$$

In fact

$$\widetilde{\mu_2}(s) = \frac{2}{b_1 s^{\beta_1+1} + b_2 s^{\beta_2+1}}, \quad \text{so } \mu_2(t) \sim \begin{cases} \dfrac{2}{b_2\Gamma(\beta_2+1)}t^{\beta_2}, & t \to 0, \\ \dfrac{2}{b_1\Gamma(\beta_1+1)}t^{\beta_1}, & t \to \infty. \end{cases} \tag{3.5}$$

[3] We find an earlier idea of fractional derivative of distributed order in time in the 1969 book by Caputo [3], that was later developed by Caputo himself, see [4,5] and by Bagley and Torvik, see [1].

In [6], see Eq. (16), the authors were able to provide the analytical expression of $\mu_2(t)$ in terms of a 2-parameter Mittag–Leffler function.

The second case is *super-slow diffusion* (logarithmic growth) where

$$b(\beta) = 1, \quad 0 \leqslant \beta \leqslant 1.$$

In fact

$$\widetilde{\mu_2}(s) = \frac{s-1}{\log s}, \quad \text{so } \mu_2(t) \sim \begin{cases} 2t\log(1/t), & t \to 0, \\ 2\log(t), & t \to \infty. \end{cases} \tag{3.6}$$

In [6], see Eqs. (23)–(26), the authors were able to provide the analytical expression of $\mu_2(t)$ in terms of an exponential integral function.

Inverting the Laplace transform, in virtue of a theorem by Titchmarsh we obtain the remaining Fourier transform as

$$\hat{u}(\kappa, t) = -\frac{1}{\pi}\int_0^\infty \mathrm{e}^{-rt}\mathrm{Im}\{\hat{\tilde{u}}(r\mathrm{e}^{\mathrm{i}\pi})\}\mathrm{d}r, \tag{3.7}$$

that requires $-\mathrm{Im}\{B(s)/[s(B(s)+\kappa^2]\}$ along the ray $s = r\mathrm{e}^{\mathrm{i}\pi}$ with $r > 0$ (the branch cut of the functions s^β and $s^{\beta-1}$). By writing

$$B(r\mathrm{e}^{\mathrm{i}\pi}) = \rho\cos(\pi\gamma) + \mathrm{i}\rho\sin(\pi\gamma), \quad \begin{cases} \rho = \rho(r) = |B|(r\mathrm{e}^{\mathrm{i}\pi})|, \\ \gamma = \gamma(r) = \frac{1}{\pi}\arg[B(r\mathrm{e}^{\mathrm{i}\pi})], \end{cases} \tag{3.8}$$

we get after simple calculations

$$\hat{u}(\kappa, t) = \int_0^\infty \frac{\mathrm{e}^{-rt}}{r}K(\kappa, r)\mathrm{d}r, \tag{3.9}$$

where

$$K(\kappa, r) = \frac{1}{\pi}\frac{\kappa^2\rho\sin(\pi\gamma)}{\kappa^4 + 2\kappa^2\rho\cos(\pi\gamma) + \rho^2}. \tag{3.10}$$

Since $u(x,t)$ is symmetric in x, Fourier inversion yields

$$u(x,t) = \frac{1}{\pi}\int_0^{+\infty}\cos(\kappa x)\left\{\int_0^\infty \frac{\mathrm{e}^{-rt}}{r}K(\kappa, r)\mathrm{d}r\right\}\mathrm{d}\kappa. \tag{3.11}$$

To calculate this Fourier integral we use the Mellin transform. Let

$$\mathscr{M}\{f(\xi); s\} = f^*(s) = \int_0^{+\infty} f(\xi)\xi^{s-1}\mathrm{d}\xi, \quad \gamma_1 < \Re(s) < \gamma_2, \tag{3.12}$$

be the Mellin transform of a sufficiently well-behaved function $f(\xi)$, and let

$$\mathscr{M}^{-1}\{f^*(s); \xi\} = f(\xi) = \frac{1}{2\pi\mathrm{i}}\int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} f^*(s)\xi^{-s}\mathrm{d}s, \tag{3.13}$$

be the inverse Mellin transform, where $\xi > 0$, $\gamma = \Re(s)$, $\gamma_1 < \gamma < \gamma_2$. Denoting by $\overset{\mathscr{M}}{\leftrightarrow}$ the juxtaposition of a function $f(\xi)$ with its Mellin transform $f^*(s)$, the Mellin convolution theorem implies

$$h(\xi) = f(\xi) \otimes g(\xi) := \int_0^\infty \frac{1}{\eta}f(\eta)g(\xi/\eta)\mathrm{d}\eta \overset{\mathscr{M}}{\leftrightarrow} h^*(s) = f^*(s)g^*(s). \tag{3.14}$$

