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Accelerating Brownian motion: A fractional dynamics approach to fast diffusion

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Abstract. – Superdiffusion in the sub-ballistic regime with a non-diverging mean-squared displacement is studied on the basis of a linear, fractional kinetic equation with constant coefficients which is non-local in time and leads to an exponential tail of the corresponding probability density function. It is shown that sub-ballistic superdiffusion can be regarded as ballistic motion with a memory, much as slow diffusion can be thought of as a random walk with a memory. This suggests that fractional kinetic equations are useful in describing both sub- and superdiffusion processes.

Stochastic processes whose mean-squared displacement grows faster than linearly in time have been under discussion since Richardson's seminal study of the relative diffusion of two particles in fully developed turbulence for which he established the famed t^3 law [1]. The description of Richardson diffusion, among others, has been based on modified diffusion equations with position- or time-dependent diffusion coefficients which are local in time and lead to a (stretched) Gaussian shape of the probability density function (pdf) [1–3], or on Lévy walk models [4–6], the latter being non-local in time.

In general, transport processes characterised by a mean-squared displacement $\langle x^2(t)\rangle \propto t^\kappa$ which deviates from the linear time dependence ($\kappa = 1$) of Brownian motion are called anomalous [7]. Slow diffusion corresponds to $0 < \kappa < 1$, and has been studied extensively in the absence and presence of external force fields [5–8], fractional diffusion and Fokker-Planck equations having been recognised as an especially suited tool for its description [8–10].

In what follows, we concentrate on the one-dimensional description of diffusion processes in the domain of sub-ballistic superdiffusion (SSD) corresponding to $1 < \kappa < 2$. In that course, we investigate the fractional kinetic equation

$$\frac{\partial^2 P}{\partial t^2} = K_{2-\alpha}\, {}_0D_t^\alpha \frac{\partial^2}{\partial x^2} P(x,t), \qquad 0 < \alpha < 1, \tag{1}$$

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which has been derived from a long-range correlated dichotomous stochastic process [11], from a fractional Kramers equation [12], and from the generalised Chapman-Kolmogoroff equation [13]. Equation (1) was called fractional wave equation in the hallmark paper of Schneider and Wyss [9]. In eq. (1), the generalised diffusion constant $K_{2-\alpha}$ is of dimension $[K_{2-\alpha}] = \mathrm{cm}^2\,\mathrm{s}^{-(2-\alpha)}$ the dynamical origin of which is derived in ref. [13]. The fractional Riemann-Liouville operator ${}_0D_t^{\alpha} \equiv \frac{\partial}{\partial t}\,{}_0D_t^{-\alpha}$ is defined in terms of the convolution [14]

$$ {}_0D_t^{-\alpha}P(x,t) \equiv \frac{1}{\Gamma(\alpha)}\int_0^t \mathrm{d}t' \frac{P(x,t')}{(t-t')^{1-\alpha}}\,, \tag{2}$$

for which the generalisation $\mathcal{L}\{\,{}_0D_t^{-\alpha}P(x,t)\} = u^{-\alpha}P(x,u)$ of the integration theorem of the Laplace transformation holds. Note that, according to eq. (2), the fractional dynamics approach in eq. (1) is explicitly non-local in time. We will show that at the same time, the tail of the pdf decays exponentially. Furthermore, the solution of eq. (1) features propagating humps, underlining the proximity to the standard wave equation. Interestingly, our approach to describe SSD in a way resembles Monin and Yaglom's third-order equation $\frac{\partial^3 P}{\partial t^3} = K_3\frac{\partial^2}{\partial x^2}P(x,t)$ to obtain the Richardson t^3 law [15].

The integral form of eq. (1), $P(x,t) - P_0(x) = {}_0D_t^{\alpha-2}K_{2-\alpha}\frac{\partial^2}{\partial x^2}P(x,t)$, is obtained through the twofold application of the integral operator ${}_0D_t^{-1}$. This form explicitly features the initial value $P_0(x) \equiv \lim_{t\to 0+} P(x,t)$. Note that norm conservation implies that the initial field velocity vanishes, $\lim_{t\to 0+}\left[\frac{\partial}{\partial t}P(x,t)\right] \equiv 0$. The mean-squared displacement associated with eq. (1) follows by integration, yielding

$$\langle x^2(t)\rangle = \frac{2K_{2-\alpha}}{\Gamma(3-\alpha)}t^{2-\alpha}. \tag{3}$$

Equations (1) and (3) reduce to the wave equation in the ballistic limit $\alpha \to 0$, with $\langle x^2(t)\rangle \propto t^2$, and to the diffusion equation in the Brownian case $\alpha \to 1$, with $\langle x^2(t)\rangle \propto t$ [16].

