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Convergence of the Grünwald–Letnikov scheme for time-fractional diffusion

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Abstract

Using bivariate generating functions, we prove convergence of the Grünwald–Letnikov difference scheme for the fractional diffusion equation (in one space dimension) with and without central linear drift in the Fourier–Laplace domain as the space and time steps tend to zero in a well-scaled way. This implies convergence in distribution (weak convergence) of the discrete solution towards the probability of sojourn of a diffusing particle. The difference schemes allow also interpretation as discrete random walks. For fractional diffusion with central linear drift we show that in the Fourier–Laplace domain the limiting ordinary differential equation coincides with that for the solution of the corresponding diffusion equation.

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1. Introduction

During the last 20 years many numerical methods have been developed using discrete approximations to fractional differential equations. There exists already a rich literature on the subject that we cannot survey here giving full justice to each contribution. But let us mention the pioneering paper by Lubich [19], also [7] and the references therein. As a newer reference let us quote [4]. Fractional diffusion processes have found growing interest among scientists and have been applied to many different topics, e.g., in physics and chemistry, see [24] and for a grand survey about these applications and the collection of articles [17]. For them there are (besides many papers on continuous time random walks) already available many publications on approximations by difference schemes. Without going into details let us quote only the papers [12,18,20,22,23,30]. In some of these papers the essential role is played by the Grünwald–Letnikov approximation of fractional derivatives.

Being interested in the Grünwald–Letnikov discretization of the space–time-fractional diffusion equation we prove its convergence in the Fourier–Laplace domain to the solution of the differential equation. In doing this we generalize

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the method used in [11] for the Markovian case $\beta = 1$. We begin with the space–time-fractional diffusion equation, namely the Cauchy problem

$$\underset{t\ *}{D}^{\beta} u(x,t) = \underset{x\ 0}{D}^{\alpha} u(x,t), \quad u(x,0) = \delta(x), \quad 0 < \beta \leqslant 1, \quad 0 < \alpha \leqslant 2, \tag{1.1}$$

for $x \in \mathbb{R}$, $t \geqslant 0$. Here $\underset{x\ 0}{D}^{\alpha}$ denotes the linear pseudo-differential operator with symbol $-|\kappa|^{\alpha}$, the *Riesz* space-fractional derivative operator. Its Fourier representation for a sufficiently smooth function $f(x)$, $x \in \mathbb{R}$, has the form

$$\mathscr{F}\{\underset{x\ 0}{D}^{\alpha} f(x); \kappa\} = \widehat{f}(\kappa) = -|\kappa|^{\alpha} \widehat{f}(\kappa), \quad \kappa \in \mathbb{R}, \tag{1.2}$$

with the Fourier transform of a (generalized) function $f(x)$ defined as

$$\mathscr{F}\{f(x); \kappa\} = \widehat{f}(\kappa) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\kappa x} f(x)\,\mathrm{d}x, \quad \kappa \in \mathbb{R}. \tag{1.3}$$

The operator $\underset{t\ *}{D}^{\beta}$ denotes the Caputo time-fractional derivative operator, see [10,26] for more information. For our purpose we use the definition

$$\underset{t\ *}{D}^{\beta} f(t) = \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{f'(\tau)}{(t-\tau)^{\beta}}\,\mathrm{d}\tau \ \text{ for } 0 < \beta < 1, \quad f'(t) = \frac{\mathrm{d}f(t)}{\mathrm{d}t} \ \text{ for } \beta = 1. \tag{1.4}$$

This fractional derivative has the Laplace image

$$\mathscr{L}\{\underset{t\ *}{D}^{\beta} f(t); s\} = s^{\beta} \widetilde{f}(s) - s^{\beta-1} f(0), \quad 0 < \beta \leqslant 1, \quad s > 0,$$

with the Laplace transform of a (generalized) function $g(t)$ defined as

$$\mathscr{L}\{g(t); s\} = \widetilde{g}(s) = \int_0^{\infty} \mathrm{e}^{-st} g(t)\,\mathrm{d}t. \tag{1.5}$$

For the proof of convergence we distinguish several cases:

(a) $\alpha = 2$, $\beta = 1$: classical diffusion, which is Markovian,
(b) $\alpha = 2$, $0 < \beta < 1$: time-fractional diffusion,
(c) $0 < \alpha < 2$, $\beta = 1$: space-fractional diffusion, which is Markovian,
(d) $0 < \alpha < 2$, $\alpha \neq 1$, $0 < \beta < 1$: space–time-fractional diffusion,
(e) $\alpha = 1$, $0 < \beta < 1$: a singular case of space–time-fractional diffusion.

Case (a) is formally contained in case (b). By extending all formulas to $\beta = 1$, the proof remains valid. The convergence in case (a) is well-known from classical random walk theory and from numerical analysis. Case (c) has been treated by Gorenflo and Mainardi, see [11]. We treat here case (b), because the proofs for (d) and (e) can easily be carried out by modifying those for (b) and (c).