Then, following [24, pp. 160–161], we identify the Fourier integral in (3.11) as a Mellin convolution in κ, that is $u(x,t) = f(\kappa, t) \otimes g(\kappa, x)$, if we set (see (3.14) with $\xi = 1/x$, $\eta = \kappa$)

$$f(\kappa, t) := \int_0^\infty \frac{\mathrm{e}^{-rt}}{r}K(\kappa, r)\mathrm{d}r \overset{\mathscr{M}}{\leftrightarrow} f^*(s, t), \tag{3.15}$$

$$g(\kappa, x) := \frac{1}{\pi x\kappa}\cos\left(\frac{1}{\kappa}\right) \overset{\mathscr{M}}{\leftrightarrow} \frac{\Gamma(1-s)}{\pi x}\sin\left(\frac{\pi s}{2}\right) := g^*(s, x), \tag{3.16}$$

with $0 < \Re(s) < 1$. The next step thus consists in computing the Mellin transform $f^*(s,t)$ of the function $f(\kappa,t)$ and then inverting the product $f^*(s,t)g^*(s,x)$ using (3.16) in the Mellin inversion formula, namely

$$u(x,t) = \frac{1}{\pi x}\frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} f^*(s,t)\Gamma(1-s)\sin(\pi s/2)x^s\mathrm{d}s$$
$$= \frac{1}{x}\frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} f^*(s,t)\frac{\Gamma(1-s)}{\Gamma(s/2)\Gamma(1-s/2)}x^s\mathrm{d}s. \tag{3.17}$$

The required Mellin transform $f^*(s,t)$ is

$$f^*(s,t) = \int_0^\infty \frac{\mathrm{e}^{-rt}}{r}\left\{\frac{1}{\pi}\int_0^\infty \frac{\kappa^2\rho\sin(\pi\gamma)}{\kappa^4+2\rho\cos(\pi\gamma)\kappa^2+\rho^2}\kappa^{s-1}\mathrm{d}\kappa\right\}\mathrm{d}r. \tag{3.18}$$

By the variable change $\kappa^2 \to \rho\mu$ the term in braces becomes

$$\frac{\rho^{s/2+1}}{2\rho}\frac{1}{\pi}\int_0^\infty \frac{\sin(\pi\gamma)}{\mu^2+2\mu\cos(\pi\gamma)+1}\mu^{(s/2+1)-1}\mathrm{d}\mu = -\frac{\rho^{s/2}}{2}\left\{\frac{\Gamma(s/2+1)\Gamma[1-(s/2+1)]}{\Gamma(\gamma s/2)\Gamma(1-\gamma s/2)}\right\}, \tag{3.19}$$

where we use a formula from the Handbook by Marichev, see [27, p. 156, Eq. 15 (1)], under the condition $0 < \Re(s/2+1) < 2$, $|\gamma| < 1$. As a consequence of (3.18) and (3.19) we get

$$f^*(s,t) = -\int_0^\infty \frac{\mathrm{e}^{-rt}}{r}\frac{\rho^{s/2}}{2}\left\{\frac{\Gamma(s/2+1)\Gamma[1-(s/2+1)]}{\Gamma(\gamma s/2)\Gamma(1-\gamma s/2)}\right\}\mathrm{d}r. \tag{3.20}$$

Now, using Eqs. (3.17) and (3.20) we can finally write the solution as

$$u(x,t) = \frac{1}{2\pi x}\int_0^\infty \frac{\mathrm{e}^{-rt}}{r}F(\rho^{1/2}x)\mathrm{d}r, \tag{3.21}$$

where $F(\rho^{1/2}x)$ is expressed in terms of Mellin–Barnes integrals:

$$F(\rho^{1/2}x) = \frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty}\frac{\pi\Gamma(1-s)}{\Gamma(\gamma s/2)\Gamma(1-\gamma s/2)}(\rho^{1/2}x)^s\mathrm{d}s = \frac{1}{2\pi\mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty}\Gamma(1-s)\sin(\pi\gamma s/2)(\rho^{1/2}x)^s\mathrm{d}s, \tag{3.22}$$

with $\rho = \rho(r)$, $\gamma = \gamma(r)$. We remind that $\rho(r)$ and $\gamma(r)$ are related to the order-density $b(\beta)$ according to Eqs. (3.3) and (3.8). By evaluating the Mellin–Barnes integrals via the residue theorem we arrive at the series representations in powers of $(\rho^{1/2}x)$,

$$F(\rho^{1/2}x) = \pi\rho^{1/2}x\sum_{k=0}^\infty \frac{(-\rho^{1/2}x)^k}{k!\Gamma(\gamma k/2+\gamma/2)\Gamma(-\gamma k/2+1-\gamma/2)}$$
$$= \rho^{1/2}x\sum_{k=0}^\infty \frac{(-\rho^{1/2}x)^k}{k!}\sin(\pi\gamma(k+1)/2). \tag{3.23}$$

