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Characterizations and simulations of a class of stochastic processes to model anomalous diffusion

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Abstract
In this paper, we study a parametric class of stochastic processes to model both fast and slow anomalous diffusions. This class, called generalized grey Brownian motion (ggBm), is made up of self-similar with stationary increments processes (H-**sssi**) and depends on two real parameters $\alpha \in (0, 2)$ and $\beta \in (0, 1]$. It includes fractional Brownian motion when $\alpha \in (0, 2)$ and $\beta = 1$, and time-fractional diffusion stochastic processes when $\alpha = \beta \in (0, 1)$. The latter have a marginal probability density function governed by time-fractional diffusion equations of order β. The ggBm is defined through the explicit construction of the underlying probability space. However, in this paper we show that it is possible to define it in an unspecified probability space. For this purpose, we write down explicitly all the finite-dimensional probability density functions. Moreover, we provide different ggBm characterizations. The role of the M-Wright function, which is related to the fundamental solution of the time-fractional diffusion equation, emerges as a natural generalization of the Gaussian distribution. Furthermore, we show that the ggBm can be represented in terms of the product of a random variable, which is related to the M-Wright function, and an independent fractional Brownian motion. This representation highlights the H-**sssi** nature of the ggBm and provides a way to study and simulate the trajectories. For this purpose, we developed a random walk model based on a finite difference approximation of a partial integro-differential equation of a fractional type.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Diffusive processes are generally classified as normal or anomalous if their variance grows linearly in time or not, respectively. Furthermore, the normal diffusion is associated with the Gaussian probability density function (PDF) for particle positions.

Several physical phenomena show anomalous diffusion. They range from dispersion in complex plasmas [1] to self-diffusion of surfactant molecules [2], or from light in a cold atomic cloud [3] to donor–acceptor electron pair within a protein [4], to mention only some of the more recent experimental evidences. Such anomalous behaviours cover the full range of anomalous diffusion, e.g. from slow diffusion [4–6], when the variance grows slower than linear, to fast diffusion [1–3, 7], when the variance grows faster than linear. In order to model with a unique mathematical framework both slow and fast anomalous diffusions, a class of stochastic processes is introduced here and analysed. We would like this work to be a first step towards a comprehensive description of all dispersive mechanisms. Moreover, the PDF of particle positions of this class turns out to be related to the M-Wright function, which is a natural generalization of the Gaussian density.

A Gaussian anomalous diffusion can be obtained from a standard diffusion equation with time-dependent diffusivity. The latter is mainly based on the empirical flux–gradient relation and, for this reason, it is considered a simple particular case.

Anomalous diffusion processes can also be obtained as Gaussian processes with time subordination (see remark 1). As a consequence, the particle density is not Gaussian. This fact is often seen as the origins and the physical interpretation of anomalous diffusion. In fact, let $f(x,t)$ be the density function of a diffusive process and $G(x,t)$ a standard Gaussian density function. Namely, with $t \geqslant 0$,

$$G(x,t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right), \qquad \sigma_G^2(t) := \int_{\mathbb{R}} x^2 G(x,t)\,\mathrm{d}x = 2t. \tag{1}$$

Let $\varphi_\beta(\tau,t) = t^{-\beta}\phi(\tau t^{-\beta})$, with $\tau \geqslant 0$, $t > 0$ and $\beta > 0$, be the marginal probability density function of a self-similar stochastic process, which is interpreted as a randomized operational time. Therefore, in agreement with the monotonic growing of time, such a process is required to be a non-negative non-decreasing random process. Hereinafter, it is called the marginal probability density function, the one-dimensional PDF of a certain stochastic process (e.g. the one-point and one-time PDF of particle position)[3]. Furthermore, we remember that a process $X(t)$, $t \geqslant 0$, is said to be self-similar with a self-similarity exponent H if, for all $a \geqslant 0$, the processes $X(at)$, $t \geqslant 0$, and $a^H X(t)$, $t \geqslant 0$, have the same finite-dimensional distributions. We also suppose that ϕ has moments of any order. Then, if the subordination formula

$$f(x,t) = \int_0^{+\infty} G(x,\tau)\varphi_\beta(\tau,t)\,\mathrm{d}\tau \tag{2}$$

holds, $f(x,t)$ is the marginal density function of an anomalous diffusion process. In fact,

$$\begin{aligned}\sigma_f^2(t) &= \int_{-\infty}^{+\infty} x^2 f(x,t)\,\mathrm{d}x = \int_{-\infty}^{+\infty} x^2 \left\{\int_0^{+\infty} G(x,\tau)\varphi_\beta(\tau,t)\,\mathrm{d}\tau\right\}\mathrm{d}x \\ &= \int_0^{+\infty}\left\{\int_{-\infty}^{+\infty} x^2 G(x,\tau)\,\mathrm{d}x\right\}\varphi_\beta(\tau,t)\,\mathrm{d}\tau \\ &= 2\int_0^{+\infty} \tau\varphi_\beta(\tau,t)\,\mathrm{d}\tau = Dt^\beta,\end{aligned}$$

[3] This notation is a physical analogue of probability theory notation. In fact, this marginal density corresponds to the result of the integration over an n-dimensional joint density (e.g. the n-points and n-times density associated with an n-steps particle trajectory).

where we set

$$D = 2\int_0^{+\infty} \zeta\phi(\zeta)\,\mathrm{d}\zeta,$$

which is finite by hypothesis.

We observe that it is desirable having a random time process that for $\beta = 1$ gives a Gaussian process with a linear growing variance in time. Thus, from equation (2), we require that $\varphi_1(\tau, t) = \delta(\tau - t)$.

A ready-made example is given by the *M*-function (see the appendix), which is related to the fundamental solution of the so-called *time-fractional diffusion equation* of order β (see [8–12]) which, in an integral form, reads

$$u(x,t) = u_0(x) + \frac{1}{\Gamma(\beta)}\int_0^t (t-s)^{\beta-1}\partial_{xx}u(x,s)\,\mathrm{d}s, \qquad t \geqslant 0, \tag{3}$$

with $u_0(x) = u(x, 0)$.

In fact, suppose that the marginal density function of the random time process is

$$\varphi(\tau,t) = t^{-\beta}M_\beta(\tau t^{-\beta}) \equiv \mathcal{M}_\beta(\tau,t),$$

with $0 < \beta < 1$. With this choice, equation (2) becomes

$$f(x,t) = \int_0^{+\infty} G(x,\tau)\mathcal{M}_\beta(\tau,t)\,\mathrm{d}\tau,$$

which, by using (A.6) and (A.2), becomes

$$f(x,t) = \frac{1}{2}\int_0^{+\infty} \mathcal{M}_{1/2}(|x|,\tau)\mathcal{M}_\beta(\tau,t)\,\mathrm{d}\tau = \frac{1}{2}\mathcal{M}_{\beta/2}(|x|,t). \tag{4}$$

That is just the fundamental solution of (3). Moreover, when $\beta = 1$, equation (3) becomes a standard diffusion equation and indeed, using (A.5), one finds

$$f(x,t) = \int_0^{+\infty} G(x,\tau)\mathcal{M}_1(\tau,t)\,\mathrm{d}\tau = G(x,t).$$

Example 1. Consider a Brownian motion $B(t), t \geqslant 0$, such that $E(B(1)^2) = 2$ (we call it standard Brownian motion), and consider a random time $l_\beta(t), t \geqslant 0$, defined by the local time[4] in zero at time t of a $d = 2(1-\beta)$-dimensional Bessel process, with $0 < d < 2$ (see [13–16]). Furthermore, let l_β be independent of B. It is known that l_β is a self-similar process with the scaling parameter $H = \beta$. Therefore, the subordinated process

$$D_\beta(t) = B(l_\beta(t)), \qquad t \geqslant 0, \tag{5}$$

is a model for slow anomalous diffusion, and its marginal probability density function is the fundamental solutions of the time-fractional diffusion equation of order $0 < \beta \leqslant 1$ (also see [17]). Actually, the local time $l_\beta(t)$ is defined up to a multiplicative constant (see [18]). Here, we suppose that $l_\beta(t), t \geqslant 0$, is defined such that its marginal density function is $\mathcal{M}_\beta(x,t), x, t \geqslant 0$.

Example 2. Consider again a standard Brownian motion $B(t), t \geqslant 0$. Another possible choice of an independent random time process $l_\beta(t)$, for which the subordinated process $B(l_\beta(t))$ has still marginal density governed by the time-fractional diffusion equation of order β, is the

[4] Heuristically, the local time $l(t, x)$ of a diffusion process characterizes the 'time spent by the process at a given level x up to time t' (we shortly write $l(t)$ if $x = 0$). For instance, in the case of Brownian motion, the local time can be written as $l(t,x) = \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\int_0^t 1_{[x-\epsilon,x+\epsilon]}(B(s))\,\mathrm{d}s$, where $1_{[a,b]}(x)$ is the indicator function of the interval.

inverse of the totally skewed strictly β-stable process, as founded in the context of continuous time random walk (CTRW) by Meerschaert *et al* [19] (see also [20–24]).

Remark 1. The stochastic interpretation through subordinated processes turns out to be very natural. A subordinated process is defined as $Y(t) = X(l(t)), t \geqslant 0$, where $X(t)$ is a Markovian diffusion and $l(t)$ is a (non-negative) random time process independent of $X(t)$ (see [25, 26]), so that $Y(t)$ has a direct physical interpretation. For instance, $X(t)$ can be interpreted as the state of a system at time t, while $l(t)$ can be interpreted as the 'effective activity' up to time t. In this way, even if the process $X(t)$ is Markovian, the resulting subordinated process $Y(t)$ is in general non-Markovian, and the non-local memory effects are attributable to the random time process $l(t)$ and to its evolution, which is in general non-local in time.

Examples 1 and 2 provide two different stochastic processes with the same marginal density function (equation (4)). Indeed, it is important to remark that, starting from a master equation which describes the time evolution of a probability density function $f(x,t)$, it is always possible to define an equivalence class of stochastic processes with the same marginal density function $f(x,t)$. The above two examples represent only particular cases of subordinated-type processes. However, processes which are not of a subordinated type can also serve as models for anomalous diffusion described by time-fractional diffusion equations (see [27]). It is clear that additional requirements may be stated in order to fix the probabilistic model.

