Two-particle anomalous diffusion: Probability density functions and self-similar stochastic processes

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Two-particle dispersion is investigated in the context of the Anomalous Diffusion. Two different modelling approaches related to time-subordination are considered and unified in the framework of self-similar stochastic processes. By assuming a single-particle fractional Brownian motion and the two-particle correlation function decreasing in time with a power law, the particle relative separation density is computed for the cases with time-subordination directed by a unilateral M-Wright density and by an extremal Lévy stable density. Looking for advisable mathematical properties (for instance, the stationarity of the increments), the corresponding self-similar stochastic processes are represented in terms of fractional Brownian motions with stochastic variance, whose profile is modelled by using the M-Wright density or the Lévy stable density.

Key words: Two-particle diffusion, anomalous diffusion, self-similar stochastic processes, Brownian motion, fractional Brownian motion, generalized grey Brownian motion, M-Wright function, Lévy stable density.

1. Introduction

Diffusion phenomena occur in many natural systems and they are investigated in several disciplines. In particular, to study diffusion is important to compute the statistics of a tracer concentration field $\theta(x,t)$. In fact, let $p(x;t|y,t_0)$ be the probability density function (PDF) of finding a particle in x at time t knowing that it was in y at time t_0 and let $S(y,t_0)$ be the initial tracer source, then it is well-known that for the single-particle diffusion the mean value of the tracer

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Phil. Trans. R. Soc. A 1–15; doi: 10.1098/rspa.00000000

concentration field $\langle\theta\rangle$ is

$$\langle\theta(x,t)\rangle = \int p(x;t|y,t_0)S(y,t_0)\,dy\,dt_0\,, \quad t_0 \le t\,, \tag{1.1}$$

and for the two-particle diffusion the two-point covariance is

$$\langle\theta(x_1,t_1)\theta(x_2,t_2)\rangle = \int p(x_1,x_2;t_1,t_2|y_1,y_2,t_{01},t_{02}) \times S(y_1,t_{01})S(y_2,t_{02})\,dy_1dy_2\,dt_{01}dt_{02}\,, \quad t_{01} \le t_1\,, \quad t_{02} \le t_2\,. \tag{1.2}$$

Studying two-particle separation is of paramount importance in applied sciences because it is related to the local fluctuations of the concentration field $\theta' = \theta - \langle\theta\rangle$, whose variance, i.e.,

$$\langle\theta'^2(x,t)\rangle = \langle\theta^2(x,t)\rangle - \langle\theta(x,t)\rangle^2\,, \tag{1.3}$$

is strongly relevant for what concerns, for example, the overcoming of a safe concentration threshold in industrial accidents (Nielsen et al., 2002) or the segregation coefficient in non-premixed reacting mixtures (Komori et al., 1991).

In the formula of the concentration fluctuation variance (1.3), $\langle\theta^2(x,t)\rangle$ is obtained from (1.2) by setting $x_1 = x_2 = x$ and $t_1 = t_2 = t$, then it emerges to be established by the *backward diffusion* of two particles with very close initial positions, in the limit $x_1 = x_2 = x$, at the instant $t_1 = t_2 = t$ and the separation is estimated at $t_{01} = t_{02} = t_0 < t$ (Sawford, 2001). Hereinafter the dependence on the initial condition of the PDFs will be dropped because initial particle positions are assumed to be coincident and stated equal to 0.

From (1.2) it follows that diffusion differences generate different quantitative results, which are important in the applied problems connected to concentration fluctuations. Diffusive processes are generally classified as *normal* when particle displacement variance grows linearly in time and otherwise classified as *anomalous*. Moreover, normal diffusion is associated also to the Gaussian PDF for particle displacement and, by using the stochastic process terminology, normal diffusion is also called Brownian motion (Bm). A Gaussian anomalous diffusion can be obtained from normal diffusion by assuming a diffusion coefficient dependent on time. This can lead, for instance, to a Gaussian process like the *fractional Brownian motion* (fBm) that generalizes the standard Brownian motion.

Anomalous diffusion appears in several different fields and Fractional Calculus emerged to be a powerful tool to manage memory effects and long range dependence (Baleanu et al., 2012). Recently, fractional systems have been investigated in their dynamic evolution by Lyapunov exponent analysis (Li et al., 2010) as well as to encode memory in nuclear magnetic resonance phenomena (Magin et al., 2009; Bhalekar et al., 2011).

Anomalous diffusion is named *fast diffusion*, when the variance of the particle spreading grows according to a power law with exponent greater than 1, and *slow diffusion*, when such exponent is lower than 1.

In this paper, two-particle diffusion is analyzed in the context of *Anomalous Diffusion*.

A physical idea useful to model anomalous diffusion is related to time-subordination of the Gaussian process. The resulting PDF is no longer Gaussian and the particle displacement variance grows no longer linearly in time. In this paper two modelling approaches of anomalous diffusion based on time-subordination are discussed and unified into the framework of self-similar stochastic processes by showing that the resulting one-time PDFs share the same integral representation. The two time-subordination mechanisms are the parent-directing process (Feller, 1971) and the product of two independent random variables (Mainardi et al., 2003, 2006).

The paper is organized as follows. In Section 2, the two time-subordination mechanisms, namely the parent-directing process and the product of random variables, are introduced and unified in the context of self-similar stochastic processes. In Section 3, two-particle anomalous diffusion is studied by assuming a fractional Brownian motion for single-particle trajectory and a correlation function decreasing in time with a power law. In Section 4, the resulting integral representations of the one-time PDFs are evaluated and the representations in terms of H-function and by series are given together with their asymptotic behaviours. In Section 5, a class of stochastic processes are chosen to model the two-particle anomalous diffusion corresponding to the derived PDFs. In Section 6, conclusions are discussed.