For the time-fractional diffusion equation with central linear drift, we have the Cauchy problem for $x \in \mathbb{R}$, $t \geqslant 0$, $0 < \beta \leqslant 1$:

$$\underset{t\ *}{D}^{\beta} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) + \frac{\partial}{\partial x}(x u(x,t)), \quad u(x,0) = \delta(x - x^*), \tag{1.6}$$

with $x^* \in \mathbb{R}$ as the initial position of the particle. Avoiding confusion with the grid point $x_0 = 0h$, we denote the initial position by x^*. Eq. (1.6) is a time-fractional continuous version of the Ehrenfest model describing diffusion in a potential well, see [1] for more information and [3] for other effects of non-linear oscillators driven by Lévy noise. We distinguish the two cases:

(f) $\beta = 1$: classical diffusion with central linear drift (the continuous version of the Ehrenfest model),
(g) $0 < \beta < 1$: time-fractional diffusion with central linear drift.

Case (f) is formally contained in case (g), but we treat it separately because its transition probabilities are much simpler than those of case (g). For all these cases, we show that by properly scaled transition to the limit of vanishing step sizes, in space and time, there is convergence in the Fourier–Laplace domain, implying convergence in distribution (weak convergence) of the corresponding probability densities for the location of the particle.

This paper is organized as follows: in Section 2, the discretization of case (b) will be discussed. We outline the theory of convergence to the corresponding fundamental solution in Section 3. In Section 4, the convergence of case (f) is treated. In Section 5, we prove the convergence of case (g). Finally, in Section 6, we state our Conclusions. Our proofs by help of bivariate generating functions amount to show convergence in the Fourier–Laplace domain and to use the continuity theorems of probability theory to obtain weak convergence (convergence in distribution) in the physical domain.

2. Discretization of the time-fractional diffusion equation and general conditions

We discuss here case (b) of Section 1,

$$\underset{t\,*}{D}^{\beta} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), \quad u(x,0) = \delta(x), \quad 0 < \beta \leqslant 1, \tag{2.1}$$

in the Fourier–Laplace domain $s^{\beta}\widehat{\widetilde{u}}(\kappa, s) - s^{\beta-1} = -\kappa^2 \widehat{\widetilde{u}}(\kappa, s)$, implying

$$\widehat{\widetilde{u}}(\kappa, s) = \frac{s^{\beta-1}}{s^{\beta} + \kappa^2}, \quad s > 0, \quad \kappa \in \mathbb{R}. \tag{2.2}$$

Inverting the Laplace transform of (2.2) gives $\widehat{u}(\kappa, t) = E_{\beta}(-|\kappa|^2 t^{\beta})$, with the Mittag-Leffler function

$$E_{\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+k\beta)}, \quad \beta \in \mathbb{R}, \quad z \in \mathbb{C} \tag{2.3}$$

introduced in [25]. It arises naturally in the solution of many fractional differential equations, see [10,21]. Actually it appears as the solution of the Abel integral equation of the second type, see e.g., [5,14,29]. For applications in anomalous diffusion, see e.g., [2,16,28].

The solution $u(x,t)$ of Eq. (2.1) with the initial condition $u(x,0) = \delta(x)$ is known as the *Green function* or *fundamental solution* or *propagator* and can be interpreted as a probability density. We have the conservation property

$$u(x,t) \geqslant 0, \quad \int_{-\infty}^{\infty} u(x,t)\, \mathrm{d}x = 1 \quad \forall t \geqslant 0.$$

Now, to generate a discrete approximate solution to Eq. (2.1), we discretize the space variable x by grid points $x_j = jh$, with $h > 0$, $j \in \mathbb{Z}$, the time variable t by grid points $t_n = n\tau$, with $\tau > 0$, $n \in \mathbb{N}_0$. The dependent variable is then discretized by introducing $y_j(t_n)$ intended as approximations:

$$y_j(t_n) \approx \int_{x_j - h/2}^{x_j + h/2} u(x, t_n)\, \mathrm{d}x \approx h u(x_j, t_n). \tag{2.4}$$

The $y_j(t_n)$ can be visualized as clumps of probability of sojourn in points x_j, collected from intervals of length h at time t_n.

The discretization of the time-fractional diffusion equation (2.1) is based first on the backward Grünwald–Letnikov scheme in time. The discretization of the fractional derivative operators (in space or in time), has been widely used. Gorenflo and Vivoli [15] used it for constructing fully discrete random walk models for the space–time-fractional diffusion equation. See [11] for the special case $\beta = 1$. Recently Meerschaert et al. have published a series of papers in which they used the Grünwald–Letnikov difference scheme in approximating the fractional diffusion equation, see e.g., [22,23].