Since $0 < \beta < 1$, equation (3) depicts a system with a slow-anomalous diffusion behaviour. In order to study the full range (slow and fast) of anomalous diffusion, we introduce a suitable *time-stretching* $g(t) = t^{\alpha/\beta}$, $0 < \beta \leqslant 1$ and $\alpha > 0$. Let $f(x,t)$ be a solution of (3); then the function $f_{\alpha,\beta}(x,t) = f(x, t^{\alpha/\beta})$ is a solution of the *stretched time-fractional diffusion equation*:

$$u(x,t) = u_0(x) + \frac{1}{\Gamma(\beta)}\frac{\alpha}{\beta}\int_0^t s^{\frac{\alpha}{\beta}-1}\left(t^{\frac{\alpha}{\beta}} - s^{\frac{\alpha}{\beta}}\right)^{\beta-1}\frac{\partial^2}{\partial x^2}u(x,s)\,\mathrm{d}s, \tag{6}$$

with the same initial condition. Then, the fundamental solution of equation (6) is $u(x,t) = \frac{1}{2}\mathcal{M}_{\beta/2}(|x|, t^{\alpha/\beta})$ and defines a self-similar PDF of order $H = \alpha/2$. That is,

$$u(x,t) = \frac{t^{-\alpha/2}}{2}M_{\beta/2}(|x|t^{-\alpha/2}), \qquad x \in \mathbb{R}. \tag{7}$$

The diffusion is slow when $\alpha < 1$, standard when $\alpha = 1$ and fast when $\alpha > 1$. We observe that when $\beta = 1$, $u(x,t)$ is a 'stretched' Gaussian density:

$$u(x,t) = \frac{t^{-\alpha/2}}{2}M_{1/2}(|x|/t^{\alpha/2}) = \frac{1}{\sqrt{4\pi t^{\alpha}}}\exp\left(-\frac{x^2}{4t^{\alpha}}\right), \qquad t > 0. \tag{8}$$

Moreover, in the case $\alpha = \beta, 0 < \beta < 1$, the non-Gaussian probability density $u(x,t) = \frac{1}{2}\mathcal{M}_{\beta/2}(|x|, t)$ is recovered, i.e. the fundamental solutions of equation (3). The diffusion is always slow and becomes standard when $\beta \to 1$. Finally, in the general case $0 < \beta < 1$ and $\alpha > 0$, we have a non-Gaussian full-ranged anomalous diffusion.

Our main goal is to develop stochastic processes that serve as models for the anomalous diffusion described by this class of equations (equation (6)). To do this, we require some constraints. Let $X(t), t \geqslant 0$, be a self-similar stochastic process with the scaling parameter $H = \alpha/2$ and marginal probability density function defined by equation (7). We have already observed that there is a whole equivalence class of such stochastic processes. For instance, looking at examples 1 and 2, one could immediately take $X(t) = B(l_\beta(t^{\alpha/\beta})), t \geqslant 0$, with a suitable choice of the independent random time $l_\beta(t)$. In order to choose a specific model, we add the requirement that the process $X(t)$ be also a stationary increments process. Namely, we require that the process $X(t)$ be H-**sssi** (self-similar of order H with the stationary increments process), with $H = \alpha/2$.

Remark 2. The latter requirement forces the α-parameter to be in the range $0 < \alpha < 2$ [28]. Moreover, it automatically excludes the subordinated processes of examples 1 and 2, which have in general no stationary increments.

Summarizing, we ask that the stochastic process $X(t), t \geqslant 0$, satisfies the following requirements: let $0 < \beta \leqslant 1$ and $0 < \alpha < 2$; then

(i) $X(t)$ is self-similar with index $H = \alpha/2$.
(ii) $X(t)$ has a marginal density function $f_{\alpha,\beta}(x,t) = \frac{t^{-\alpha/2}}{2} M_{\beta/2}(|x|t^{-\alpha/2})$ (see (7)).
(iii) $X(t)$ has stationary increments.

In [27], the authors have shown that a stochastic process which satisfies all the above properties is the so-called *generalized grey Brownian motion* (ggBm) $B_{\alpha,\beta}(t), t \geqslant 0$, [29, 30]. It represents a generalization of Brownian motion (Bm) and fractional Brownian motion (fBm) as well. Moreover, it serves as a stochastic model for equation (6). Hence, in this paper, we will focus on the study of this process.

Remark 3. Because of the stationarity of the increments, the anomalous diffusion appears deeply related to the long-range dependence characterization of $B_{\alpha,\beta}(t)$. We remember that an H-**sssi** process has *long-range dependence* (or *long memory*) if $1/2 < H < 1$. This means that the discrete time process of its increments exhibits long-range correlation. That is, the increments' autocorrelation function $\gamma(k)$ tends to zero with a power law as k goes to infinity and in such a manner that it does not become integrable [28, 31, 32]. Therefore, when $0 < \alpha < 1$ the diffusion is *slow* and the process has *short memory*. While when $1 < \alpha < 2$ the diffusion is *fast* and the process has *long memory*.

The rest of the paper is organized as follows. In the following section, we briefly introduce the mathematical definition of the ggBm. In the third section, we characterize the ggBm through the study of its finite-dimensional probability density functions. The last two sections are devoted to trajectory simulations and final remarks.

2. The generalized grey Brownian motion

The generalized grey noise space is the probability space $(\mathcal{S}'(\mathbb{R}), \mathcal{B}, \mu_{\alpha,\beta})$, where $\mathcal{S}'(\mathbb{R})$ is the space of tempered distribution defined on $\mathbb{R}$, $\mathcal{B}$ is the Borel's σ-algebra generated by the weak topology on $\mathcal{S}'(\mathbb{R})$ and $\mu_{\alpha,\beta}$ is the so-called generalized grey noise measure. The measure $\mu_{\alpha,\beta}$ satisfies

$$\int_{\mathcal{S}'(\mathbb{R})} \mathrm{e}^{\mathrm{i}\langle\omega,\xi\rangle}\,\mathrm{d}\mu_{\alpha,\beta}(\omega) = E_\beta\left(-\|\xi\|_\alpha^2\right), \qquad \xi \in \mathcal{S}(\mathbb{R}), \qquad 0 < \beta \leqslant 1, \qquad 0 < \alpha < 2, \tag{9}$$

where $\langle\cdot,\cdot\rangle$ is the canonical bilinear pairing between $\mathcal{S}(\mathbb{R})$ and $\mathcal{S}'(\mathbb{R})$ (see [27]) and $E_\beta(t)$ is the Mittag–Leffler function of order β:

$$E_\beta(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(\beta n + 1)}, \qquad x \in \mathbb{R}. \tag{10}$$

Moreover,

$$\|f\|_\alpha^2 = \Gamma(1+\alpha)\sin\frac{\pi}{2}\alpha \int_{\mathbb{R}} \mathrm{d}x|x|^{1-\alpha}|\widetilde{f}(x)|^2, \qquad f \in \mathcal{S}(\mathbb{R}), \tag{11}$$

with

$$\widetilde{f}(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}y \mathrm{e}^{\mathrm{i}xy} f(y), \qquad f \in \mathcal{S}(\mathbb{R}).$$

The range $0 < \beta \leqslant 1$ ensures the complete monotonicity of the function $E_\beta(-t), t \geqslant 0$ (see [33]), as required by equation (9), while the range $0 < \alpha < 2$ is chosen in order to have $\|1_{[a,b)}\|_\alpha^2 < \infty$, where $1_{[a,b)}$ is the indicator function of the interval $[a, b)$. In fact, in this case one has

$$\|1_{[a,b)}\|_\alpha^2 = (b-a)^\alpha, \qquad 0 < \alpha < 2, \qquad 0 \leqslant a < b. \tag{12}$$

It is possible to show (see [27, 29, 30]) that for each $t > 0$, the real random variable

$$X_{\alpha,\beta}(1_{[0,t)})(\cdot) = \langle \cdot, 1_{[0,t)} \rangle \tag{13}$$

is defined almost everywhere on $\mathcal{S}'(\mathbb{R})$. Moreover, it follows from (9) that it belongs to $L^2(\mathcal{S}'(\mathbb{R}), \mu_{\alpha,\beta})$ and

$$E(X_{\alpha,\beta}(1_{[0,t)})^2) = \frac{2}{\Gamma(1+\beta)} t^\alpha.$$

The generalized grey Brownian motion is then defined as the process

$$B_{\alpha,\beta}(t) = X_{\alpha,\beta}(1_{[0,t)}), \qquad t \geqslant 0. \tag{14}$$

The $B_{\alpha,\beta}(t)$ marginal density function, indicated with $f_{\alpha,\beta}(x, t)$, is the fundamental solution of equation (6). Namely, $f_{\alpha,\beta}(x, t) = \frac{t^{-\alpha/2}}{2} M_{\beta/2}(|x|t^{-\alpha/2})$ (see remark 5). Moreover, the linearity of definition (14) can be used to show many of the fundamental properties of $B_{\alpha,\beta}(t)$. For instance, $B_{\alpha,\beta}(t)$ turns out to be H-**sssi** with $H = \alpha/2$. Furthermore, one can calculate characteristic functions. For example in the one-dimensional case, for any real y and $t > 0$,

$$\widetilde{f}_{\alpha,\beta}(y, t) = E(\mathrm{e}^{\mathrm{i}y(B_{\alpha,\beta}(t))}) = E(\mathrm{e}^{\mathrm{i}X_{\alpha,\beta}(y1_{[0,t)})}).$$

By using equations (9) and (12), one has

$$\widetilde{f}_{\alpha,\beta}(y, t) = E_\beta\left(-y^2\|1_{[0,t)}\|_\alpha^2\right) = E_\beta(-y^2 t^\alpha).$$

In the multidimensional case, given a sequence of real numbers $\{\theta_1, \theta_2, \ldots, \theta_n\}$, for any collection $\{B_{\alpha,\beta}(t_1), \ldots, B_{\alpha,\beta}(t_n)\}$ with $0 < t_1 < t_2 < \cdots < t_n$, using linearity again, one can show that [27]

$$E\left(\exp\left(\mathrm{i}\sum_{j=1}^n \theta_j B_{\alpha,\beta}(t_j)\right)\right) = E_\beta\left(-\Gamma(1+\beta)\frac{1}{2}\sum_{i,j=1}^n \theta_i\theta_j\gamma_{\alpha,\beta}(t_i, t_j)\right), \tag{15}$$

where

$$\gamma_{\alpha,\beta}(t, s) = \frac{1}{\Gamma(1+\beta)}\left(t^\alpha + s^\alpha - |t-s|^\alpha\right), \qquad t, s \geqslant 0, \tag{16}$$

is the autocovariance matrix of $B_{\alpha,\beta}(t)$.