2. Two time-subordination mechanisms and their unification for self-similar stochastic processes

(a) *The parent-directing subordination process*

At the microscopic level, time-subordination is defined as a process $X(t) = Y(T(t))$ that is obtained by randomizing the time clock of a stochastic process $Y(\tau)$ using a new clock $\tau = T(t)$, where $T(t)$ is a random process with non-negative increments, see e.g. (Feller, 1971).

The resulting process $Y(T(t))$ is said to be subordinated to $Y(\tau)$, which is called the *parent process*, and is directed by $T(t)$, which is called the *directing process*. The time variable τ is often referred to as the *operational time*. The process $t = t(\tau)$, inverse of $\tau = T(t)$, is called the *leading process* and it plays a fundamental role in the parametric approach, introduced by Gorenflo and Mainardi (2011, 2012), to simulate fractional diffusion processes. Even if the parent process $Y(\tau)$ is Markovian, the resulting subordinated process $X(t)$ is in general non-Markovian and the non-local memory effects are due to the random time process $\tau = T(t)$ and to its evolution, which is in general non-local in time.

At the macroscopic-level, i.e., in terms of the particle PDF, the time-subordination is embodied by the following integral formula

$$p(x;t) = \int_0^\infty \mathcal{G}(x;\tau)\,\varphi(\tau;t)\,d\tau\,, \qquad (2.1)$$

where $\mathcal{G}(x;\tau)$ is the PDF (of x evolving in τ) of the parent process, and $\varphi(\tau,t)$ is the PDF (of τ evolving in t) of the directing process.

(b) Independent random variables product and the time-subordination integral

It is well-known that the PDF of the product of two independent random variables is given by the Mellin convolution[1] of the two corresponding PDFs (Mainardi et al., 2003, 2006). Let Z_1 and Z_2 be two real independent random variables whose PDFs are $p_1(z_1)$ and $p_2(z_2)$, respectively, with $z_1 \in R$ and $z_2 \in R^+$. Then, the joint PDF is $p(z_1, z_2) = p_1(z_1)p_2(z_2)$. Let Z be the random variable obtained by the product of Z_1 and Z_2^γ, i.e.,

$$Z = Z_1\, Z_2^\gamma\,, \tag{2.2}$$

so that $z = z_1 z_2^\gamma$, then, carrying out the variable transformations $z_1 = z/\xi^\gamma$ and $z_2 = \xi$, it follows that $p(z,\tau)dzd\xi = p_1(z/\xi^\gamma)p_1(\tau)Jdzd\xi$, where $J = 1/\xi^\gamma$ is the Jacobian of the transformation. Integrating in $d\xi$, the PDF of Z emerges to be

$$p(z) = \int_0^\infty p_1\left(\frac{z}{\xi^\gamma}\right) p_2(\xi)\, \frac{d\xi}{\xi^\gamma}\,. \tag{2.3}$$

By applying the changes of variable $z = xt^{-\gamma\omega}$ and $\xi = \tau t^{-\omega}$, the typical time-subordination integral (2.1) is recovered from (2.3) by setting

$$\frac{1}{t^{\gamma\omega}} p\left(\frac{x}{t^{\gamma\omega}}\right) = p(x;t)\,, \quad \frac{1}{\tau^\gamma} p_1\left(\frac{x}{\tau^\gamma}\right) = \mathcal{G}(x;\tau)\,, \quad \frac{1}{t^\omega} p_2\left(\frac{\tau}{t^\omega}\right) = \varphi(\tau;t)\,. \tag{2.4}$$

(c) Unification of time-subordination mechanisms for self-similar stochastic processes

A process $W(t)$, $t \ge 0$, is a self-similar process with self-similarity exponent H (Hurst exponent) if, for all $a > 0$, the processes $W(at)$ and $a^H W(t)$ have the same finite-dimensional distributions.

If the parameter a is turned into a random variable, by setting $Y(\tau) = W(\tau)$ and $T(t) = at$, according to definitions given in §2(a), so that $X(t) = Y(T(t)) = W(at)$, and by setting $Z = Z_1 Z_2^\gamma = a^H W(t)$, according to definitions given in §2(b), it is recovered a time-subordination where the parent process is a self-similar process and the operational time is simply a line with stochastic slope.

Then, in the case described above, both mechanisms, i.e., explicit time-subordination with a stochastic operational time and product of random variables, can be seen as equivalent in the context of subordinated processes.

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[1] The Mellin transform pair $\psi(r) \stackrel{\mathcal{M}}{\longleftrightarrow} \psi^*(s)$, with $r \in R^+$ and $s \in C$, is defined by

$$\psi^*(s) = \int_0^\infty \psi(r)\, r^{s-1}\, dr\,, \quad \psi(r) = \frac{1}{2\pi i}\int_{\sigma - i\infty}^{\sigma + i\infty} \psi^*(s) r^{-s}\, ds\,, \quad \sigma = \mathrm{Re}(s)\,. \tag{N1}$$

The transformed function $\psi^*(s)$ exists if the integral $\int_0^\infty |\psi(r)| r^{s-1}\, dr$ is bounded and this constraint is met in the vertical strip $a < \sigma = \mathrm{Re}(s) < b$, where the boundary values a and b follow from the analytic structure of $\psi(r)$ provided that $|\psi(r)| \le Mr^{-a}$ when $r \to 0^+$ and $|\psi(r)| \le Mr^{-b}$ when $r \to +\infty$. The Mellin convolution integral corresponds to the pair

$$\psi(r) = \int_0^\infty f\left(\frac{r}{\xi}\right) g(\xi)\, \frac{d\xi}{\xi} \stackrel{\mathcal{M}}{\longleftrightarrow} f^*(s) g^*(s) = \psi^*(s)\,. \tag{N2}$$