This function can be interpreted again in terms of generalized Wright or H-Fox functions, as outlined in [26]. From Eqs. (3.21) and (3.23), interchanging integration and summation, we get the series representation of the fundamental solution:

$$u(x,t) = \frac{1}{2\pi}\sum_{k=0}^\infty \frac{(-x)^k}{k!}\varphi_k(t), \tag{3.24}$$

where, with $\rho = \rho(r)$, $\gamma = \gamma(r)$,

$$\varphi_k(t) = \int_0^\infty \frac{\mathrm{e}^{-rt}}{r}\sin[\pi\gamma(k+1)/2]\rho^{(k+1)/2}\mathrm{d}r. \tag{3.25}$$

In order to check the consistency of this general analysis we find it instructive to derive from Eqs. (3.24) and (3.25) the results of Section 2 concerning the fractional subdiffusion of a single order. We denote this (fixed) order by ν in distinction from the variable β in the distributed order case. This means to consider in Eq. (3.1) the particular case

$$b(\beta) = \delta(\beta - \nu), \quad 0 < \nu < 1, \tag{3.26}$$

so that $B(s) = s^{\nu}$ and Eq. (3.8) yields

$$\rho = \rho(r) = r^{\nu}, \quad \gamma = \text{constant} = \nu. \tag{3.27}$$

In the series representation of the fundamental solution (3.24) and (3.25) the functions $\varphi_k(t)$ now turn out as

$$\varphi_k(t) = \sin[\pi\nu(k+1)/2] \int_0^{\infty} \frac{\mathrm{e}^{-rt}}{r} r^{\nu(k+1)/2} \mathrm{d}r = \sin[\pi\nu(k+1)/2] \frac{\Gamma[\nu(k+1)/2]}{t^{\nu(k+1)/2}}. \tag{3.28}$$

As a consequence, the solution reads

$$u(x,t) = \frac{1}{2} t^{-\nu/2} \cdot \frac{1}{\pi} \sum_{k=0}^{\infty} \frac{(-x/t^{\nu/2})^k}{k!} \Gamma[\nu(k+1)/2] \sin[\pi\nu(k+1)/2] = \frac{1}{2} t^{-\nu/2} M_{\frac{\nu}{2}}\left(\frac{x}{t^{\nu/2}}\right), \tag{3.29}$$

in agreement with Eqs. (2.13) and (2.14). Of course, only in this special case it is possible to single out a common time factor ($t^{-\nu/2}$) from all the functions $\varphi_k(t)$ and get a self-similar solution. In general the set of functions $\varphi_k(t)$ gives rise to a distribution of different time scales related to the order density $b(\beta)$.

4. Conclusions

After outlining the basic theory of the Cauchy problem for the spatially one-dimensional and symmetric time fractional diffusion equation (with its main equivalent formulations), we have paid special attention to transform methods for finding its fundamental solution or (exploiting self-similarity) the corresponding reduced Green function. We have stressed the importance of the transforms of Fourier, Laplace and Mellin and of the functions of Mittag–Leffler and Wright type, avoiding however the cumbersome H-Fox function notations.

A natural first step for construction of the fundamental solution consists in applying in either succession the transforms of Fourier in space and Laplace in time to the Cauchy problem. This yields in the Fourier-Laplace domain the solution in explicit form, but for the space-time domain we must invert both transforms in sequence for which there are two choices, both leading to the same power series in the spatial variable with time-dependent coefficients. The strategy, called by us the "second", of first doing Laplace inversion and then the Fourier inversion yields the reduced Green function as a Mellin–Barnes integral form which, by the calculus of residues, the power series is obtained. This strategy can be adapted to the treatment of the more general case of the distributed order time fractional diffusion equation. Now the fundamental solution can be expressed as an integral over a Mellin–Barnes integral containing two parameters having the form of functionals of the order-density. Finally, again for the fundamental solution a power series comes out whose coefficients, however, are time-dependent functionals of the order-density. But, if there is more than one time derivative-order present, self-similarity is lost.