For discretizing the Caputo time-fractional derivative operator ${}_{t}D_{*}^{\beta}$ starting at level $t = t_{n+1}$, see [7,26,27], we use the formula

$$ {}_{\tau}D_{*}^{\beta} y_j(t_{n+1}) = \sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} \frac{y_j(t_{n+1-k}) - y_j(t_0)}{\tau^\beta}, \quad 0<\beta\leqslant 1 \ \ \forall n \in \mathbb{N}_0, \tag{2.5}$$

observing that ${}_{\tau}D_{*}^{1} y_j(t_{n+1}) = (1/\tau)(y_j(t_{n+1}) - y_j(t_n))$. Approximating the operator $\partial^2/\partial x^2$, symmetrically we get the discretization of Eq. (2.1) $\forall n \in \mathbb{N}_0,\ \ \forall j \in \mathbb{Z}$ as

$$\sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} (y_j(t_{n+1-k}) - y_j(t_0)) = \mu y_{j+1}(t_n) - 2\mu y_j(t_n) + \mu y_{j-1}(t_n), \tag{2.6}$$

with the scaling parameter $\mu = \tau^\beta/h^2$. Solving for $y_j(t_{n+1})$, we obtain

$$\begin{aligned} y_j(t_{n+1}) = &\sum_{k=0}^{n} (-1)^k \binom{\beta}{k} y_j(t_0) + \sum_{k=1}^{n} (-1)^{k+1} \binom{\beta}{k} y_j(t_{n+1-k}) \\ &+ \mu y_{j+1}(t_n) - 2\mu y_j(t_n) + \mu y_{j-1}(t_n), \quad y_j(0) = \delta_{j,0}. \end{aligned} \tag{2.7}$$

Here and later we denote by $\delta_{j,m}$ the usual Kronecker symbol. $y_j(t_{n+1})$ represents the probability for where to find the particle at time t_{n+1}. It depends on $y_{j-1}(t_n),\ y_j(t_n),\ y_{j+1}(t_n),\ y_j(t_{n-1}),\ \ldots,\ y_j(t_1),\ y_j(t_0)$. So this equation represents a discrete process with memory. According to Eq. (2.4), we introduce a vector

$$y(t_n) = \{\ldots, y_{-1}(t_n), y_0(t_n), y_1(t_n), \ldots\} \quad \forall n \in \mathbb{N}_0.$$

For the interpretation of $y(t_n)$ as a vector of probabilities we need the condition of preservation of non-negativity which requires that $y_j(t_{n+1})$ is a linear combination of all $y_j(t_k)$, $k\leqslant n$ with non-negative coefficients. To achieve this we impose the condition

$$0 < \mu = \tau^\beta/h^2 \leqslant \beta/2. \tag{2.8}$$

For proving the conservation property, we suitably use in Eq. (2.7) the initial value $y_j(t_0) = y_j(0) = \delta_{j,0}$ corresponding to $u(x,0) = \delta(x)$ and implying $\sum_{j\in\mathbb{Z}} y_j(t_0) = 1$. To imitate the conservation property we want $\sum_{j\in\mathbb{Z}} y_j(t_n) = 1\ \forall n \in \mathbb{N}_0$. Gorenflo et al. [12] have proved this discrete conservation property by induction and interpreted Eq. (2.6) as a *random walk* on the spatial grid in discrete time. See also [12,13]. This random walk stands in conceptual contrast to the method of approximating time-fractional diffusion by continuous time random walks, see e.g., [2] that, however, can also be given a discrete version (see [15]).

Remark. In order to obtain in Eq. (2.7) an explicit scheme we have in Eq. (2.6) discretized the spatial part of the operator at the old time t_n.

3. Proof of convergence

For dealing with the system (2.6) of difference equations we apply the method of generating functions. For $n \in \mathbb{N}_0$, we define

$$q_n(z) = \sum_{j\in\mathbb{Z}} y_j(t_n) z^j, \tag{3.1}$$

for the two-sided sequence of the sojourn probabilities

$$\{\ldots, y_{-2}(t_n), y_{-1}(t_n), y_0(t_n), y_1(t_n), y_2(t_n), \ldots\} \quad \forall n \in \mathbb{N}_0. \tag{3.2}$$

We note that this sequence satisfies the conservation property and the non-negativity preservation because all $y_j(t_n) \geqslant 0$ and $\sum_{j=-\infty}^{\infty} y_j(t_n) = 1$. Therefore, the series (3.1) converges absolutely on the circle $|z| = 1$. From now on we assume

$|z|=1$. Introducing the generalized function $\sum_{j\in\mathbb{Z}}\delta(x-x_j)y_j(t_n)$, $\forall n\in\mathbb{N}_0$ and applying the Fourier transform, we obtain

$$\mathscr{F}\left\{\sum_{j\in\mathbb{Z}}\delta(x-x_j)y_j(t_n);\kappa\right\}=\sum_{j\in\mathbb{Z}}\mathrm{e}^{\mathrm{i}\kappa x_j}y_j(t_n)=q_n(\mathrm{e}^{\mathrm{i}\kappa h}),\quad \kappa\in\mathbb{R}. \tag{3.3}$$

By comparing Eqs. (3.1) and (3.3), we see that the Fourier-transform of the sequence (3.2) coincides with the generating function $q_n(z)$, if we replace z by $\mathrm{e}^{\mathrm{i}\kappa h}$. In other words, the Fourier transform of the sequence of clumps $y_j(t_n)$, $j\in\mathbb{Z}$, is represented by $q_n(\mathrm{e}^{\mathrm{i}\kappa h})$.