(d) The M-Wright and Lévy directing processes

Two noteworthy examples of PDFs for anomalous diffusion are obtained, *despite the effective microscopic stochastic formulation*, by subordination-type integral (2.1) ot (2.3) of the Markovian Bm, with PDF

$$\mathcal{G}(x;t) = \frac{1}{\sqrt{4\pi t}} \exp\left\{-\frac{x^2}{4t}\right\}, \tag{2.5}$$

and variance $\langle x^2 \rangle = 2t$, by selecting as PDF of the directing process either a unilateral M-Wright function, as introduced in the so-called *generalized grey Brownian motion* (ggBm) (Mura, 2008; Mura and Pagnini, 2008; Mura and Mainardi, 2009), named also Erdélyi–Kober fractional diffusion (Pagnini, 2012; Pagnini et al., 2012), or an extremal Lévy stable density, as considered in (Mainardi et al., 2001). In fact, in the former case, for $0 < \beta \leq 1$ and $0 < \alpha < 2$, it holds (Pagnini, 2012)

$$\begin{aligned} p_M(x;t) &= \int_0^\infty \frac{1}{\sqrt{4\pi\tau}} \exp\left\{-\frac{x^2}{4\tau}\right\} M_\beta\left(\frac{\tau}{t^\alpha}\right) \frac{d\tau}{t^\alpha} \\ &= \frac{1}{t^{\alpha/2}} \int_0^\infty \frac{1}{\sqrt{4\pi\xi}} \exp\left\{-\frac{(xt^{-\alpha/2})^2}{4\xi}\right\} M_\beta(\xi)\, d\xi \\ &= \frac{1}{2\, t^{\alpha/2}} M_{\beta/2}\left(\frac{|x|}{t^{\alpha/2}}\right), \end{aligned} \tag{2.6}$$

which includes as special cases the fBm for $\beta = 1$, the grey Brownian motion, in the sense of Schneider (1990, 1992), for $0 < \alpha = \beta < 1$, and the Bm for $\alpha = \beta = 1$ (Mainardi et al., 2010). In the latter case, for $0 < \alpha \leq 2$, we have (Mainardi et al., 2003, 2006)

$$\begin{aligned} p_L(x;t) &= \int_0^\infty \frac{1}{\sqrt{4\pi\tau}} \exp\left\{-\frac{x^2}{4\tau}\right\} L_{\alpha/2}^{-\alpha/2}\left(\frac{\tau}{t^{2/\alpha}}\right) \frac{d\tau}{t^{2/\alpha}} \\ &= \frac{1}{t^{1/\alpha}} \int_0^\infty \frac{1}{\sqrt{4\pi\xi}} \exp\left\{-\frac{(xt^{-1/\alpha})^2}{4\xi}\right\} L_{\alpha/2}^{-\alpha/2}(\xi)\, d\xi \\ &= \frac{1}{t^{1/\alpha}} L_\alpha^0\left(\frac{x}{t^{1/\alpha}}\right). \end{aligned} \tag{2.7}$$

The function M_ν (with $0 < \nu \leq 1$) is the so-called M-Wright function, also named Mainardi function, and L_α^θ is the Lévy stable density of order $\alpha \in 0, 2]$ and asymmetry parameter $|\theta| \leq \min\{\alpha, 2-\alpha\}$, which is symmetric for $\theta = 0$ and one-sided on the positive semi-axis for $\theta = -\alpha$ $(0 < \alpha < 1)$. These functions can be defined respectively by their Mellin transform pairs (N1) as, see Eq. (6.1) in (Mainardi et al., 2003),

$$M_\nu(r) \overset{\mathcal{M}}{\longleftrightarrow} \frac{\Gamma[1+(s-1)]}{\Gamma[1+\nu(s-1)]}, \quad 0 < \nu < 1, \quad 0 < r < \infty, \tag{2.8}$$

and, see Eq. (5.1) in (Mainardi et al., 2003),

$$L_\alpha^\theta(r) \stackrel{\mathcal{M}}{\longleftrightarrow} \frac{1}{\alpha} \frac{\Gamma\left(-\dfrac{s-1}{\alpha}\right)\Gamma(1+(s-1))}{\Gamma(1+\rho(s-1))\Gamma(-\rho(s-1))}\,, \quad \rho = \frac{\alpha-\theta}{2\alpha}\,, \quad 0 < r < \infty\,. \tag{2.9}$$

It is reminded here that the symmetric M-Wright function and the Lévy stable density provide the Green functions of the time-fractional and the space-fractional diffusion equations, respectively (Mainardi et al., 2001).

3. Two-particle anomalous diffusion

The problem of two-particle diffusion can be restated taking into account the single-particle motion and the relative separation between the particles. In terms of PDF it means $p(x_1, x_2; t)\, dx_1\, dx_2 = p(x, \delta r; t)\, dx\, d\delta r$, after the change of variable $x_1 = x$ and $x_2 = x - \delta r$.

However, following turbulent dispersion literature (Durbin, 1980; Thomson, 1990), the problem of two-particle diffusion can be analyzed in terms of the particle separation $\delta r = x_1 - x_2$ and of the centre-of-mass position $x_{CM} = (x_1 + x_2)/2$ that, for mathematically convenience (i.e., the Jacobian of the variable trasformation is equal to 1), are transformed into: $\Delta = (x_1 - x_2)/\sqrt{2}$ and $\Sigma = (x_1 + x_2)/\sqrt{2}$.