Remark 4. From equation (15), it follows that, with β fixed, $B_{\alpha,\beta}(t)$ is defined only by its covariance structure. In other words, the ggBm, which is not Gaussian in general, is an example of a process defined only through its first and second moments, which is a property of Gaussian processes indeed.

3. Characterization of the ggBm

We now want to characterize the ggBm through its finite-dimensional structure. From equation (15), we know that all the ggBm finite-dimensional probability density functions are defined only by their autocovariance matrix. The following proposition holds.

Proposition 1. *Let $B_{\alpha,\beta}$ be a ggBm; then for any collection $\{B_{\alpha,\beta}(t_1), \dots, B_{\alpha,\beta}(t_n)\}$, the joint probability density function is given by*

$$f_{\alpha,\beta}(x_1,\dots,x_n;\gamma_{\alpha,\beta}) = \frac{(2\pi)^{-\frac{n-1}{2}}}{\sqrt{2\Gamma(1+\beta)^n \det\gamma_{\alpha,\beta}}} \int_0^\infty \frac{1}{\tau^{n/2}} M_{1/2}\left(\frac{\xi}{\tau^{1/2}}\right) M_\beta(\tau)\,\mathrm{d}\tau, \tag{17}$$

with

$$\xi = \left(2\Gamma(1+\beta)^{-1}\sum_{i,j=1}^{n} x_i {\gamma_{\alpha,\beta}}^{-1}(t_i,t_j)x_j\right)^{1/2},$$

$$\gamma_{\alpha,\beta}(t_i,t_j) = \frac{1}{\Gamma(1+\beta)}\left(t_i^\alpha + t_j^\alpha - |t_i - t_j|^\alpha\right), \qquad i,j = 1,\dots,n.$$

Proof. In order to show equation (17), we calculate its n-dimensional Fourier transform and find that it is equal to (15). We have

$$\int_{\mathbb{R}^n} \exp\left(\mathrm{i}\sum_{j=1}^{n}\theta_j x_j\right) f_{\alpha,\beta}(x_1,\dots,x_n;\gamma_{\alpha,\beta})\,\mathrm{d}^n x = \frac{(2\pi)^{-\frac{n-1}{2}}}{\sqrt{2\Gamma(1+\beta)^n \det\gamma_{\alpha,\beta}}}$$
$$\times \int_0^\infty \frac{1}{\tau^{n/2}} M_\beta(\tau) \int_{\mathbb{R}^n} \exp\left(\mathrm{i}\sum_{j=1}^{n}\theta_j x_j\right) M_{1/2}\left(\frac{\xi}{\tau^{1/2}}\right)\mathrm{d}^n x\,\mathrm{d}\tau.$$

We remember that $M_{1/2}(r) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{-r^2/4}$; thus we get

$$\int_0^\infty \frac{1}{\tau^{n/2}} M_\beta(\tau) \int_{\mathbb{R}^n} \exp\left(\mathrm{i}\sum_{j=1}^{n}\theta_j x_j\right)$$
$$\times \frac{(2\pi)^{-\frac{n}{2}}}{\sqrt{\Gamma(1+\beta)^n \det\gamma_{\alpha,\beta}}} \exp\left(-\sum_{i,j=1}^{n} \frac{x_i\gamma_{\alpha,\beta}^{-1}(t_i,t_j)x_j}{2\tau\Gamma(1+\beta)}\right)\mathrm{d}^n x\,\mathrm{d}\tau. \tag{18}$$

We make the change of variables $\mathbf{x} = \Gamma(1+\beta)^{1/2}\tau^{1/2}\mathbf{y}$, with $\mathbf{x},\mathbf{y} \in \mathbb{R}^n$, and we get

$$\int_0^\infty M_\beta(\tau)\int_{\mathbb{R}^n} \exp\left(\mathrm{i}\Gamma(1+\beta)^{1/2}\tau^{1/2}\sum_{j=1}^{n}\theta_j y_j\right)$$
$$\times \frac{(2\pi)^{-\frac{n}{2}}}{\sqrt{\det\gamma_{\alpha,\beta}}} \exp\left(-\sum_{i,j=1}^{n}\frac{y_i\gamma_{\alpha,\beta}^{-1}(t_i,t_j)y_j}{2}\right)\mathrm{d}^n y\,\mathrm{d}\tau$$
$$= \int_0^\infty M_\beta(\tau)\exp\left(-\Gamma(1+\beta)\tau\sum_{i,j=1}^{n}\frac{\theta_i\gamma_\alpha(t_i,t_j)\theta_j}{2}\right)\mathrm{d}\tau$$
$$= \int_0^\infty \mathrm{e}^{-\tau s} M_\beta(\tau)\,\mathrm{d}\tau = E_\beta(-s),$$

where $s = \Gamma(1+\beta)\sum_{i,j=1}^{n}\theta_i\theta_j\gamma_{\alpha,\beta}(t_i,t_j)/2$ and we have used equation (A.4). □

Applying the Kolmogorov extension theorem, the above proposition allows us to define the ggBm in an unspecified probability space. In fact, given a probability space $(\Omega, \mathcal{F}, P)$, the following proposition characterizes the ggBm.

Proposition 2. *Let $X(t), t \geqslant 0$, be a stochastic process defined in a certain probability space $(\Omega, \mathcal{F}, P)$, such that*

(i) $X(t)$ has a covariance matrix indicated by $\gamma_{\alpha,\beta}$ and finite-dimensional distributions defined by equation (17),
(ii) $E(X^2(t)) = \frac{2}{\Gamma(1+\beta)} t^\alpha$ for $0 < \beta \leqslant 1$ and $0 < \alpha < 2$,
(iii) $X(t)$ has stationary increments,

then $X(t), t \geqslant 0$, is a ggBm.

In fact, condition (ii) together with condition (iii) implies that $\gamma_{\alpha,\beta}$ must be the ggBm autocovariance matrix (16).

Remark 5. Using (A.2), for $n = 1$, equation (17) reduces to

$$f_{\alpha,\beta}(x,t) = \frac{1}{\sqrt{4t^\alpha}} \int_0^\infty \mathcal{M}_{1/2}\left(|x|t^{-\alpha/2}, \tau\right) \mathcal{M}_\beta(\tau, 1)\, \mathrm{d}\tau$$
$$= \frac{1}{2} t^{-\alpha/2} M_{\beta/2}(|x|t^{-\alpha/2}). \tag{19}$$

This means that the ggBm marginal density function is indeed the fundamental solution of equation (6).

Remark 6. Because for $\beta = 1$

$$M_1(\tau) = \delta(\tau - 1),$$

then, putting $\gamma_{\alpha,1} \equiv \gamma_\alpha$, we have that equation (17) reduces to the Gaussian distribution of the fractional Brownian motion. That is,

$$f_{\alpha,1}(x_1, x_2, \ldots, x_n; \gamma_{\alpha,1}) = \frac{(2\pi)^{-\frac{n-1}{2}}}{\sqrt{2 \det \gamma_\alpha}} M_{1/2}\left(\left(2 \sum_{i,j=1}^n x_i \gamma_\alpha^{-1}(t_i, t_j) x_j\right)^{1/2}\right).$$

We have the following corollary.

Corollary 1. *Let $X(t), t \geqslant 0$, be a stochastic process defined in a certain probability space $(\Omega, \mathcal{F}, P)$. Let $H = \alpha/2$ with $0 < \alpha < 2$ and suppose that $E(X(1)^2) = 2/\Gamma(1+\beta)$. The following statements are equivalent:*

*(i) X is H-**sssi** with finite-dimensional distribution defined by (17),*
(ii) X is a ggBm with the scaling exponent $\alpha/2$ and the 'fractional order' parameter β,
(iii) X has a zero mean, covariance function $\gamma_{\alpha,\beta}(t,s), t, s \geqslant 0$, defined by (16) and finite-dimensional distribution defined by (17).

3.1. Representation of the ggBm

Up to now, we have seen that the ggBm $B_{\alpha,\beta}(t), t \geqslant 0$, is an H-**sssi** process, which generalizes Gaussian processes (it is indeed Gaussian when $\beta = 1$) and is defined only by its autocovariance structure. These properties make us think that $B_{\alpha,\beta}(t)$ may be equivalent to a process $\Lambda_\beta X_\alpha(t), t \geqslant 0$, where $X_\alpha(t)$ is a Gaussian process and Λ_β is a suitable chosen independent random variable. Indeed, the following proposition holds.

Proposition 3. *Let $B_{\alpha,\beta}(t), t \geqslant 0$, be a ggBm; then*

$$B_{\alpha,\beta}(t) \stackrel{d}{=} \sqrt{L_\beta} X_\alpha(t), \qquad t \geqslant 0, \qquad 0 < \beta \leqslant 1, \qquad 0 < \alpha < 2, \quad (20)$$

where $\stackrel{d}{=}$ denotes the equality of the finite-dimensional distribution, $X_\alpha(t)$ is a standard fBm and L_β is an independent non-negative random variable with the probability density function $M_\beta(\tau), \tau \geqslant 0$.