Now let us introduce the *bivariate* (two-fold) generating function

$$Q(z,\zeta)=\sum_{n=0}^{\infty}q_n(z)\zeta^n=\sum_{n=0}^{\infty}\left(\sum_{j\in\mathbb{Z}}y_j(t_n)z^j\right)\zeta^n, \tag{3.4}$$

as a function of ζ for the sequence

$$\{q_0(z),q_1(z),q_2(z),\ldots\}. \tag{3.5}$$

Because all $|q_n(z)|\leqslant 1$, the sequence $Q(z,\zeta)$ converges for $|\zeta|<1$, and from now on we assume $|\zeta|<1$. By introducing the generalized function $\sum_{n=0}^{\infty}\delta(t-t_n)q_n(z)$ and applying the Laplace transform, we get

$$\mathscr{L}\left\{\sum_{n=0}^{\infty}\delta(t-t_n)q_n(z);s\right\}=\sum_{n=0}^{\infty}\mathrm{e}^{-st_n}q_n(z),\quad s>0. \tag{3.6}$$

From Eqs. (3.3) and (3.6), we deduce that with $z=\mathrm{e}^{\mathrm{i}\kappa h}$ and $\zeta=\mathrm{e}^{-s\tau}$ we get the Fourier–Laplace transform of the bivariate sequence $\{y_j(t_n)|j\in\mathbb{Z},n\in\mathbb{N}_0\}$. This means

$$Q(\mathrm{e}^{\mathrm{i}\kappa h},\mathrm{e}^{-s\tau})=\sum_{n=0}^{\infty}\left(\sum_{j\in\mathbb{Z}}y_j(t_n)\mathrm{e}^{\mathrm{i}\kappa jh}\right)\mathrm{e}^{-ns\tau},\quad \kappa\in\mathbb{R},\quad s>0. \tag{3.7}$$

Our aim now is to prove that $Q(\mathrm{e}^{\mathrm{i}\kappa h},\mathrm{e}^{-s\tau})$ is related asymptotically to the Fourier–Laplace transform of $u(x,t)$ which represents the fundamental solution of the time-fractional diffusion equation (2.1). By considering (2.4), we find that the discretization of the Fourier-transform of $u(x,t)$ formally gives the approximation

$$\widehat{u}(\kappa,t_n)\approx q_n(\mathrm{e}^{\mathrm{i}\kappa h}),\quad \kappa\in\mathbb{R}.$$

By taking its Laplace transform and imitating a rectangle rule for numerical integration, we get the formal approximation

$$\widehat{\widetilde{u}}(\kappa,s)\approx\tau Q(\mathrm{e}^{\mathrm{i}\kappa h},\mathrm{e}^{-s\tau}),\quad s>0. \tag{3.8}$$

To find the explicit form of $\tau Q(\mathrm{e}^{\mathrm{i}\kappa h},\mathrm{e}^{-s\tau})$, we fix $\kappa\in\mathbb{R}$ and $s>0$, use the condition (2.8), and intend to show that

$$\lim_{h,\tau\to 0}\tau Q(\mathrm{e}^{\mathrm{i}\kappa h},\mathrm{e}^{-s\tau})=\widehat{\widetilde{u}}(\kappa,s),$$

namely that the Fourier–Laplace transform of the discrete solution approximates the Fourier–Laplace transform of the corresponding fundamental solution. To this aim, we construct $Q(z,\zeta)$ with the initial condition $q_0(z)=\widehat{\delta}(\kappa)\equiv 1$. Multiplying Eq. (2.6) by z^j and summing over all j, we get

$$\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(q_{n+1-k}(z)-1)=\mu(z^{-1}-2+z)q_n(z),\quad \sum_{j\in\mathbb{Z}}y_j(0)z^j=1. \tag{3.9}$$

Multiplying Eq. (3.9) by ζ^n and summing over $n\in\mathbb{N}_0$ we get

$$\sum_{n=0}^{\infty}\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(q_{n+1-k}(z)-1)\zeta^n=\mu(z^{-1}-2+z)\sum_{n=0}^{\infty}q_n(z)\zeta^n. \tag{3.10}$$

Using the definition (3.4), setting $m = n + 1$, and summing the RHS of Eq. (3.10) over $m \in \mathbb{N}$, we obtain

$$\sum_{m=1}^{\infty} \sum_{k=0}^{m} (-1)^k \binom{\beta}{k} (q_{m-k}(z) - 1)\zeta^m = \mu(z^{-1} - 2 + z) Q(z, \zeta). \tag{3.11}$$

Since $q_0(z) \equiv 1$, we can begin the summation over m with $m = 0$.