Since the two particles are identical, it holds $\langle x_1^2 \rangle = \langle x_2^2 \rangle = \sigma^2$ and in general their motion is correlated $\langle x_1 x_2 \rangle = \sigma^2 \rho$, then the joint Gaussian PDF is

$$\begin{aligned}
\mathcal{G}(x_1, x_2; t) &= \frac{1}{2\pi\sigma^2\sqrt{1-\rho^2}} \exp\left\{-\frac{x_1^2 - 2\rho x_1 x_2 + x_2^2}{2\sigma^2(1-\rho^2)}\right\} \\
&= \frac{1}{\sqrt{2\pi\sigma^2(1-\rho)}} \exp\left\{-\frac{\Delta^2}{2\sigma^2(1-\rho)}\right\} \times \\
&\qquad \frac{1}{\sqrt{2\pi\sigma^2(1+\rho)}} \exp\left\{-\frac{\Sigma^2}{2\sigma^2(1+\rho)}\right\} = \mathcal{G}(\Delta, \Sigma; t)\,,
\end{aligned} \tag{3.1}$$

so that $\mathcal{G}(\Delta, \Sigma; t) = \mathcal{G}(\Delta; t)\mathcal{G}(\Sigma; t)$ and the following three normalization conditions hold: $\int \mathcal{G}(x_1, x_2; t)\, dx_1 dx_2 = 1$, $\int G(\Delta; t)\, d\Delta = 1$ and $\int \mathcal{G}(\Sigma; t)\, d\Sigma = 1$. From (3.1) it follows that $\langle \Delta^2 \rangle = \sigma^2(1-\rho)$ and $\langle \Sigma^2 \rangle = \sigma^2(1+\rho)$.

Assuming that, before the Einstein regime, i.e., $\sigma^2 = 2t$ for $t \gg 1$, the trajectories x_1 and x_2 follows a fBm, then the same holds for x, and assuming also that the correlation function decreases in time according to a power law then

$$\begin{cases} \sigma^2 \simeq 2\, t^q\,, & t \ll 1\,, \quad 0 < q < 2\,, \\ \sigma^2 \simeq 2\, t\,, & t \gg 1\,, \end{cases} \quad , \quad \begin{cases} \rho \simeq 1 - t^\zeta\,, & t \ll 1\,, \quad \zeta \geq 0\,, \\ \rho \simeq 0\,, & t \gg 1\,. \end{cases} \tag{3.2}$$

What concerns the particle separation type variable Δ it holds

$$\begin{cases} \langle\Delta^2\rangle = \sigma^2(1-\rho) \simeq 2\,t^\mu\,, \quad t \ll 1\,, \quad \mu = q+\zeta > 0\,, \\ \langle\Delta^2\rangle = \sigma^2(1-\rho) \simeq 2\,t\,, \quad\ \ t \gg 1\,. \end{cases} \tag{3.3}$$

It is worth noting to remark that the regime established for $t \ll 1$ in (3.3) is a generalization of that in the most common Ornstein–Uhlenbeck process, i.e., the combination of the ballistic regime $\sigma^2 \simeq t^2$ with the exponential correlation function $\rho = e^{-t} \simeq 1-t$ so that $\sigma^2(1-\rho) \simeq t^3$.

On the other side, for what concerns the center-of-mass type variable Σ, it emerges that in the considered context its variance is $\langle\Sigma^2\rangle = \sigma^2(1+\rho) \simeq 4\,t^\mu\left(\dfrac{1}{t^\zeta} - \dfrac{1}{2}\right)$, when $t \ll 1$, and $\langle\Sigma^2\rangle = 2\,t$, when $t \gg 1$, so that the simple power law scaling when $t \ll 1$ is lost.

Hence, in the range $t \ll 1$, it results that, according to the notation introduced at the beginning of the section, i.e., $x = x_1$, Σ and $\Delta = \delta r/\sqrt{2}$, it holds

$$\mathcal{G}(x;t) = \mathcal{G}_q(x;t) = \frac{1}{\sqrt{4\pi t^q}} \exp\left\{-\frac{x^2}{4\,t^q}\right\}\,, \tag{3.4}$$

and

$$\mathcal{G}(\Sigma;t) = \mathcal{G}_{\mu,\zeta}(\Sigma;t) = \frac{1}{\sqrt{2\pi\langle\Sigma^2\rangle}} \exp\left\{-\frac{\Sigma^2}{2\,\langle\Sigma^2\rangle}\right\}\,, \quad \langle\Sigma^2\rangle \simeq 4\,t^\mu\left(\frac{1}{t^\zeta} - \frac{1}{2}\right)\,, \tag{3.5}$$

$$\mathcal{G}(\Delta;t) = \mathcal{G}_\mu(\Delta;t) = \frac{1}{\sqrt{4\pi t^\mu}} \exp\left\{-\frac{\Delta^2}{4\,t^\mu}\right\}\,. \tag{3.6}$$

However, since the center-of-mass motion is a single-point trajectory then, in agreement with the assumed single-particle trajectory for x_1 and x_2, it is governed by the fBm and its time-dependent diffusion coefficient is $\mathcal{D}_\Sigma(t) = \dfrac{1}{2}\dfrac{d\langle\Sigma^2\rangle}{dt}$, but the two-point trajectory Δ can have long range correlation and show an anomalous diffusion. Then, hereinafter, the analysis is performed solely for $\Delta = \delta r/\sqrt{2} = (x_1 - x_2)/\sqrt{2}$. Such non-local memory effects can be modelled by the subordination integral (2.1) and, in this framework, the PDF of particle relative separation emerges to be determined by

$$p(\Delta;t) = \int_0^\infty \mathcal{G}_\mu(\Delta;\tau)\,\varphi(\tau;t)\,d\tau\,. \tag{3.7}$$