In fact, after some manipulation, equation (18) can be written as follows:

$$\int_{\mathbb{R}^n} \int_0^\infty \exp\left(\mathrm{i} \sum_{j=1}^n \theta_j y x_j\right) 2y M_\beta(y^2) \frac{(2\pi)^{-\frac{n}{2}}}{\sqrt{\det \gamma_\alpha}} \exp\left(-\sum_{i,j=1}^n x_i \gamma_\alpha^{-1}(t_i, t_j) x_j/2\right) \mathrm{d}y\, \mathrm{d}^n x$$
$$= E\left(\exp\left(\mathrm{i} \sum_{\mathrm{j}=1}^{\mathrm{n}} \theta_{\mathrm{j}} \sqrt{\mathrm{L}_\beta} \mathrm{X}_\alpha(\mathrm{t_j})\right)\right).$$

Example 3. A possible choice of L_β is the random variable $l_\beta(1)$, where $l_\beta(t), t \geqslant 0$, is the random time process of example 1 or example 2.

Remark 7. Proposition 3 highlights the *H*-**sssi** nature of the ggBm. Moreover, for $\beta = 1$ from equation (A.5) it follows that $L_1 = 1$ a.s.; thus we recover the fractional Brownian motion of order $H = \alpha/2$.

Representation (20) is very interesting. In fact, a number of questions, in particular those related to the distribution properties of $B_{\alpha,\beta}(t)$, can be reduced to questions concerning the fBm $X_\alpha(t)$, which are easier since $X_\alpha(t)$ is a Gaussian process. For instance, the Hölder continuity of the $B_{\alpha,\beta}(t)$ trajectories follows immediately from those of $X_\alpha(t)$:

$$E(|X_\alpha(t) - X_\alpha(s)|^p) = c_p |t - s|^{p\alpha/2}.$$

Moreover, this factorization is indeed suitable for path simulation (see the following section).

Remark 8. From equation (20), it is clear that the Brownian motion $(B_{1,1}(t), t \geqslant 0)$ is the only process of the ggBm class with independent increments.

4. Path simulation

In the previous section, we have shown that the ggBm could be represented by the process

$$B_{\alpha,\beta}(t) = \sqrt{L_\beta} X_\alpha(t), \qquad t \geqslant 0, \quad 0 < \beta \leqslant 1, \quad 0 < \alpha < 2,$$

where L_β is a suitable chosen random variable independent of the standard fBm $X_\alpha(t)$. Clearly, to simulate ggBm trajectories we first need a method to generate the random variable L_β.

4.1. The time-fractional drift equation

In order to generate the random variable L_β with the probability density function $M_\beta(\tau)$, we consider the so-called *time-fractional forward drift equation*, which in an integral form reads

$$u(x,t) = u_0(x) - \frac{1}{\Gamma(\beta)} \int_0^t (t-s)^{\beta-1} \frac{\partial}{\partial x} u(x,s)\, \mathrm{d}s, \qquad x \in \mathbb{R}, \quad t \geqslant 0, \quad 0 < \beta \leqslant 1. \tag{21}$$

The fundamental solution of equation (21) is [15, 16]

$$u(x,t) = \mathcal{M}_\beta(x,t), \qquad x, t \geqslant 0. \tag{22}$$

This function can be interpreted as the marginal density function of a non-negative self-similar stochastic process with the scaling parameter $H = \beta$ (see examples 1 and 2).

Remark 9. The name '*drift equation*' refers to the fact that when $\beta = 1$ equation (21) turns out to be the one-dimensional (forward) drift, equation $\partial_t u(x,t) = -\partial_x u(x,t)$, whose fundamental solution is $\delta(x-t)$.

Remark 10. When $\beta = 1$, we recover $\mathcal{M}_1(x,t) = \delta(x-t)$ (see (A.5)).

We write equation (21) in terms of the fractional derivative of order β. Let us introduce the *Caputo–Dzherbashyan* derivative:

$$_*D_t^\beta f(t) = J_t^{1-\beta} \frac{\partial f}{\partial t} = \frac{1}{\Gamma(1-\beta)} \int_0^t (t-s)^{-\beta} \frac{\partial f(s)}{\partial s}\, \mathrm{d}s, \tag{23}$$

where J_t^α is the Riemann–Liouville fractional integral of order $0 \leqslant \alpha < 1$ such that, for $\alpha = 0$, J_t^0 is the identity operator. Then, the corresponding Cauchy problem of equation (21) can be written as

$$\begin{cases} _*D_t^\beta u(x,t) = -\partial_x u(x,t), \\ u(x,0) = u_0(x) = \delta(x), \end{cases} \tag{24}$$

with $x \in \mathbb{R}$, $t \geqslant 0$ and $0 < \beta \leqslant 1$.

Using a random walk model, one can simulate a discrete time random process $L_\beta(t)$, $t \geqslant 0$, governed by the time-fractional forward drift equation (24) (see [34, 35]). In this way, for each run, the random variable $L_\beta(1)$ has the required distribution $u(x,1) = M_\beta(x)$. The random walk construction follows two steps:

- the Grünwald–Letnikov discretization of the Caputo–Dzherbashyan derivative,
- the interpretation of the corresponding finite difference scheme as a random walk scheme.

4.2. Finite difference schemes

In order to define the finite difference model, we write the Cauchy problem (24) in a finite domain

$$\begin{cases} _*D_t^\beta u(x,t) = -\dfrac{\partial}{\partial x} u(x,t), & (x,t) \in \Omega = [-a,a] \times [0,1], \quad a > 0, \\ u(x,0) = u_0(x) = \delta(x), & \\ u(-a,t) = \Phi_1(t), \quad u(a,t) = \Phi_2(t), & t > 0. \end{cases} \tag{25}$$

Let N, M be positive integers. Then, we introduce a bi-dimensional lattice:

$$\mathcal{G}_{\delta x,\delta t}^{2M,N} = \{(j\delta x, n\delta t), (j,n) \in \mathbb{Z}_{2M} \times \mathbb{Z}_N\},$$

contained on Ω, with $\delta x = 2a/(2M-1)$ and $\delta t = 1/(N-1)$. The lattice elements are indicated with

$$(x_j, t_n) = (j\delta x, n\delta t), \quad j = 0, 1, \ldots, 2M-1, \quad n = 0, 1, \ldots N-1.$$

Let $u : \Omega \to \mathbb{R}$ be a function defined on Ω. We indicate with $u_j^n = u(x_j, t_n)$ the restriction of u to $\mathcal{G}_{\delta x,\delta t}^{2M,N}$ evaluated in (x_j, t_n).

The time-fractional forward drift equation is then replaced by the finite difference equation

$$ {}_*D_t^\beta u_j^n = -\frac{u_j^n - u_{j-1}^n}{\delta x}, \tag{26}$$

where

$$\begin{aligned} {}_*D_t^\beta u_j^n &= \sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} \frac{u_j^{n+1-k} - u_j^0}{\delta t^\beta}, \qquad u_j^0 = u_0(j\delta x), \\ \binom{\beta}{k} &= \frac{\Gamma(\beta+1)}{\Gamma(k+1)\Gamma(\beta-k+1)} \end{aligned} \tag{27}$$

is the so-called forward Grünwald–Letnikov scheme for the Caputo–Dzherbashyan derivative (23). Using the 'empty sum' convention

$$\sum_{k=p}^{q} \cdot = 0, \qquad \text{if} \quad q < p,$$

for any $n \geqslant 0$, we obtain the explicit equation

$$u_j^{n+1} = u_j^0 \sum_{k=0}^{n} (-1)^k \binom{\beta}{k} + \sum_{k=1}^{n} (-1)^{k+1} \binom{\beta}{k} u_j^{n+1-k} + \mu\left(u_{j-1}^n - u_j^n\right), \tag{28}$$

where $\mu = \delta t^\beta/\delta x$. Equation (28) can be written in the following noteworthy form:

$$u_j^{n+1} = b_n u_j^0 + \sum_{k=1}^{n} c_k u_j^{n+1-k} + \mu\left(u_{j-1}^n - u_j^n\right), \tag{29}$$

where we have defined

$$\begin{aligned} c_k &= (-1)^{k+1} \binom{\beta}{k}, \qquad && k \geqslant 1, \\ b_n &= \sum_{k=0}^{n} (-1)^k \binom{\beta}{k}, \qquad && n \geqslant 0. \end{aligned} \tag{30}$$

More precisely, the explicit scheme reads

$$\begin{cases} u_0^n = \Phi_1(t_n), \quad u_{2M-1}^n = \Phi_2(t_n), \quad n > 0, \\ u_j^1 = (1 - \mu + \mu L) u_j^0, \quad 0 < j < 2M-1, \\ u_j^{n+1} = (c_1 - \mu + \mu L) u_j^n + c_2 u_j^{n-1} + \cdots + c_n u_j^1 + b_n u_j^0, \quad n > 0, \quad 0 < j < 2M-1, \end{cases}$$

where L is the 'lowering' operator $Lf_j = f_{j-1}$.

Remark 11. When $\beta = 1$, all the coefficients c_k and b_n vanish except $b_0 = c_1 = 1$, so that we recover the finite difference approximation of the (forward) drift equation.

In order to write an implicit scheme, we have to use backward approximations for the time-fractional derivative. Therefore, for any $n \geqslant 0$, we obtain

$$u_j^{n+1} + \mu\left(u_j^{n+1} - u_{j-1}^{n+1}\right) = b_n u_j^0 + \sum_{k=1}^{n} c_k u_j^{n+1-k}. \tag{31}$$

Namely,

$$\begin{cases} u_0^n = \Phi_1(t_n), \quad u_{2M-1}^n = \Phi_2(t_n), \quad n > 0, \\ (1+\mu-\mu L)u_j^1 = u_j^0, \quad 0 < j < 2M-1, \\ (1+\mu-\mu L)u_j^{n+1} = c_1 u_j^n + c_2 u_j^{n-1} + \cdots + c_n u_j^1 + b_n u_j^0, \quad n > 0, \quad 0 < j < 2M-1. \end{cases}$$

The above equation can be rewritten in matrix notation:

$$\begin{cases} \Lambda_{ij} u_j^1 = u_i^0 + \psi_i^1, \\ \Lambda_{ij} u_j^{n+1} = c_1 u_i^n + c_2 u_i^{n-1} + \cdots + c_n u_i^1 + b_n u_i^0 + \psi_i^{n+1}, n \geqslant 1. \end{cases} \tag{32}$$

Λ is the following $2M \times 2M$ matrix, divided into four $M \times M$ blocks:

$$\Lambda = \left(\begin{array}{c|c} \Lambda_1 & 0 \\ \hline \Lambda_2 & A \end{array}\right)$$

$$\Lambda = \left(\begin{array}{ccccc|ccccc} 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & \cdots & 0 \\ -\mu & 1+\mu & 0 & \cdots & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & -\mu & 1+\mu & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -\mu & 1+\mu & 0 & 0 & \cdots & 0 & 0 \\ \hline 0 & 0 & 0 & \cdots & -\mu & 1+\mu & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\mu & 1+\mu & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -\mu & 1+\mu & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & -\mu & 1 \end{array}\right). \tag{33}$$

Moreover, for any $n \geqslant 0$, ψ^n is a suitable vector which takes into account for the boundary terms.