To proceed further, we need the convolution of two general sequences which is equivalent to the multiplication of their generating functions (see [6]). If $\{\alpha_n\}$ and $\{\beta_k\}$ are two numerical sequences with absolutely convergent power series

$$\alpha(\zeta) = \sum_{n=0}^{\infty} \alpha_n \zeta^n, \quad \beta(\zeta) = \sum_{k=0}^{\infty} \beta_k \zeta^k,$$

then

$$\alpha(\zeta)\beta(\zeta) = c(\zeta) = \sum_{r=0}^{\infty} c_r \zeta^r, \quad c_r = \sum_{n=0}^{r} \alpha_n \beta_{r-n}.$$

This means that the LHS of Eq. (3.11) can be represented as a product of the two generating functions

$$\alpha(\zeta) = \sum_{k=0}^{\infty} (-1)^k \binom{\beta}{k} \zeta^k = (1 - \zeta)^\beta, \quad \beta(\zeta) = \sum_{m=0}^{\infty} (q_m(z) - 1)\zeta^m.$$

By a simple index shift equation (3.11) goes over in

$$\frac{(1-\zeta)^\beta}{\zeta} \left(Q(z, \zeta) - \frac{1}{1-\zeta} \right) = \mu(z^{-1} - 2 + z) Q(z, \zeta). \tag{3.12}$$

Solving for $Q(z, \zeta)$, we get

$$Q(z, \zeta) = \frac{(1-\zeta)^{\beta-1}}{(1-\zeta)^\beta - \zeta\mu(z^{-1} - 2 + z)}. \tag{3.13}$$

With $z = \mathrm{e}^{\mathrm{i}\kappa h}$, $\zeta = \mathrm{e}^{-s\tau}$, we get asymptotically for $h \to 0$, $\tau \to 0$

$$(z^{-1} - 2 + z) \sim -(\kappa h)^2, \quad (1-\zeta)^\beta \sim s^\beta \mu h. \tag{3.14}$$

Now multiplying by τ, using the scaling relation (2.8), and passing to the limit in Eq. (3.13), we find

$$\lim_{h \to 0, \tau \to 0} \tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau}) = \frac{s^{\beta-1}}{s^\beta + \kappa^2} = \widehat{\widetilde{u}}(\kappa, s). \tag{3.15}$$

Using the continuity theorems of probability theory (see [6]) we deduce from this equation with the scaling relation (2.8) that the solution of the difference scheme of the time-fractional diffusion equation converges in distribution to the corresponding fundamental solution. Let us remark that by applying the inverse Laplace transform to Eq. (3.15) we get $\widehat{u}(\kappa, t) = E_\beta(-\kappa^2 t^\beta)$. So the second moment of the density $u(x, t)$ is $(\sigma(t))^2 = -(\partial^2/\partial\kappa^2)\widehat{u}(\kappa, t)|_{\kappa=0} = 2t^\beta/\Gamma(1+\beta)$, see [8]. In the special case $\beta = 1$ we have $\widehat{u}(\kappa, t) = \mathrm{e}^{-\kappa^2 t}$ and consequently $(\sigma(t))^2 = 2t$. We summarize our results as

Theorem 1. *With the notations $x_j = jh$, $h > 0$, $t_n = n\tau$, $\tau > 0$, $j \in \mathbb{Z}$, $n \in \mathbb{N}_0$, the intended approximation* (2.4), *and under the restriction $2\tau^\beta \leqslant h^2$, the solution of the difference scheme* (2.7) *converges, for $h \to 0$, weakly* (*in distribution*) *to the time-dependent probability distribution whose density is $u(x, t)$, the solution of the Cauchy problem* (2.1).

4. Convergence for classical diffusion with central linear drift

We devote this section to case (f) of Section 1

$$\frac{\partial}{\partial t}u(x,t)=\frac{\partial^2}{\partial x^2}u(x,t)+\frac{\partial}{\partial x}(xu(x,t)),\quad u(x,0)=\delta(x-x^*), \tag{4.1}$$

with $x^*\in\mathbb{R}$. In the Fourier–Laplace domain this means

$$\kappa\frac{\partial}{\partial\kappa}\widehat{\widetilde{u}}(\kappa,s)+(\kappa^2+s)\widehat{\widetilde{u}}(\kappa,s)=\mathrm{e}^{\mathrm{i}\kappa x^*},\quad \widehat{\widetilde{u}}(0,s)=1/s. \tag{4.2}$$