Finally, adopting the same directing processes of formulae (2.6) and (2.7), the resulting PDFs for the two-particle anomalous diffusion emerge to be, with $0 < \beta \le 1$ and $0 < \alpha < 2$,

$$\begin{aligned} P_M(\Delta;t) &= \int_0^\infty \frac{1}{\sqrt{4\pi\tau^\mu}} \exp\left\{-\frac{\Delta^2}{4\,\tau^\mu}\right\} M_\beta\left(\frac{\tau}{t^\alpha}\right) \frac{d\tau}{t^\alpha} \\ &= \frac{1}{t^{\mu\alpha/2}} \int_0^\infty \frac{1}{\sqrt{4\pi\xi^\mu}} \exp\left\{-\frac{(\Delta t^{-\mu\alpha/2})^2}{4\,\xi^\mu}\right\} M_\beta(\xi)\,d\xi\,, \end{aligned} \tag{3.8}$$

and

$$P_L(\Delta;t) = \int_0^\infty \frac{1}{\sqrt{4\pi\tau^\mu}} \exp\left\{-\frac{\Delta^2}{4\,\tau^\mu}\right\} L_{\alpha/2}^{-\alpha/2}\left(\frac{\tau}{t^{2/\alpha}}\right) \frac{d\tau}{t^{2/\alpha}}$$

$$= \frac{1}{t^{\mu/\alpha}} \int_0^\infty \frac{1}{\sqrt{4\pi\xi^\mu}} \exp\left\{-\frac{(\Delta t^{-\mu/\alpha})^2}{4\,\xi^\mu}\right\} L_{\alpha/2}^{-\alpha/2}(\xi)\, d\xi\,. \quad (3.9)$$

Clearly if anomalous diffusion is assumed also for the single-particle trajectory x, the analysis follows from the present one by setting $\mu=q$. Moreover it is important to highlight here also that, if the single-particle trajectory is assumed to be Gaussian, i.e., $q=1$, then in the anomalous diffusion framework the PDF of x is given by (2.6) or (2.7) depending on the selected directing process.

4. Evaluation, representations and asymptotic behaviour of the P_M and of the P_L PDFs

(*a*) *The P_M PDF*

What concerns the determination of the P_M PDF defined in (3.8), by applying the Mellin transform (N1) to the first line of (3.8) and the change of variable $\Delta^2 = 4\tau^\mu\xi$, the RHS becomes

$$\frac{1}{2}\frac{2^{s-1}}{\sqrt{\pi}} \int_0^\infty \mathrm{e}^{-\xi}\xi^{s/2-1}\, d\xi \int_0^\infty M_\beta\left(\frac{\tau}{t^\alpha}\right) \tau^{\mu(s-1)/2}\,\frac{d\tau}{t^\alpha}\,. \quad (4.1)$$

Then, by the change of variable $\tau = t^\alpha z$ and reminding the Gamma function definition, i.e., $\Gamma(s) = \int_0^\infty \mathrm{e}^{-\xi}\xi^{s-1}\, d\xi$, expression (4.1) turns into

$$\frac{t^{\alpha\mu(s-1)/2}}{2}\frac{2^{s-1}}{\sqrt{\pi}}\,\Gamma\left(\frac{s}{2}\right) \int_0^\infty M_\beta(z)\, z^{\mu(s-1)/2}\, dz\,. \quad (4.2)$$

To conclude, by the Gamma function property $\Gamma(s)\Gamma(s+1/2) = 2^{1-2s}\sqrt{\pi}\,\Gamma(s)$ and the Mellin transform pair for the M-Wright function (2.8), after the Mellin inverse transformation (N1), the Mellin–Barnes integral representation of the P_M PDF is

$$P_M(\Delta;t) = \frac{1}{2t^{\alpha\mu/2}}\,\frac{1}{2\pi i}\int_{\mathcal{L}} \frac{\Gamma(s)\,\Gamma\left(1-\frac{\mu}{2}+\frac{\mu}{2}s\right)}{\Gamma\left(\frac{1}{2}+\frac{s}{2}\right)\,\Gamma\left(1-\frac{\beta\mu}{2}+\frac{\beta\mu}{2}s\right)} \left(\frac{\Delta}{t^{\alpha\mu/2}}\right)^{-s} ds\,, \quad (4.3)$$

where $\mathcal{L}$ is the contour path encircling the poles of $\Gamma(s)$ and those of $\Gamma(1-\mu/2+\mu s/2)$.