Remark 12. Because Λ is lower diagonal, Λ^{-1} is

$$\Lambda^{-1} = \left(\begin{array}{c|c} \Lambda_1^{-1} & 0 \\ \hline -A^{-1}\Lambda_2\Lambda_1^{-1} & A^{-1} \end{array}\right). \tag{34}$$

As usual, the explicit scheme is subjected to a stability condition, while the implicit scheme is always stable. For example, if we take $\mu \leqslant \beta$, namely

$$\delta x \geqslant \delta t^\beta / \beta, \tag{35}$$

then the explicit scheme becomes indeed stable and preserves non-negativity as well. This means that if we suppose $u_j^0 \geqslant 0$ for any $0 \leqslant j \leqslant 2M-1$, then $u_j^n \geqslant 0$ for any $n > 0$ and $0 < j < 2M-1$. Actually, this is crucial because we interpret $\{u_j^n\}$ as sojourn probabilities. In order to show this, it is convenient to write equations (29) and (31) in the Fourier domain. Namely, we apply the *discrete Fourier transform* with respect to the 'space' index j to both sides of (29) and (31). We remember that, given a collection of complex numbers $\{x_j, j = 0, 1, \ldots, 2M-1\}$[5], its discrete Fourier transform is usually defined as

$$\mathcal{F}_d(x_l)_k := \widehat{x}_k = \sum_{j=0}^{2M-1} x_j \mathrm{e}^{-\mathrm{i}2\pi jk/2M}, \qquad k = 0, \ldots, 2M-1.$$

[5] Actually, we are considering $\{x_j\}$, for any $j \in \mathbb{Z}_+$, as a periodic sequence, such that $x_{j+2M} = x_j$ for any non-negative integer j.

One can show that, for any real number a, one has

$$\mathcal{F}(x_{j+a})_k = \mathrm{e}^{\mathrm{i}2\pi ak/2M}\widehat{x}_k.$$

Thus, heuristically, the effect of applying the Fourier transform to our finite difference equations is just to 'line up' the points in the Fourier space. In fact, for any $n > 0$, we get

$$\begin{cases} \widehat{u}_k^{n+1} = \xi_e(k)\widehat{u}_k^n + (\cdots)_k, & \text{explicit case,} \\ \xi_i(k)^{-1}\widehat{u}_k^{n+1} = \beta\widehat{u}_k^n + (\cdots)_k, & \text{implicit case,} \end{cases} \tag{36}$$

where $\xi_e(k) = (\beta - \mu + \mu\mathrm{e}^{-\mathrm{i}\pi k/M})$ and $\xi_i(k) = (1 + \mu - \mu\mathrm{e}^{-\mathrm{i}\pi k/M})^{-1}$ correspond to the so-called *amplification factors*. Then, heuristically, the schemes are stable if $|\xi(k)| \leqslant 1$ for any k. Namely, one has to require

$$\begin{cases} \max\limits_k((\beta-\mu)^2 + \mu^2 + 2\mu(\beta-\mu)\cos(\pi k/M)) \leqslant 1, & \text{explicit case,} \\ \min\limits_k((1+\mu)^2 + \mu^2 - 2\mu(1+\mu)\cos(\pi k/M)) \geqslant 1, & \text{implicit case.} \end{cases} \tag{37}$$

Clearly, while the second one is always satisfied, the first condition is indeed true if (35) holds[6].

4.3. *Random walk models*

We observe that, for $0 < \beta < 1$,

$$\sum_{k=1}^{\infty} c_k = 1, \qquad 1 > \beta = c_1 > c_2 > \cdots \to 0. \tag{38}$$

Moreover,

$$\begin{cases} b_0 = 1 = \sum\limits_{k=1}^{\infty} c_k, \qquad b_m = 1 - \sum\limits_{k=1}^{m} c_k = \sum\limits_{k=m+1}^{\infty} c_k, \\ 1 = b_0 > b_1 > b_2 > \cdots \to 0. \end{cases} \tag{39}$$

Thus, the coefficients c_k and b_n are a sequence of positive numbers, which do not exceed unity and decrease strictly monotonically to zero.

4.3.1. *Explicit random walk.*

In order to build a random walk model, we consider first the explicit scheme. Omitting the boundary terms, we have

$$\begin{cases} u_j^1 = (1-\mu)u_j^0 + \mu u_{j-1}^0, \\ u_j^{n+1} = (c_1 - \mu)u_j^n + \mu u_{j-1}^n + c_2 u_j^{n-1} + \cdots + c_n u_j^1 + b_n u_j^0, \quad n \geqslant 1. \end{cases}$$

We consider a walker which starts in zero at time zero, namely $x(t = 0) = 0$. We interpret u_j^n as the probability of sojourn in $x_j = j\delta x$ at time $t_n = n\delta t$. Then, we indicate with $x(t_n)$ the position of the particle at time t_n.

At time $t_1 = \delta t$ the walker could be at the position $x(1) = x_1$ with probability μ (that is the probability to come from one space-step behind) or in $x(1) = x_0 = 0$ with probability $1 - \mu$ (that is the probability to remain in the starting position).

[6] This follows from the fact that if $(\beta - \mu)$ is non-negative, the maximum is reached when the cosine equals +1, then one has $\beta^2 \leqslant 1$, which is in fact true by hypothesis.

From equations (38) and (39), it is clear that the parameters $c_1, c_2, \ldots c_n, b_n$ can be interpreted as probabilities. Then, the position at time t_{n+1} is determined as follows. We define a partition of events $\{E_{c_1}, E_{c_2}, \ldots, E_{c_n}, E_{b_n}\}$, with $P(E_{c_k}) = c_k$, $P(E_{b_n}) = b_n$, $n \geqslant 1$, such that

- E_{c_1} ={*the particle starts in the previous position* $x(t_n)$ *and jumps in* $x(t_n) + \delta x$ *with probability* μ *or stays in* $x(t_n)$ *with probability* $1 - \mu$}.
- E_{c_k} ={*the particle backs to the position* $x(t_{n+1-k})$}.
- E_{b_n} ={*the particle backs to the initial position* $x(t_0)$}.

4.3.2. Implicit random walk. Consider the implicit case

$$\begin{cases} u^1 = \Lambda^{-1} u^0, \\ u^{n+1} = \Lambda^{-1}[c_1 u^n + c_2 u^{n-1} + \cdots + c_n u^1 + b_n u^0], \end{cases}$$

where Λ is given by (34). The probability interpretation of the parameters c_k and b_n is still valid. In this case, however, we must use the *transpose matrix* P of A^{-1} to define the transition probabilities. Indeed, the $M \times M$ matrix A^{-1} propagates in the positive semi-axis. Moreover, from (33), it can be shown that P defines a transition matrix (all the elements are positive numbers less than 1 and all the rows sum to 1; see the example below).

Example 4. In the four-dimensional case, the matrix P is

$$P = \begin{pmatrix} 1/(1+\mu) & \mu/(1+\mu)^2 & \mu^2/(1+\mu)^3 & \mu^3/(1+\mu)^3 \\ 0 & 1/(1+\mu) & \mu/(1+\mu)^2 & \mu^2/(1+\mu)^2 \\ 0 & 0 & 1/(1+\mu) & \mu/(1+\mu) \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In the implicit case, the random walk is defined as follows. Let the particle start at zero; at the first step, it could jump up to $M - 1$ steps ahead with probabilities defined by the first P row. Then we have the following partition of events:

- E_{c_1} ={*the particle starts in the previous position* $x(t_n)$, *for instance* x_j. *Then, it could jump up to* $M - j - 1$ *steps ahead with probabilities defined by the* $j + 1$*th P row*};
- E_{c_k} = {*the particle backs to the position* $x(t_{n+1-k})$, *for instance* x_j. *Then it could jump up to* $M - j - 1$ *steps ahead with probabilities defined by the* $j + 1$*th P row*};
- E_{b_n} = {*the particle backs to the initial position* $x(t_0)$ *and then could jump up to* $M - 1$ *steps ahead with probabilities defined by the first P row*}.

Remark 13. The implicit method is slower than the explicit one. However, we observe that, because of the stability constraint (equation (35)), the implicit scheme is advisable for small β. Indeed, we have $\delta x \sim \delta t^\beta/\beta$, with $0 < \beta < 1$, and we are forced to raise the time steps in order to improve 'spatial' resolution.