The scaling relation (2.8), for $\beta=1$, takes the form

$$0<\mu=\tau/h^2\leqslant\tfrac{1}{2}. \tag{4.3}$$

Conveniently with the scaling relation (4.3), we discretize by central differences (4.1) as

$$\begin{aligned}y_j(t_{n+1})-y_j(t_n)&=\mu(y_{j+1}(t_n)-2y_j(t_n)+y_{j-1}(t_n))\\&\quad+\frac{\mu h^2}{2}\{(j+1)y_{j+1}(t_n)-(j-1)y_{j-1}(t_n)\},\quad y_j(0)=\delta_{j,x^*/h}.\end{aligned} \tag{4.4}$$

As we have discussed in [1,9], Eq. (4.1) describes the elastic diffusion of a bounded particle. Allowing only values h with $2/h^2=R\in\mathbb{N}$, restricting the index j to $\{-R,-R+1,\ldots,R-1,R\}$, we write (4.4) as

$$y_j(t_{n+1})=\gamma y_j(t_n)+\lambda_{j+1}y_{j+1}(t_n)+\rho_{j-1}y_{j-1}(t_n),\quad -R\leqslant j\leqslant R, \tag{4.5}$$

with

$$\rho_j=\mu\left(1-\frac{j}{R}\right),\quad \gamma=(1-2\mu),\quad \lambda_j=\mu\left(1+\frac{j}{R}\right). \tag{4.6}$$

These coefficients (as transition probabilities) satisfy the condition

$$\rho_j+\lambda_j+\gamma=1,\quad \rho_R=\lambda_{-R}=0\ \ \forall j\in[-R,R]. \tag{4.7}$$

We interpret $y_j(t_{n+1})$ in Eq. (4.5) as the probability of finding the diffusing particle at the point x_j, $j\in[-R,R]$, at the time instant t_{n+1}, $n\in\mathbb{N}_0$. In [1] the reader can find interpretation of our discretization as a particular form of the classical Ehrenfest urn model with specific meanings of N, R and μ. To get an initial condition for the probability vector

$$y(t_n)=\{y_{-R}(t_n),y_{-R+1}(t_n),\ldots,y_0(t_n),\ldots,y_{R-1}(t_n),y_R(t_n)\}\quad\forall n\in\mathbb{N}_0, \tag{4.8}$$

we set in the initial condition of Eq. (1.6) $x^*=mh$ with $m\in\{-R,-R+1,\ldots,R-1,R\}$ and correspondingly

$$y_j(t_0)=\delta_{j,m}. \tag{4.9}$$

We can use Eq. (4.7) and the condition (4.9) to show that

$$\sum_{j=-R}^{R}y_j(t_n)=\sum_{j=-R}^{R}y_j(t_0)=1, \tag{4.10}$$

where $y_j(t_n)\geqslant 0\ \forall j\in[-R,R]$. See [9] and the thesis [1], for the full proof of these non-negativity and conservation properties. We concentrate here on the proof of the convergence using our previous results as a tool. Since all $x_j\in\{-Rh,(-R+1)h,\ldots,0\ldots,(R-1)h,Rh\}$ and no jump goes outside of this set we can fix $y_j(t_n)=0$, $\forall|j|\geqslant R+1$, $n\in\mathbb{N}_0$. This guarantees us a finite Markov chain with the states $x_j=jh$, $j\in\{-R,-R+1,\ldots,R-1,R\}$. We can extend Eq. (4.10) to

$$\sum_{j\in\mathbb{Z}}y_j(t_n)=\sum_{j\in\mathbb{Z}}y_j(t_0)=1. \tag{4.11}$$

Hence we can use the generating function $q_n(z)$ defined in (3.1) for the infinitely extended sequence of sojourn probabilities

$$y(t_n) = \{\ldots, 0, y_{-R}(t_n), y_{-R+1}(t_n), \ldots, y_0(t_n), \ldots, y_{R-1}(t_n), y_R(t_n), 0, \ldots\}, \tag{4.12}$$

$\forall n \in \mathbb{N}_0$. Here the series $q_n(z)$ is convergent on $|z| = 1$. We use the definition (3.4) of the generating function $Q(z, \zeta)$ for the sequence (4.12), having convergence for $|\zeta| < 1$. Our aim is to prove that in the limit $h \to 0, \tau \to 0$, the sequence $\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})$ satisfies the ordinary differential equation (4.2). Multiplying Eq. (4.4) by z^j and summing over all j, we find

$$\begin{aligned} q_{n+1}(z) - q_n(z) = \mu q_n(z) &\left\{(z^{-1} - 2 + z) - \frac{y_{-R}}{z^{R+1}} - y_R z^{R+1}\right\} \\ &+ \frac{\mu h^2}{2}\left\{(z^{-1} - z)\sum_{j\in\mathbb{Z}} j y_j(t_n) z^j + \frac{R y_{-R}}{z^{R+1}} + R y_R z^{R+1}\right\}. \end{aligned} \tag{4.13}$$