The exact solution for the propagator of eq. (1) is given in closed form in terms of the Fox function

$$P(x,t) = \frac{1}{\sqrt{4K_{2-\alpha}t^{2-\alpha}}} H^{1,0}_{1,1}\left[\frac{|x|}{\sqrt{K_{2-\alpha}t^{2-\alpha}}}\,\middle|\, \begin{matrix}\left(\frac{\alpha}{2},\frac{2-\alpha}{2}\right)\\ (0,1)\end{matrix}\right], \tag{4}$$

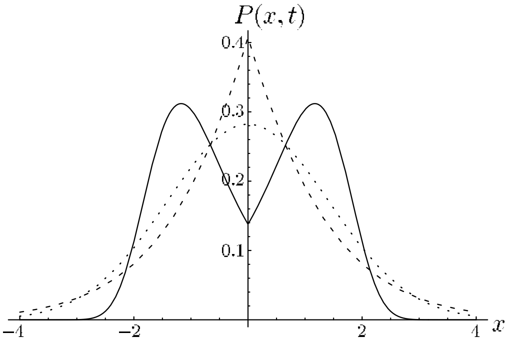
which can be represented in computable form through the series [17]

$$P(x,t) = \frac{1}{\sqrt{4K_{2-\alpha}t^{2-\alpha}}}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!\Gamma(1-(2-\alpha)[n+1]/2)}\left(\frac{x^2}{K_{2-\alpha}t^{2-\alpha}}\right)^{n/2}. \tag{5}$$

The pdf (4) is equivalent to the result reported by Schneider and Wyss who proved that $P(x,t)$ is non-negative [9]. In the asymptotic region $|x|/\sqrt{K_{2-\alpha}t^{2-\alpha}} \gg 1$, the tails of the pdf (4) are given by the compressed Gaussian shape ($0 < \alpha \le 1$)

$$\begin{aligned} P(x,t) \sim\ & \frac{\left(2/(2-\alpha)\right)^{(\alpha-1)/\alpha}}{\sqrt{4\pi\alpha K_{2-\alpha}t^{2-\alpha}}}\left(\frac{|x|}{\sqrt{K_{2-\alpha}t^{2-\alpha}}}\right)^{(1-\alpha)/(\alpha)} \times \\ & \times \exp\left[-\frac{\alpha}{2}\left(\frac{2-\alpha}{2}\right)^{(2-\alpha)/\alpha}\left[\frac{|x|}{\sqrt{K_{2-\alpha}t^{2-\alpha}}}\right]^{2/\alpha}\right]. \end{aligned} \tag{6}$$

From the Fox function representation in eq. (4), one infers the Gaussian pdf $P_d(x,t) = (4\pi K_1 t)^{-1/2}e^{-x^2/(4K_1t)}$ in the Brownian limit $\alpha \to 1$, and the moving delta peaks $P_w(x,t) =$