4.4. ggBm trajectories

Along this section, we have provided a method to generate the random variable L_β, and the simulation results are shown in figures 1–3. In particular,

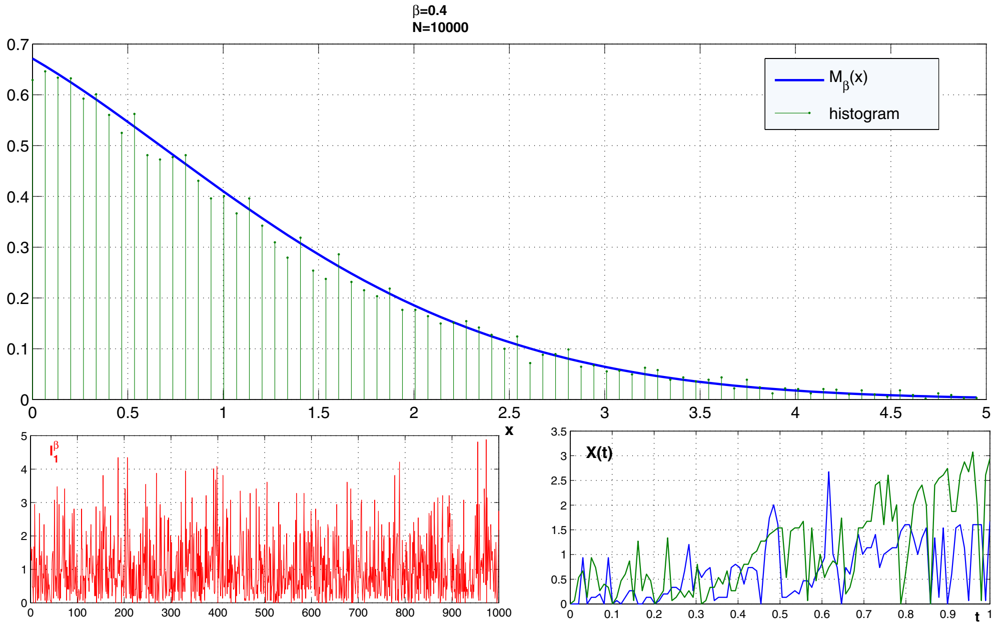

Figure 1. In the top panel, the histogram of L_β, which is calculated from a sample of $N = 10\,000$ outcomes, is obtained with an implicit random walk scheme and is compared with the exact PDF $M_\beta(x), x \geqslant 0$, with $\beta = 0.4$. In the bottom panels, the random variable L_β (left) and two trajectory examples (right) are shown.

- Figure 1 shows a random walk simulation with $\beta = 0.4$. In this case, we used an implicit random walk scheme. Moreover, we compared the histogram evaluated over $N = 10\,000$ simulations and the density function $M_{2/5}(x), x \geqslant 0$.
- Figure 2 shows a random walk when $\beta = 0.5$. Because $M_{1/2}(x) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{-x^2/4}, x \geqslant 0$, in this case $L_{1/2} \stackrel{d}{=} |Z|$ where Z is a Gaussian random variable.
- Figure 3 shows a random walk with $\beta = 0.8$. We used an explicit random walk scheme. Then, we compared the histogram with the corresponding probability density function $M_{4/5}(x), x \geqslant 0$.

In all the studied cases, we have found a good agreement between the histograms and the theoretical density functions.

At this point, in order to obtain examples of the $B_{\alpha,\beta}(t) = \sqrt{L_\beta}X_\alpha(t)$ trajectories, we just have to simulate the fractional Brownian motion $X_\alpha(t)$. For this purpose, we have used an exact Cholesky method (see [36]).

Path simulations of $B_{\beta,\beta}(t)$ (shortly B_β) and $B_{2-\beta,\beta}(t)$, with $\beta = 1/2$, are shown in figures 4–9. The first process provides an example of a stochastic model for slow diffusion (short memory) and the second provides a stochastic model for fast diffusion (long memory).

- Figure 4 shows some typical paths. In the bottom panel, we present the corresponding increment process. Namely,
$$Z_\beta(t_k) = B_\beta(t_k) - B_\beta(t_{k-1}), \qquad t_k = k\delta t, \qquad k = 1, 2, \ldots, M - 1.$$
- Figure 5 shows the agreement between simulations and the theoretical densities at times $t = 1$ and $t = 2$.

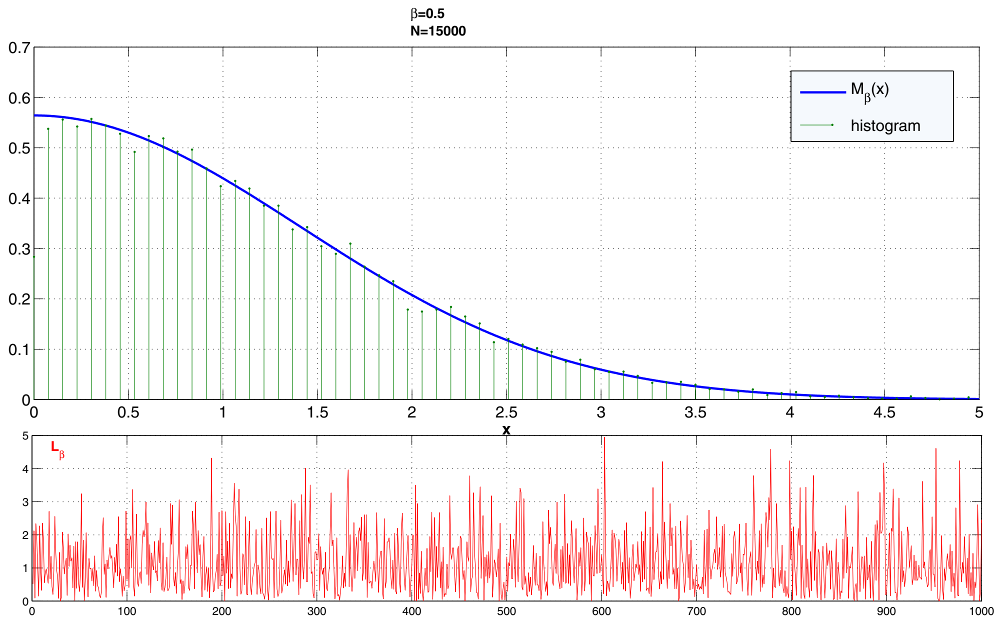

Figure 2. In the top panel, the histogram for the case $\beta = 0.5$ is calculated from a sample of $N = 15\,000$ outcomes, which are obtained simulating independent Gaussian random variables. The corresponding L_β is shown in the bottom.

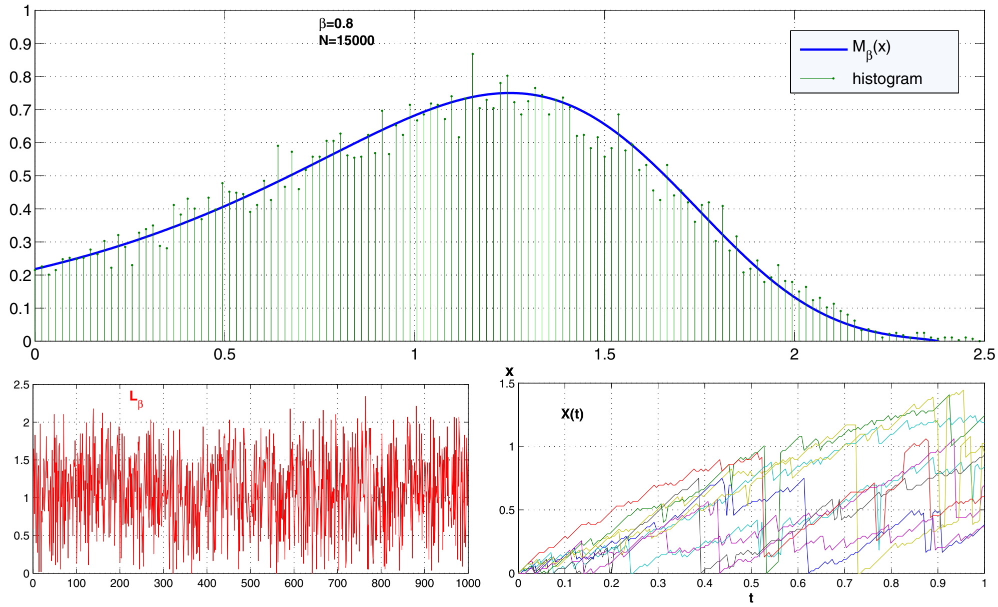

Figure 3. In the top panel, the histogram of L_β, which is calculated from a sample of $N = 15\,000$ outcomes, is obtained with an explicit random walk scheme and is compared with the exact PDF $M_\beta(x)$, $x \geqslant 0$, with $\beta = 0.8$. In the bottom panels, the random variable L_β (left) and many trajectory examples (right) are shown.

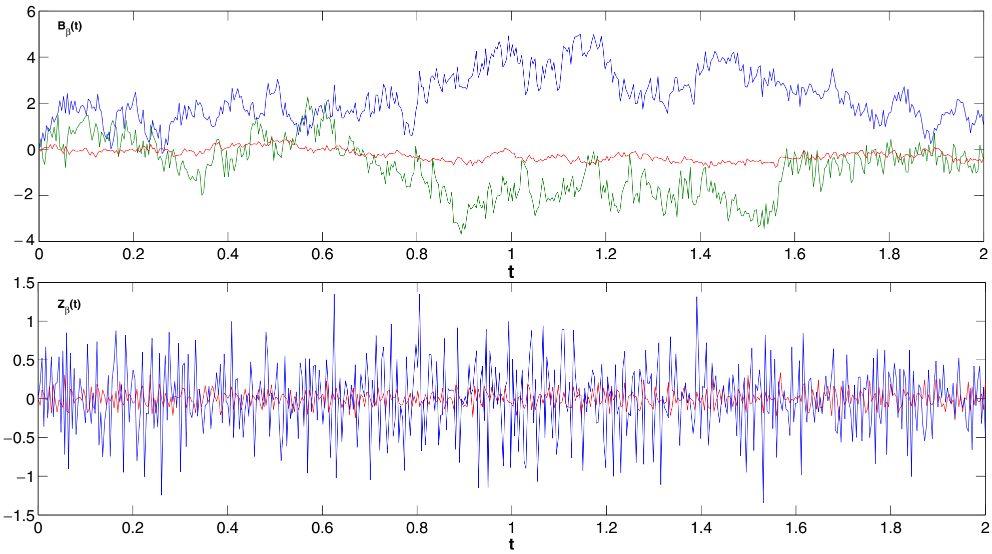

Figure 4. $B_\beta(t)$ trajectories in the case $\beta = 0.5$ (top panel) for $0 \leqslant t \leqslant 2$. The time series of the corresponding stationary noise $Z_\beta(t)$ is presented in the bottom panel.