With $R = 2/h^2$ and the identity

$$\sum_{j\in\mathbb{Z}} j y_j(t_n) z^j = z\frac{\mathrm{d}}{\mathrm{d}z}\sum_{j\in\mathbb{Z}} y_j(t_n) z^j, \tag{4.14}$$

we get

$$q_{n+1}(z) - q_n(z) = \mu q_n(z)(z^{-1} - 2 + z) + \frac{\mu h^2}{2}(z^{-1} - z) z \frac{\mathrm{d}}{\mathrm{d}z} q_n(z). \tag{4.15}$$

Now multiplying by ζ^n and summing over all $n \in \mathbb{N}$, we obtain

$$\frac{1}{\zeta}(Q(z,\zeta) - z^m) - Q(z,\zeta) = \mu Q(z,\zeta)(z^{-1} - 2 + z) + \frac{\mu h^2}{2}(1 - z^2)\frac{\mathrm{d}}{\mathrm{d}z} Q(z,\zeta). \tag{4.16}$$

Rearranging, we find

$$\frac{\mu h^2}{2}(1 - z^2)\frac{\mathrm{d}}{\mathrm{d}z} Q(z,\zeta) + \{\zeta\mu(z^{-1} - 2 + z) - (1 - \zeta)\} Q(z,\zeta) = -z^m. \tag{4.17}$$

For $h \to 0$, $\tau \to 0$, using Eq. (3.14) and multiplying by τ, we get

$$\kappa\frac{\mathrm{d}}{\mathrm{d}\kappa}(\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})) + (\kappa^2 + s)(\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})) = \mathrm{e}^{\mathrm{i}\kappa m h}. \tag{4.18}$$

So far, we have proved that $\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})$ under our scaling relation asymptotically solves the ordinary differential equation (4.2) which is exact for $\widehat{\widetilde{u}}(\kappa, s)$. Hence the discrete solution of the classical diffusion equation with central linear drift tends asymptotically for $h \to 0$, $\tau \to 0$, to the corresponding solution of Eq. (4.1) in the Fourier–Laplace domain in spite of vanishing outside of a finite interval (the exterior however being exhausted for h tending to zero).

Theorem 2. *With the notations as in Theorem* 1, *and under the condition* $2\tau \leqslant h^2$, *the solution of the difference scheme* (4.4) *provided with the initial condition* (4.9) *and intended as approximation* (2.4) *converges*, *for* $h \to 0$, *weakly* (*in distribution*) *to the time-dependent probability distribution whose density is* $u(x,t)$, *the solution of the Cauchy problem* (4.1).

5. Convergence for time-fractional diffusion with central linear drift

We consider now case (g) of Section 1. Again the particle is moving in the bounded interval $[-Rh, Rh]$ with $R = 2/h^2$ and again we have the scaling relation (2.8) but here we have $0 < \beta < 1$, and hence Eq. (1.6) in the Fourier–Laplace domain reads

$$\kappa\frac{\partial}{\partial\kappa}\widehat{\widetilde{u}}(\kappa, s) + (\kappa^2 + s^\beta)\widehat{\widetilde{u}}(\kappa, s) = \mathrm{e}^{\mathrm{i}\kappa x^*} s^{\beta-1}, \quad \widehat{\widetilde{u}}(0, s) = 1/s. \tag{5.1}$$

Its solution $\widehat{\widehat{u}}(\kappa, s)$ has the form of a complicated expression which we do not write down here. By using Eq. (2.5), we write the discretization of Eq. (1.6) as

$$\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(y_j(t_{n+1-k})-y_j(t_0))$$
$$=\mu(y_{j+1}(t_n)-2y_j(t_n)+y_{j-1}(t_n))+\frac{\mu h^2}{2}\{(j+1)y_{j+1}(t_n)-(j-1)y_{j-1}(t_n)\},\quad y_j(0)=\delta_{j,x^*/h}. \tag{5.2}$$

Solving for $y_j^{(n+1)}$, we get

$$y_j(t_{n+1})=\sum_{k=0}^{n}(-1)^k\binom{\beta}{k}y_j(t_0)+\sum_{k=1}^{n}(-1)^{k+1}\binom{\beta}{k}y_j(t_{n+1-k})$$
$$+y_{j+1}(t_n)\left[\mu+\frac{\mu h^2}{2}(j+1)\right]-2\mu y_j(t_n)+y_{j-1}(t_n)\left[\mu-\frac{\mu h^2}{2}(j-1)\right]. \tag{5.3}$$

Again $y_j(t_{n+1})$ is the probability for where to find the particle at time t_{n+1}.