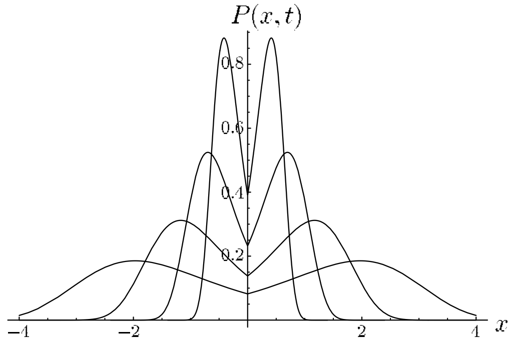


Fig. 1 – Left: pdf $P(x,t)$ of the fractional wave equation (1) for $\alpha = 1/2$ (full line), in comparison to the Gaussian $P_d(x,t)$ (dotted line). The humps of the SSD pdf strongly contrast the cusp shape of the subdiffusive pdf which is represented by the dashed line for the case $\kappa = 1/2$ in eq. (3), see the fractional diffusion equation $\frac{\partial}{\partial t}P = K_{1/2}\, {}_0D_t^{1/2}\frac{\partial^2}{\partial x^2}P(x,t)$ in ref. [8]. Both the humps in the SSD case and the cusp shape for slow diffusion are related to the persisting initial condition which implies a moving front in the SSD motion and a spatial sticking in the latter case. All curves are drawn for the dimensionless time $t = 1$. Right: fractional wave pdf $P(x,t)$ for $\alpha = 1/2$, eq. (4), for four consecutive dimensionless times, $t = 1/4,\ 1/2,\ 1,\ 2$ (decay and broadening of humps in the course of time).

$\frac{1}{2}\big(\delta(x-\sqrt{K_2}t)+\delta(x+\sqrt{K_2}t)\big)$ with velocity $|\sqrt{K_2}|$, in the ballistic limit $\alpha \to 0$ [18]. Note that the ballistic limit is equivalent to the results from refs. [4,19].

From eq. (4), one infers the asymptotic scaling behaviour ($0 < \alpha < 1$)

$$g(\xi) \sim \begin{cases} e^{c\xi}, & \xi < 1\,, \\ (\xi)^{1/\alpha-1}\exp\big[-c(\xi)^{2/\alpha}\big], & \xi > 1\,, \end{cases} \tag{7}$$

where the scaling function g is related to the pdf (4) through $P(x,t) = t^{(2-\alpha)/2}g(\xi)$, employing the scaling variable $\xi \equiv |x|/t^{(2-\alpha)/2}$. This behaviour is remarkable as, close to the origin, the function grows initially, before turning to the compressed Gaussian tail at around $\xi \approx 1$. The numerical evaluation in fig. 1 illustrates this turnover behaviour manifested in the distinct humps, in comparison to the Brownian and subdiffusive cases. On the right of fig. 1, we depict the evolution of the fractional wave solution $P(x,t)$ in the course of time.

In fig. 2, the gradual transition from the Gaussian to the travelling-wave behaviour is illustrated. The increasing depletion around the origin in favour of the humps, as well as the more and more pronounced decay of the tails of the pdf indicate the parametric approach of the pdf $P(x,t)$, eq. (4), to the propagating δ-peaks of the wave equation. Accordingly, the dispersive-diffusive character of the transport is continuously diminished, being replaced by the non-dispersive ballistic nature of wave motion.

Let us further pursue the relation of eq. (1) to the wave equation. To this end, we note that Fourier-Laplace transformation produces an algebraic equation in the wave number k and the Laplace variable u whose solution is given by the (k,u)-form of the pdf,

$$P(k,u) = \frac{1}{u + K_{2-\alpha}u^{\alpha-1}k^2}, \tag{8}$$

which corresponds to the asymptotic form obtained in ref. [19]. From eq. (8) we derive the connection of the fractional pdf $P(x,t)$ with the solution of the wave equation $\frac{\partial^2}{\partial t^2}P_w =$

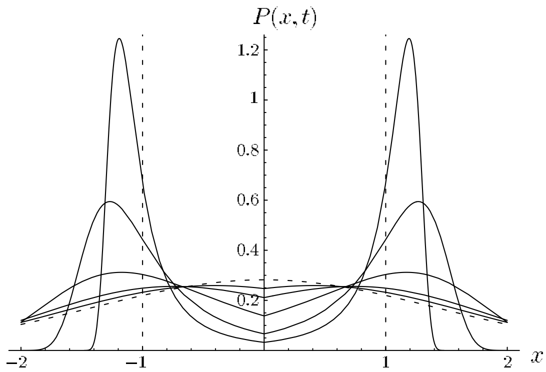


Fig. 2 – Kaleidescope picture of the turnover from Gaussian to travelling-wave character: fractional dynamics solutions, eq. (4) (full lines), at the dimensionless time $t = 1$. The larger $(2-\alpha)$ becomes, the more distinct is the depletion at the origin, and the sharper the humps are pronounced. $P(x,t)$ for $2-\alpha = 9/8$, $5/4$, $3/2$, $7/4$, $15/8$. The dashed lines show the travelling δ-peaks, $P_w(x,t)$, and the Gaussian pdf, $P_d(x,t)$.