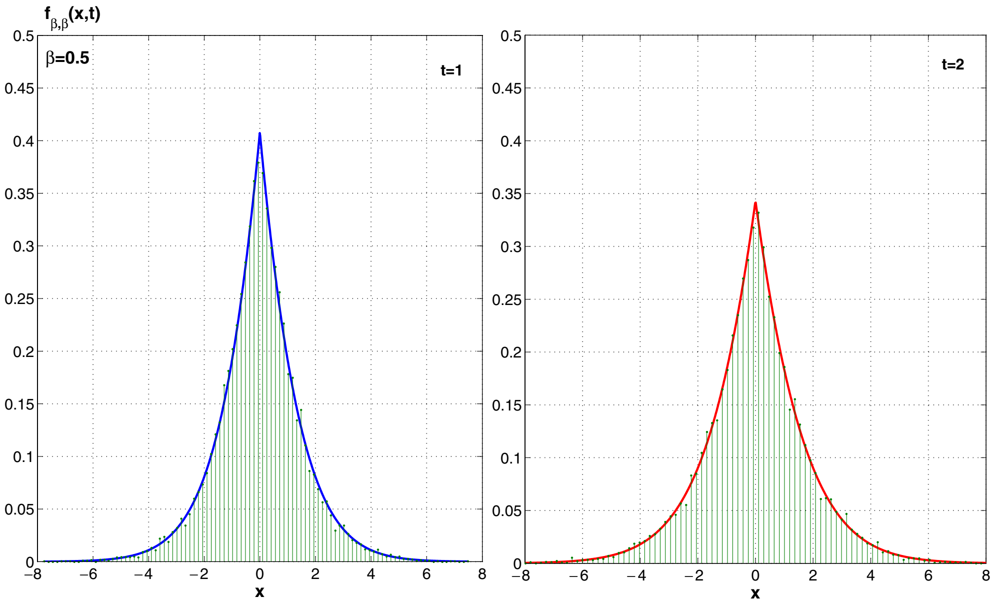

Figure 5. Histograms of $N = 15\,000$ simulations with $\beta = 0.5$ and exact marginal density at $t = 1$ and $t = 2$.

- Figure 6 presents the plot of the sample variance in the logarithmic scale. Moreover, we evaluated a linear fitting, which shows a good agreement with the theoretical result.
- Figure 7 shows some typical paths for the long-memory process $B_{2-\beta,\beta}(t)$.

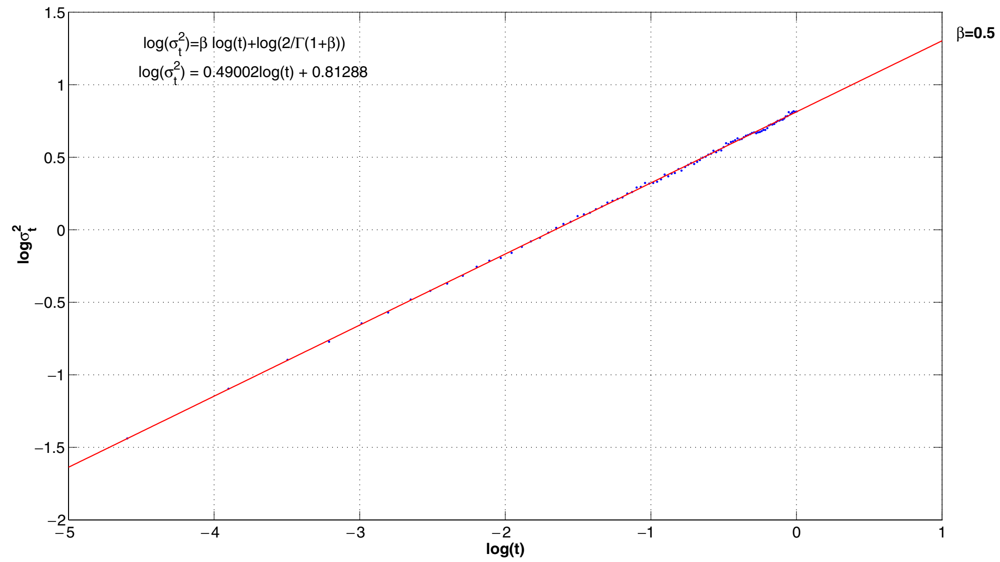

Figure 6. Sample variance in the logarithmic scale and linear fitting ($N = 10^4$).

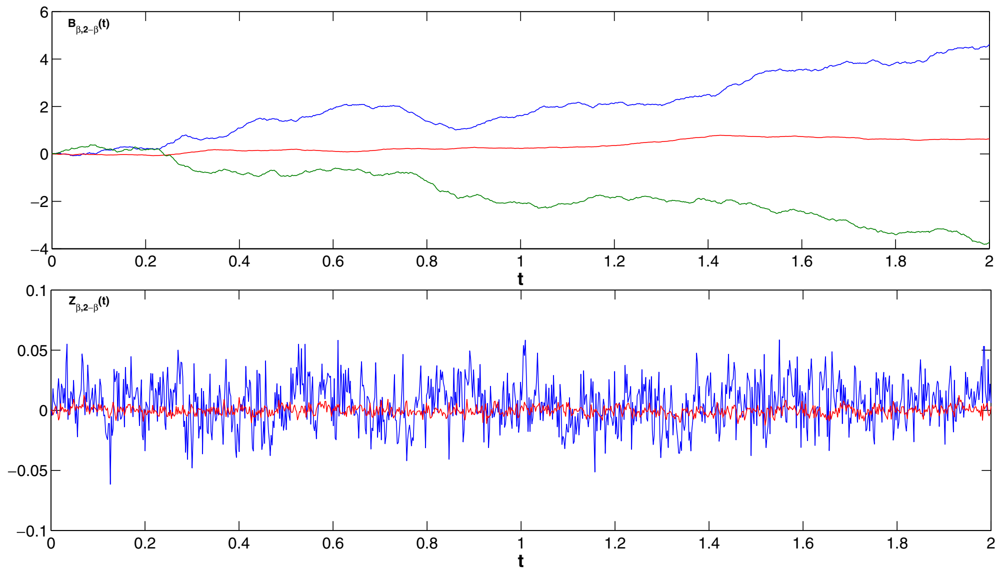

Figure 7. $B_{2-\beta,\beta}(t)$ trajectories in the case $\beta = 0.5$ (top panel) for $0 \leqslant t \leqslant 2$. The corresponding stationary noise time series is presented in the bottom panel.

- Figure 8 collects the histograms in the case $\alpha = 2 - \beta$ at times $t = 1$ and $t = 2$. The super-diffusive behaviour (that is the rapid increasing of the variance in time) is highlighted.
- Figure 9 presents the plot of the sample variance in the logarithmic scale. Even in this case, we evaluated a linear fitting.

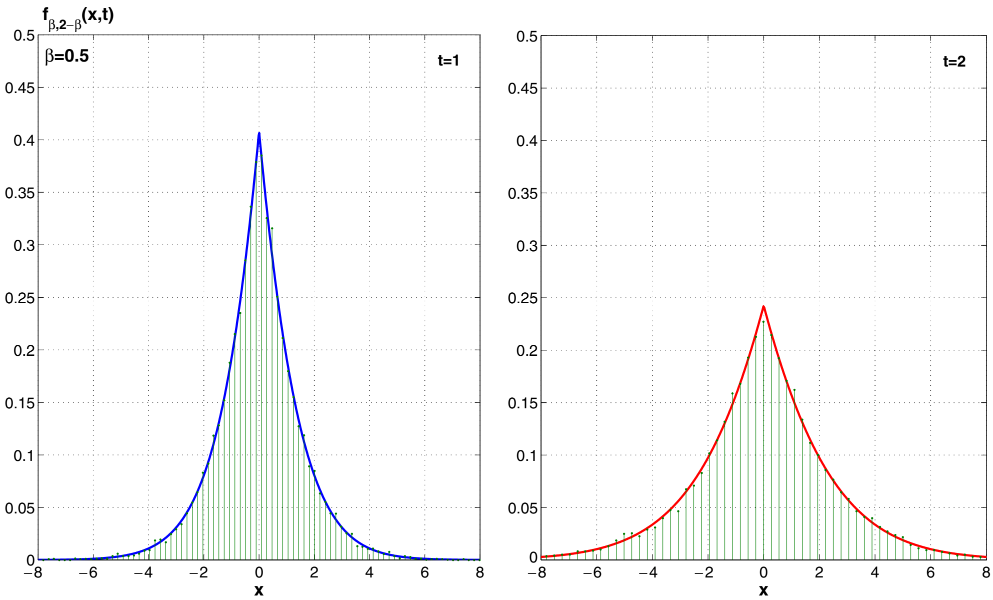

Figure 8. Histograms of two 15 000 running simulations of $B_{2-\beta,\beta}(t)$ with $\beta = 0.5$ and exact distributions at different times $t = 2$ and $t = 1$.

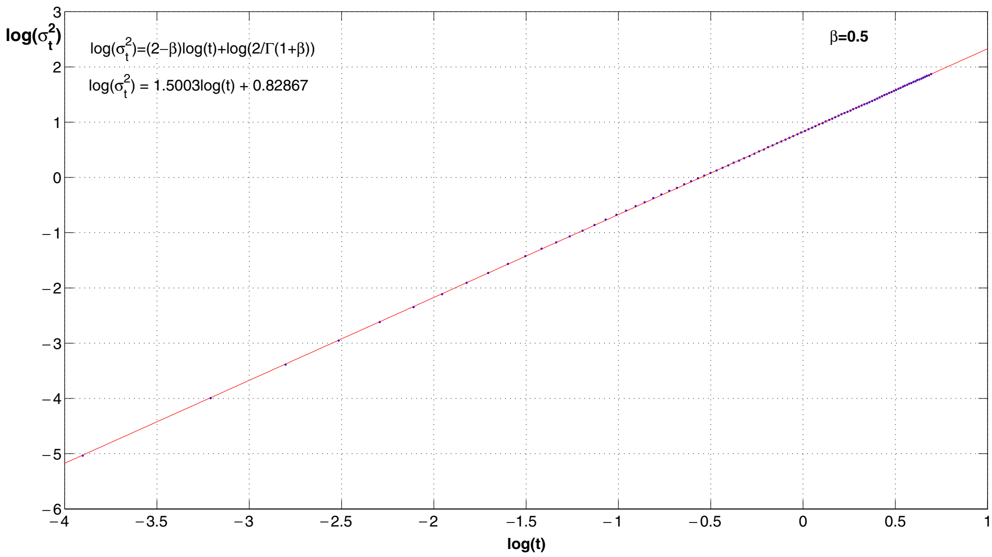

Figure 9. Sample variance in logarithmic scale and linear fitting ($N = 10^4$).