In terms of H-function (see Appendix), when $|\Delta/t^{\alpha\mu/2}| \to 0$, the density P_M is

$$P_M(\Delta;t) = \frac{1}{2t^{\alpha\mu/2}}\, H^{2,0}_{2,2}\left[\frac{\Delta}{t^{\alpha\mu/2}}\,\middle|\, \begin{array}{c} -;\left(\frac{1}{2},\frac{1}{2}\right),\left(1-\beta\frac{\mu}{2},\beta\frac{\mu}{2}\right) \\ (0,1),\left(1-\frac{\mu}{2},\frac{\mu}{2}\right);- \end{array}\right], \tag{4.4}$$

and, by applying the residue theorem, the series representation of (4.3) is

$$P_M(\Delta;t) = \frac{1}{2t^{\alpha\mu/2}}\left\{\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{\Gamma\left(1-\frac{\mu}{2}-\frac{\mu}{2}k\right)}{\Gamma\left(\frac{1}{2}-\frac{k}{2}\right)\Gamma\left(1-\frac{\beta\mu}{2}-\frac{\beta\mu}{2}k\right)}\left(\frac{\Delta}{t^{\alpha\mu/2}}\right)^k + \right.$$

$$\left.\frac{2}{\mu}\left(\frac{\Delta}{t^{\alpha\mu/2}}\right)^{2/\mu-1}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{\Gamma\left(1-\frac{2}{\mu}-\frac{2}{\mu}k\right)}{\Gamma\left(1-\frac{1}{\mu}-\frac{k}{\mu}\right)\Gamma(1-\beta-\beta k)}\left(\frac{\Delta}{t^{\alpha\mu/2}}\right)^{2k/\mu}\right\}. \tag{4.5}$$

The asymptotic behaviour for $|\Delta/t^{\alpha\mu/2}| \to +\infty$ can be computed by formula (A.3) and it emerges to be of exponential type as follows

$$P_M(\Delta;t) \simeq \frac{1}{2\,t^{\alpha\mu/2}}\,\mathcal{O}\left\{\left(\frac{\Delta}{t^{\alpha\mu/2}}\right)^{-\Omega/(1+\Omega)}\right\}\exp\left\{-\Theta\left(\frac{\Delta}{2\,t^{\alpha\mu/2}}\right)^{2/(1+\Omega)}\right\}, \tag{4.6}$$

where

$$\Omega = \mu(1-\beta)\,, \quad \Theta = (1+\Omega)\,(\beta\mu)^{-\Omega/(1+\Omega)}\,\beta^{\mu/(1+\Omega)}\,.$$

(b) The P_L PDF

The determination of the P_L PDF defined in (3.9) is analog to the determination of the PDF P_M. Actually, by applying the Mellin transform (N1) to the first line of (3.9) and after the change of variable $\Delta^2 = 4\tau^\mu\xi$, the RHS becomes

$$\frac{1}{2}\frac{2^{s-1}}{\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-\xi}\xi^{s/2-1}\,d\xi\int_0^\infty L_{\alpha/2}^{-\alpha/2}\left(\frac{\tau}{t^{2/\alpha}}\right)\tau^{\mu(s-1)/2}\,\frac{d\tau}{t^{2/\alpha}}\,. \tag{4.7}$$

Then, by the change of variable $\tau = t^{2/\alpha}z$ and using the Gamma function definition, expression (4.7) becomes

$$\frac{t^{\mu(s-1)/\alpha}}{2}\frac{2^{s-1}}{\sqrt{\pi}}\,\Gamma\left(\frac{s}{2}\right)\int_0^\infty L_{\alpha/2}^{-\alpha/2}(z)\,z^{\mu(s-1)/2}\,dz\,. \tag{4.8}$$

To conclude, by the Gamma function property $\Gamma(s)\Gamma(s+1/2) = 2^{1-2s}\sqrt{\pi}\,\Gamma(s)$ and the Mellin transform pair for the Lévy stable density (2.9), after the Mellin inverse transformation (N1), the Mellin–Barnes integral representation of the PDF P_L is

$$P_L(\Delta;t) = \frac{1}{\alpha t^{\mu/\alpha}}\,\frac{1}{2\pi i}\int_{\mathcal{L}}\frac{\Gamma(s)\,\Gamma\left(\frac{\mu}{\alpha}-\frac{\mu}{\alpha}s\right)}{\Gamma\left(\frac{\mu}{2}-\frac{\mu}{2}s\right)\,\Gamma\left(\frac{1}{2}+\frac{s}{2}\right)}\left(\frac{\Delta}{t^{\mu/\alpha}}\right)^{-s}ds\,, \tag{4.9}$$

where $\mathcal{L}$ is the contour path encircling the poles of $\Gamma(s)$.

In terms of H-function (see Appendix), it holds

$$P_L(\Delta;t) = \frac{1}{\alpha t^{\mu/\alpha}} H^{1,1}_{2,2}\left[\frac{\Delta}{t^{\mu/\alpha}}\left|\begin{array}{c}\left(1-\frac{\mu}{\alpha},\frac{\mu}{\alpha}\right);\left(\frac{1}{2},\frac{1}{2}\right)\\ \\ (0,1);\left(1-\frac{\mu}{2},\frac{\mu}{2}\right)\end{array}\right.\right], \quad \left|\frac{\Delta}{t^{\mu/\alpha}}\right| \to 0\,, \qquad (4.10)$$

and

$$P_L(\Delta;t) = \frac{1}{\alpha t^{\mu/\alpha}} H^{1,1}_{2,2}\left[\frac{t^{\mu/\alpha}}{\Delta}\left|\begin{array}{c}(1,1);\left(\frac{\mu}{2},\frac{\mu}{2}\right)\\ \\ \left(\frac{\mu}{\alpha},\frac{\mu}{\alpha}\right);\left(\frac{1}{2},\frac{1}{2}\right)\end{array}\right.\right], \quad \left|\frac{\Delta}{t^{\mu/\alpha}}\right| \to +\infty\,. \qquad (4.11)$$

Then, by applying the residue theorem, the corresponding series representations of (4.9) are

$$p_M(\Delta;t) = \frac{1}{\alpha t^{\mu/\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{\Gamma\left(\frac{\mu}{\alpha}+\frac{\mu}{\alpha}k\right)}{\Gamma\left(\frac{\mu}{2}+\frac{\mu}{2}k\right)\Gamma\left(\frac{1}{2}-\frac{k}{2}\right)} \left(\frac{\Delta}{t^{\mu/\alpha}}\right)^k, \qquad (4.12)$$

when $|\Delta/t^{\mu/\alpha}| \to 0$, and

$$P_L(\Delta;t) = \frac{1}{\mu t^{\mu/\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{\Gamma\left(1+\frac{\alpha}{\mu}k\right)}{\Gamma\left(1+\frac{\alpha}{2\mu}k\right)\Gamma\left(-\frac{\alpha}{2}k\right)} \left(\frac{\Delta}{t^{\mu/\alpha}}\right)^{-\alpha k/\mu-1}, \qquad (4.13)$$

when $|\Delta/t^{\mu/\alpha}| \to +\infty$.