Using the initial condition (4.9) and the scaling relation (2.8), we can prove the non-negativity and the conservation properties by induction, see [9] and the thesis [1] where we have also simulated the random walks for different values of β. To prove convergence we first note that at $n=0$, it is analogous to case (f) where $\beta=1$. Then at $n\geqslant 1$, we use the generating function $q_n(z)$ defined in Eq. (3.1) for the extended sequence of the sojourn probabilities (4.12), which is convergent on $|z|=1$. Again we use the bivariate generating function $Q(z,t)$ defined in Eq. (3.4) for the sequence (3.5), the series being convergent on $|\zeta|<1$.

Our aim now is to prove that $\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})$ satisfies asymptotically the ordinary differential equation (5.1). Multiplying Eq. (4.4) by z^j and summing over all j, we get

$$\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(q_{n+1-k}(z)-z^m)=\mu q_n(z)\left\{(z^{-1}-2+z)-\frac{y_{-R}}{z^{R+1}}-y_R z^{R+1}\right\}$$
$$+\frac{\mu h^2}{2}\left\{(z^{-1}-z)\sum_{j\in\mathbb{Z}} j y_j(t_n)z^j+\frac{Ry_{-R}}{z^{R+1}}+Ry_R z^{R+1}\right\}. \tag{5.4}$$

Again using the definition of R and the identity (4.14), we get

$$\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(q_{n+1-k}(z)-z^m)=\mu q_n(z)(z^{-1}-2+z)+\frac{\mu h^2}{2}(z^{-1}-z)z\frac{\mathrm{d}}{\mathrm{d}z}q_n(z), \tag{5.5}$$

and multiplying by ζ^n, summing over n and using (3.12),

$$\sum_{n=0}^{\infty}\sum_{k=0}^{n+1}(-1)^k\binom{\beta}{k}(q_{n+1-k}(z)-z^m)\zeta^n=\mu Q(z,\zeta)(z^{-1}-2+z)+\frac{\mu h^2}{2}(1-z^2)\frac{\mathrm{d}}{\mathrm{d}z}Q(z,\zeta). \tag{5.6}$$

In analogy to Eq. (3.12), we find

$$\frac{(1-\zeta)^\beta}{\zeta}\left(Q(z,\zeta)-\frac{z^m}{1-\zeta}\right)=\mu Q(z,\zeta)(z^{-1}-2+z)+\frac{\mu h^2}{2}(1-z^2)\frac{\mathrm{d}}{\mathrm{d}z}Q(z,\zeta). \tag{5.7}$$

A rearrangement gives

$$\frac{\zeta\mu h^2}{2}(1-z^2)\frac{\mathrm{d}}{\mathrm{d}z}Q(z,\zeta)+Q(z,\zeta)(\zeta\mu(z^{-1}-2+z)-(1-\zeta)^\beta)=-z^m(1-\zeta)^{\beta-1}. \tag{5.8}$$

With $h \to 0$, $\tau \to 0$, using the scaling relation (2.8) and Eq. (3.14), we get after multiplying by τ

$$\kappa \frac{\mathrm{d}}{\mathrm{d}\kappa}(\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})) + (\kappa^2 + s^\beta)(\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})) \sim s^{\beta-1}\,\mathrm{e}^{\mathrm{i}\kappa m h}, \quad \kappa > 0, \tag{5.9}$$

where $\tau Q(0, s) = 1/s$. So far, we have found that the asymptotic ordinary differential equation (5.9) with $x^* = mh$ is structured like the ordinary differential equation (5.1) and $\tau Q(\mathrm{e}^{\mathrm{i}\kappa h}, \mathrm{e}^{-s\tau})$ represents an approximation to $\widehat{\widetilde{u}}(\kappa, s)$.

We can interpret this result in the following words: the Fourier–Laplace transform of the discrete solution of Eq. (1.6) satisfies the ordinary differential equation (5.1) asymptotically as $h \to 0$ and $\tau \to 0$. The results of this section are confirmed by the numerical results discussed in our previous papers, see [1,9]. Summarizing, we have

Theorem 3. *With the notations as in Theorem* 1, *the intended approximation* (2.4), *and under the condition* $\mu = \tau^\beta/h^2 \leqslant \beta/2$, *the solution of the difference scheme* (5.3) *with the initial condition* (4.9) *converges*, *for* $h \to 0$, *weakly* (*in distribution*) *to the time-dependent probability distribution whose density is the solution* $u(x,t)$ *of the Cauchy problem* (1.6).

6. Conclusions

Using bivariate generating functions for working in the Fourier–Laplace domain we have proved weak convergence of discrete solutions of space–time-fractional diffusion processes to the solution of the corresponding equations for time derivative orders in (0, 1]. These discrete solutions are interpreted as random walk models. Thus, inspired by their usefulness in probability theory, we have applied the discrete and continuous transforms of Fourier and Laplace for constructing our proofs, leaving aside the questions of numerical accuracy in the supremum norm. In her thesis, Abdel-Rehim [1] has presented case studies illustrating the numerical convergence of the discrete solutions for the explicit and for the here not treated implicit difference scheme and simulated random walks via the Monte Carlo method.

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