5. Concluding remarks

The marginal probability density function (equation (19)) of the generalized grey Brownian motion $B_{\alpha,\beta}(t), t \geqslant 0$, evolves in time according to a 'stretched' time-fractional diffusion equation of order β (see equation (6)). Therefore, the ggBm serves as a stochastic model for the anomalous diffusion described by these classes of fractional equations.

The ggBm is defined canonically (see equation (14)) in the so-called grey noise space $(\mathcal{S}'(\mathbb{R}), \mathcal{B}, \mu_{\alpha,\beta})$, where the grey noise measure satisfies (9). However, the ggBm is an *H*-**sssi** process of order $H = \alpha$, and proposition 2 provides a characterization of $B_{\alpha,\beta}(t)$ not withstanding the underline probability space.

There are many other processes which serve as stochastic models for a given master equation. In fact, given a master equation for a PDF $f(x,t)$, it is always possible to define an equivalence class of stochastic processes with the same marginal density function $f(x,t)$. The ggBm defines a subclass $\{B_{\alpha,\beta}(t), t \geqslant 0\}$ associated with the non-Markovian equation (6). In this case, the memory effects are enclosed in the typical dependence structure of a *H*-**sssi** process, while, for instance, in the case of a subordinated process (examples 1 and 2), these are due to the memory properties of the *random time process*. The latter are preferable because they provide a ready-made physical interpretation (remark 3). However, $B_{\alpha,\beta}(t)$ is interesting because of the stationarity of its increments.

Proposition 3 provides an enlightened representation of the ggBm. Thus, the ggBm turns out to be merely a fractional Brownian motion with stochastic variance, that is $B_{\alpha,\beta}(t) = \Lambda_\beta X_\alpha(t), t \geqslant 0$, where Λ_β is a suitable independent random variable (see equation (20)). As a final remark, we observe that such a process is not ergodic, as, heuristically, follows by the multiplication with the random variable Λ_β. This also appears from the simulated trajectories. Indeed, it is impossible with a single realization of the system $B_{\alpha,\beta}(t,\omega), \omega \in \Omega$, to distinguish a ggBm from a fBm with variance $2\Lambda_\beta^2(\omega)t^\alpha$, where $\Lambda_\beta(\omega)$ indicates a single realization of the random variable Λ_β.

As a further development of the present research, it is interesting to wonder if the ggBm is the only one stationary increment process which serves as a model for time-fractional diffusion equations like (6).

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Appendix A. The *M*-function

Let us define the function $M_\beta(z), 0 < \beta < 1$, as follows:

$$\begin{aligned} M_\beta(r) &= \sum_{k=0}^{\infty} \frac{(-r)^k}{k!\Gamma[-\beta k + (1-\beta)]} \\ &= \frac{1}{\pi}\sum_{k=0}^{\infty} \frac{(-r)^k}{k!}\Gamma[(\beta(k+1))]\sin[\pi\beta(k+1)], \qquad r \geqslant 0. \end{aligned} \tag{A.1}$$

The above series defines a transcendental function (entire of order $1/(1-\beta/2)$) of the Wright type, introduced by Mainardi in [15, 37] (also see [9, 16]). It is useful to recall some important properties of the M-function. The best way to express these properties is in terms of the function

$$\mathcal{M}_\beta(\tau, t) = t^{-\beta} M_\beta(\tau t^{-\beta}), \qquad \tau, t \geqslant 0,$$

which defines a probability density function in $\tau \geqslant 0$ for any $t \geqslant 0$ and $0 < \beta < 1$.

(i) The following convolution formula holds:

$$\mathcal{M}_\nu(x, t) = \int_0^\infty \mathcal{M}_\eta(x, \tau)\mathcal{M}_\beta(\tau, t)\,\mathrm{d}\tau, \quad \nu = \eta\beta, \quad x \geqslant 0, \tag{A.2}$$

where $\nu, \eta, \beta \in (0, 1)$.

(ii) The Laplace transform of $\mathcal{M}_\beta(\tau, t)$ with respect to t is

$$\mathcal{L}\{\mathcal{M}_\beta(\tau, t); t, s\} = s^{\beta-1}\,\mathrm{e}^{-\tau s^\beta}, \qquad \tau, s \geqslant 0. \tag{A.3}$$

(iii) The Laplace transform of $\mathcal{M}_\beta(\tau, t)$ with respect to τ is

$$\mathcal{L}\{\mathcal{M}_\beta(\tau, t); \tau, s\} = E_\beta(-st^\beta), \qquad t, s \geqslant 0, \tag{A.4}$$

where $E_\beta(x)$ is the Mittag–Leffler function (10).

(iv) The singular limit $\beta \to 1$ gives

$$\mathcal{M}_1(\tau, t) = \delta(\tau - t), \qquad \tau, t \geqslant 0. \tag{A.5}$$

(v) Let $G(x, t)$ be the Gaussian density function; then

$$G(x, t) = \frac{1}{2}\mathcal{M}_{1/2}(|x|, t) = \frac{1}{\sqrt{4\pi t}}\exp\left(-\frac{x^2}{4t}\right). \tag{A.6}$$

References

[1] Ratynskaia S, Rypdal K, Knapek C, Khrapak S, Milovanov A V, Ivlev A, Rasmussen J J and Morfill G E 2006 *Phys. Rev. Lett.* **96** 105010

[2] Gambin Y, Massiera G, Ramos L, Ligoure C and Urbach W 2005 *Phys. Rev. Lett.* **94** 110602

[3] Labeyrie G, Vaujour E, Müller C A, Delande D, Miniatura C, Wilkowski D and Kaiser R 2003 *Phys. Rev. Lett.* **91** 223904

[4] Kou S C and Xie X S 2004 *Phys. Rev. Lett.* **93** 180603

[5] Solomon T H, Weeks E R and Swinney H L 1993 *Phys. Rev. Lett.* **71** 3975

[6] Marty G and Dauchot O 2005 *Phys. Rev. Lett.* **94** 015701

[7] Liu B and Goree J 2007 *Phys. Rev.* E **75** 016405

[8] Gorenflo R and Mainardi F 1997 *Fractals and Fractional Calculus in Continuum Mechanics* ed A Carpinteri and F Mainardi (Wien: Springer) p 223 http://www.fracalmo.org

[9] Mainardi F, Luchko Y and Pagnini G 2001 *Frac. Cal. Appl. Anal.* **4** 153 http://arxiv.org/abs/cond-mat/0702419

[10] Podlubny I 1999 *Fractional Differential Equations* (San Diego: Academic)

[11] Schneider W R 1990 *Dynamics and Stochastic Processes, Theory and Applications (Lecture Notes in Physics* vol 355*)* ed R Lima *et al* (Heidelberg: Springer) p 276

[12] Schneider W R and Wyss W 1989 *J. Math. Phys.* **30** 134

[13] Revuz D and Yor M 1994 *Continuous Martingales and Brownian Motion (A Series of Comprehensive Studies in Mathematics* vol 293*)* (Berlin: Springer)

[14] Molchanov S A and Ostrovskii E 1969 *Theory Probab. Appl.* **14** 128

[15] Mainardi F 1996 *Chaos, Solitons Fractals* **7** 1461

[16] Mainardi F 1997 *Fractals and Fractional Calculus in Continuum mechanics* ed A Carpinteri and F Mainardi (Wien New York: Springer) p 291 http://www.fracalmo.org

[17] Kolsrud T 1990 *Ideas and Methods in Mathematical Analysis, Stochastics and Applications* vol 1 ed S Albeverio *et al* (Cambridge: Cambridge University Press) p 168

[18] Donati-Martin C, Roynette B, Vallois P and Yor M 2008 *Stud. Sci. Math. Hung.* **45** (2) 207–21 DOI:10.1556/SScMath.2007.1033

[19] Meerschaert M, Benson D, Scheffler H and Baeumer B 2002 *Phys. Rev.* E **65** 041103

[20] Metzler R and Klafter J 2000 *Phys. Rep.* **339** 1
[21] Barkai E 2002 *Chem. Phys.* **284** 13
[22] Gorenflo R and Mainardi F 2008 *Anomalous Transport: Foundations and Applications* ed R Klages *et al* (Weinheim: Wiley-VCH) http://arxiv.org/abs/0705.0797
[23] Stanislavsky A A 2003 *Phys. Scr.* **67** 265
[24] Fulger D, Scalas E and Germano G 2008 *Phys. Rev.* E **77** 021122
[25] Bochner S 1955 *Harmonic Analysis and the Theory of Probability* (Berkeley, CA: University of California Press)
[26] Bochner S 1962 *Proc. Natl Acad. Sci. USA* **48** 19
[27] Mura A and Mainardi F 2008 submitted http://arxiv.org/abs/0711.0665
[28] Taqqu M S 2003 *Theory and Applications of Long-Range Dependence* ed P Doukhan *et al* (Basle: Birkäuser) p 5
[29] Schneider W R 1990 *Stochastic Processes, Physics and Geometry* ed S Albeverio *et al* (Singapore: World Scientific) p 676
[30] Schneider W R 1990 *Ideas and Methods in Mathematical Analysis, Stochastics and Applications* vol 1 ed S Albeverio *et al* (Cambrdige: Cambridge University Press) p 261
[31] Mandelbrot B B 1976 *J. Hydrol.* **30** 407
[32] Mandelbrot B B and Van Ness J W 1968 *SIAM Rev.* **10** 422
[33] Schneider W R 1996 *Exposition. Math.* **14** 3
[34] Gorenflo R, Mainardi F, Moretti D and Paradisi P 2002 *Nonlinear Dyn.* **29** 129
[35] Gorenflo R, Mainardi F, Moretti D, Pagnini G and Paradisi P 2002 *Chem. Phys.* **284** 521
[36] Bardet J, Lang G, Oppenheim G, Philippe A and Taqqu M S 2003 *Theory and Applications of Long-Range Dependence* ed P Doukan *et al* (Basle: Birkäuser) p 579
[37] Mainardi F 1996 *Appl. Math. Lett.* **9** 23