5. H-sssi processes for two-particle anomalous diffusion

In order to choose a class of stochastic processes to model two-particle anomalous diffusion with PDFs according to (3.8) and (3.9), the same approach introduced by Mura (2008) (see also Mura and Pagnini, 2008; Mura and Mainardi, 2009) to characterize the so-called generalized grey Brownian motion (ggBm) is adopted.

The ggBm is a class of H-sssi processes, where sssi means self-similar with stationary increments, that generalize Gaussian processes (which are recovered as a special case) and defined by only the autocovariance structure. This property can be easily deduced by noting that the ggBm can be represented by a process $\sqrt{\Lambda_\beta}\, X_\alpha(t)$, $t \geq 0$, where $X_\alpha(t)$ is a Gaussian stochastic process and Λ_β is a suitable chosen independent non-negative random variable.

In fact, let $B_{\alpha,\beta}(t)$, $t \geq 0$, be a ggBm, then

$$B_{\alpha,\beta}(t) \stackrel{d}{=} \sqrt{\Lambda_\beta}\, X_\alpha(t)\,, \quad t \geq 0\,, \quad 0 < \alpha < 2\,, \quad 0 < \beta \leq 1\,, \qquad (5.1)$$

where the symbol $\stackrel{d}{=}$ denotes the equality of the finite-dimensional distribution, the stochastic process $X_\alpha(t)$ is a standard fBm with Hurst exponent $\alpha/2$ and Λ_β is an independent non-negative random variable with PDF $M_\beta(\tau)$, $\tau \geq 0$.

Representation (5.1) can be backwardly obtained from subordination definition given in §2(b). In fact, from comparing (2.3) and (2.4) with (2.6) it follows that $Z = Xt^{-\alpha/2}$ and, since $Z = Z_1 Z_2^\gamma$, it holds $X = Z_1 t^{\alpha/2} Z_2^\gamma$, where $\gamma = 1/2$, the variable Z_1 is Gaussian and Z_2 is distributed according to M_β. Finally, representation (5.1) is recovered with $X = B_{\alpha,\beta}(t)$, $X_\alpha = Z_1 t^{\alpha/2}$ and $\Lambda_\beta = Z_2$.

It is worth noting to highlight here that representation (5.1) permits to solve a number of questions, in particularly those related to the distribution properties of $B_{\alpha,\beta}(t)$, because they can be reduced to questions concerning the fBm $X_\alpha(t)$ that, since $X_\alpha(t)$ is a Gaussian process, has been largely studied in literature.

For instance, the Hölder continuity of the $B_{\alpha,\beta}(t)$ trajectories follows immediately from those of $X_\alpha(t)$, i.e.,

$$E(|X_\alpha(t) - X_\alpha(s)|^h) = c_h |t-s|^{h\alpha/2} \,. \tag{5.2}$$

Moreover, representation (5.1) highlights the stationary increment property of the ggBm, and it emerges to be suitable for path simulations.

With the same backward-derivation method described to obtain representation (5.1) from (2.3) plus (2.4) and (2.6), the symmetric Lévy process governed by (2.7) follows to be represented by

$$\mathcal{L}_\alpha(t) \stackrel{d}{=} \sqrt{\ell_{\alpha/2}}\, X_{2/\alpha}(t) \,, \quad t \ge 0 \,, \quad 0 < \alpha < 2 \,, \quad 0 < \beta \le 1 \,, \tag{5.3}$$

where the stochastic process $X_{2/\alpha}(t)$ is a standard fBm with Hurst exponent $1/\alpha$ and $\ell_{\alpha/2}$ is an independent non-negative random variable with PDF $L_{\alpha/2}^{-\alpha/2}(\tau)$, $\tau \ge 0$.

Finally, for the two-particle anomalous diffusion, the self-similar stochastic processes representations are straighfordwarly obtained. In fact, comparing (2.3) plus (2.4) and (3.8) it follows that

$$B_{\alpha,\beta,\mu}(t) \stackrel{d}{=} (\Lambda_\beta)^{\mu/2}\, X_{\mu\alpha}(t) \,, \quad t \ge 0 \,, \quad 0 < \alpha < 2 \,, \quad 0 < \beta \le 1 \,, \quad \mu > 0 \,, \tag{5.4}$$

where the stochastic process $X_{\mu\alpha}(t)$ is a standard fBm with Hurst exponent $\mu\alpha/2$ and Λ_β is an independent non-negative random variable with PDF $M_\beta(\tau)$, $\tau \ge 0$.