Appendix. The two fractional derivatives

For a sufficiently well-behaved function $f(t)$ ($t \in \mathbf{R}^+$) we may define the fractional derivative of order β ($m-1 < \beta \leqslant m, m \in \mathbf{N}$), see e.g. [14,32] in two different senses, that we refer here as to *Riemann–Liouville* derivative and *Caputo* derivative, respectively. Both derivatives are related to the so-called Riemann–Liouville fractional integral of order $\alpha > 0$, see [34,38], defined as

$$_tJ^{\alpha} f(t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) \mathrm{d}\tau, \quad \alpha > 0. \tag{A.1}$$

We note the convention ${}_tJ^0 = I$ (Identity) and the semigroup property

$$ {}_tJ^{\alpha}{}_tJ^{\beta} = {}_tJ^{\beta}{}_tJ^{\alpha} = {}_tJ^{\alpha+\beta}, \quad \alpha \geqslant 0,\ \beta \geqslant 0. \tag{A.2}$$

The fractional derivative of order $\beta > 0$ in the *Riemann–Liouville* sense is defined as the operator ${}_tD^{\beta}$ which is the left inverse of the Riemann–Liouville integral of order β (in analogy with the ordinary derivative), that is

$$ {}_tD^{\beta}{}_tJ^{\beta} = I, \quad \beta > 0. \tag{A.3}$$

If m denotes the positive integer such that $m-1 < \beta \leqslant m$, we recognize from Eqs. (A.2) and (A.3) ${}_tD^{\beta}f(t) := {}_tD^m{}_tJ^{m-\beta}f(t)$, hence

$$ {}_tD^{\beta}f(t) = \begin{cases} \dfrac{\mathrm{d}^m}{\mathrm{d}t^m}\left[\dfrac{1}{\Gamma(m-\beta)}\displaystyle\int_0^t \dfrac{f(\tau)\mathrm{d}\tau}{(t-\tau)^{\beta+1-m}}\right], & m-1 < \beta < m, \\ \dfrac{\mathrm{d}^m}{\mathrm{d}t^m}f(t), & \beta = m. \end{cases} \tag{A.4}$$

For completion we define ${}_tD^0 = I$. On the other hand, the fractional derivative of order $\beta > 0$ in the *Caputo* sense is defined as the operator ${}_tD_*^{\beta}$ such that ${}_tD_*^{\beta}f(t) := {}_tJ^{m-\beta}{}_tD^mf(t)$, hence

$$ {}_tD_*^{\beta}f(t) = \begin{cases} \dfrac{1}{\Gamma(m-\beta)}\displaystyle\int_0^t \dfrac{f^{(m)}(\tau)\mathrm{d}\tau}{(t-\tau)^{\beta+1-m}}, & m-1 < \beta < m, \\ \dfrac{\mathrm{d}^m}{\mathrm{d}t^m}f(t), & \beta = m. \end{cases} \tag{A.5}$$

We point out the major utility of the Caputo fractional derivative in treating initial-value problems for physical and engineering applications where initial conditions are usually expressed in terms of integer-order derivatives. This can be easily seen using the Laplace transformation, according to which

$$ \mathscr{L}\{{}_tD_*^{\beta}f(t);s\} = s^{\beta}\tilde{f}(s) - \sum_{k=0}^{m-1} s^{\beta-1-k}f^{(k)}(0^+), \quad m-1 < \beta \leqslant m, \tag{A.6}$$

where $\tilde{f}(s) = \mathscr{L}\{f(t);s\} = \int_0^{\infty} \mathrm{e}^{-st}f(t)\mathrm{d}t$, $s \in \mathbf{C}$ and $f^{(k)}(0^+) := \lim_{t\to 0^+} f^{(k)}(t)$.

The corresponding rule for the Riemann–Liouville derivative is more cumbersome: for $m-1 < \beta \leqslant m$ it reads

$$ \mathscr{L}\{{}_tD^{\beta}f(t);s = s^{\beta}\tilde{f}(s) - \sum_{k=0}^{m-1}[{}_tD_t^kJ^{(m-\beta)}]f(0^+)s^{m-1-k}, \tag{A.7}$$

where, in analogy with (A.6), the limit for $t \to 0^+$ is understood to be taken after the operations of fractional integration and derivation. As soon as all the limiting values $f^{(k)}(0^+)$ are finite and $m-1 < \beta < m$, the formula (A.7) simplifies into

$$ \mathscr{L}\{{}_tD^{\beta}f(t);s\} = s^{\beta}\tilde{f}(s). \tag{A.8}$$

In the special case $f^{(k)}(0^+) = 0$ for $k = 0, 1, m-1$, we recover the identity between the two fractional derivatives. The Laplace transform rule (A.6) was practically the starting point of Caputo [2,3] in defining his generalized derivative in the late sixties. For further reading on the theory and applications of fractional calculus we recommend the recent treatise by Kilbas, Srivastava & Trujillo [18].

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