Comparing (2.3) plus (2.4) and (3.9) it follows that

$$\mathcal{L}_{\alpha,\mu}(t) \stackrel{d}{=} (\ell_{\alpha/2})^{\mu/2}\, X_{2\mu/\alpha}(t) \,, \quad t \ge 0 \,, \quad 0 < \alpha < 2 \,, \quad 0 < \beta \le 1 \,, \quad \mu > 0 \,, \tag{5.5}$$

where the stochastic process $X_{2\mu/\alpha}(t)$ is a standard fBm with Hurst exponent μ/α and $\ell_{\alpha/2}$ is an independent non-negative random variable with PDF $L_{\alpha/2}^{-\alpha/2}(\tau)$, $\tau \ge 0$.

6. Conclusions

In the present paper two-particle dispersion is investigated in the context of the Anomalous Diffusion. Two-particle diffusion is important for the statistical analysis of fluctuations of a tracer concentration field. Since anomalous diffusion can be modelled by time-subordination of Gaussian stochastic processes, here it is shown that, in the framework of self-similar stochastic processes, two different subordination modelling approaches, namely the parent-directing process and the product of random variables, can be unified because they give the same integral formula for the resulting PDF.

By assuming a single-particle fBm and the particle correlation function decreasing in time with a power law, the centre-of-mass trajectory follows to be a fBm, too, whose variance has no longer a simple power law scaling because of the two-particle correlation. Furthermore, the two-particle separation PDF is computed for the cases with time-subordination directed by the M-Wright density and by the Lévy stable density. The resulting PDFs are evaluated and represented by the Mellin–Barnes integral, in terms of H-function and by series. Moreover, also the asymptotic behaviours are shown. In particular, in the case with operational time driven by the M-Wright density the PDF asymptotically decreases with a stretched exponential law while in the case driven by the Lévy stable density the PDF asymptotically decreases with a power law.

In order to choose a class of stochastic processes with PDFs according to those previously established, the same method introduced for the derivation of the ggBm is adopted. In analogy with the ggBm, this class of stochastic processes emerges to be determined by the product of a Gaussian process with an opportune Hurst exponent, i.e., an opportune fBm, and an independent random variable distributed according to the M-Wright density or the Lévy stable density. Then the processes belonging to such class are referred to as H-sssi and defined by only the autocovariance structure.

The determination of the master equation of this class of H-sssi processes and satisfied by the evaluated PDFs will be the issue of future developments of the present research.

Acknowledgment

GP is funded by Regione Autonoma della Sardegna (PO Sardegna FSE 2007–2013 sulla L.R. 7/2007 “Promozione della ricerca scientifica e dell’innovazione tecnologica in Sardegna”).

Appendix

The H-function is defined by means of a Mellin–Barnes type integral as follows (Mathai et al., 2010)

$$H^{m,n}_{p,q}\left[z \left| \begin{array}{c} (a_1,A_1),\dots,(a_p,A_p) \\ (b_1,B_1),\dots,(b_q,B_q) \end{array} \right. \right] = \frac{1}{2\pi i}\int_{\mathcal{L}} h(s)\, z^{-s}\, ds\,, \tag{A.1}$$

with

$$h(s) = \frac{\prod_{j=1}^{m}\Gamma(b_j+B_j s)\prod_{i=1}^{n}\Gamma(1-a_i-A_i s)}{\prod_{j=m+1}^{q}\Gamma(1-b_j-B_j s)\prod_{i=n+1}^{p}\Gamma(a_i+A_i s)}\,, \tag{A.2}$$

where an empty product is always interpreted as unity, $\{m\,,\,n\,,\,p\,,\,q\}\in N_0$ with $1\le m\le q$ and $0\le n\le p$, $\{A_i\,,\,B_j\}\in R^+$ and $\{a_i\,,\,b_j\}\in R$, or C, with $i=1,\dots,p$ and $j=1,\dots q$ such that $A_i(b_j+k)\neq B_j(a_i-\ell-1)$ with k and $\ell\in N_0$, $i=1,\dots,n$ and $j=1,\dots,m$. The poles of the integrand in (A.1) are assumed to be simple. The integration path $\mathcal{L}$ encircles all the poles of $\Gamma(b_j + B_j s)$ with $j = 1, \ldots, m$.

The H-function is an analytic function of z and exists for all $z \neq 0$ when $q \geq 1$ and $\mu > 0$ or for $0 < |z| < \Delta$ when $q \geq 1$ and $\mu = 0$ where

$$\mu = \sum_{j=1}^{q} B_j - \sum_{i=1}^{p} A_i \,, \quad \Delta = \left\{ \prod_{i=1}^{p} A_i^{-A_i} \right\} \left\{ \prod_{j=1}^{q} B_j^{B_j} \right\} .$$

For other existence conditions see (Mathai et al., 2010).

The asymptotic expansion for $|z| \to \infty$ is obtained by integration around the poles of $\Gamma(1 - a_i - A_i s)$ with $i = 1, \ldots, n$. Actually this is similar to exchange $s \to -s$ and then passing from the series of powers of z to a series of powers of $1/z$, from which the asymptotic expansion follows.

In the particular case with $n = 0$ the asymptotic behaviour for $z \to +\infty$ is of exponential type and determined for real z by the formula

$$H_{p,q}^{m,0}(z) \simeq \mathcal{O}\left(z^{[\mathrm{Re}(\omega)+1/2]/\mu} \right) \exp\left\{ \mu \cos\left(\frac{\zeta\pi}{\mu} \right) \left(\frac{z}{\Delta} \right)^{1/\mu} \right\} , \tag{A.3}$$

where

$$\omega = \sum_{j=1}^{q} b_j - \sum_{i=1}^{p} a_i + \frac{p-q}{2} \,, \quad \zeta = \sum_{j=1}^{m} B_j - \sum_{i=n+1}^{p} A_j \,.$$

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