$K_2 \frac{\partial^2}{\partial x^2} P_w(x,t)$ whose (k,u)-transform is $P_w(k,u) = \left(u + K_2 u^{-1} k^2\right)^{-1}$. This relation for the Laplace transforms reads

$$P(x,u) = \sqrt{\frac{K_2}{K_{2-\alpha}}} u^{-\alpha/2} P_w \left(x, \sqrt{\frac{K_2}{K_{2-\alpha}}} u^{1-\alpha/2} \right) , \tag{9}$$

which is analogous to the one found for subdiffusion [8, 10]. In time, relation (9) corresponds to the generalised Laplace transformation [8, 12]

$$P(x,t) = \int_0^\infty \mathrm{d}s E(s,t) P_w(x,s) , \tag{10}$$

where the kernel $E(s,t)$ is defined through

$$E(s,u) = \sqrt{K/K_{2-\alpha}} u^{-\alpha/2} \exp\left[-s^* u^{1-\alpha/2} \right] , \tag{11}$$

with $s^* \equiv \sqrt{K/K_{2-\alpha}} s$. Rewriting eq. (11) as $E(s,u) = -\left(1 - \frac{\alpha}{2}\right)^{-1} \frac{\partial}{\partial u} \exp\left[-s^* u^{1-\alpha/2}\right]$ in which the exponential is but the characteristic function of the one-sided Lévy distribution $L^+_{1-\alpha/2}\left(t/(s^*)^{1/(1-\alpha/2)}\right)$ [20], we find

$$E(s,t) = \frac{t}{(1-\alpha/2)s} L^+_{1-\alpha/2} \left(\frac{t}{(s^*)^{1/(1-\alpha/2)}} \right) . \tag{12}$$

By means of the Fox function $H^{1,0}_{1,1}$, the kernel $E(s,t)$ can be expressed in analytic form through

$$E(s,t) = \frac{1}{s} H^{1,0}_{1,1} \left[s^* t^{\alpha/2-1} \middle| \begin{array}{l} \left(1, 1 - \frac{\alpha}{2}\right) \\ (1,1) \end{array} \right] \tag{13}$$

$$= \frac{1}{s} \sum_{n=0}^{\infty} \frac{(-1)^n \left(s^* t^{\alpha/2-1}\right)^{1+n}}{n! \Gamma\left(1 - \frac{2-\alpha}{2}(1+n)\right)} . \tag{14}$$

The solution of the wave equation, for a non-negative initial condition $P_0(x)$ always remains positive due to the travelling wave similarity. Thus following eq. (10), from $E(s,t) \geq 0$ we conclude that $P(x,t) \geq 0$, *i.e.*, the pdf (4) is non-negative for all (x,t), in agreement with the findings in ref. [9]. It should be noted that there exists no such transformation mapping the Brownian pdf $P_d(x,t)$ onto $P(x,t)$ [21]. Within fractional dynamics, in order to go beyond Brownian motion, one has to borrow from the ballistic process and superimpose a memory instead of modifying a Markovian random walk.

The nature of the propagating humps can now be understood as the fractional dynamics analogue of the moving δ-peaks $P_w(x,t)$ of the wave equation for the initial condition $P_0(x) = \delta(x)$: instead of the sharp peaks moving at speed $\sqrt{K_2}$, the fractional, SSD pdf $P(x,t)$ exhibits the moving humps whose width becomes increasingly broader. As can be seen from eq. (1), even if initially the field velocity is zero, at a further instant $t_1 > 0$, there exists a non-vanishing field velocity which feeds back to the evolution equation (1), thus creating the hump motion. The persistent motion of the initial condition in turn creates the depletion in the origin.

A further remarkable property of the SSD process (1) concerns the mode relaxation for a fixed wave number k_0, given in terms of the Mittag-Leffler function $E_{2-\alpha}$ [22] through

$$P(k_0,t) = E_{2-\alpha}\left(-K_{2-\alpha}k_0^2 t^{2-\alpha}\right) \equiv \sum_{n=0}^{\infty} \frac{\left(-K_{2-\alpha}k_0^2 t^{2-\alpha}\right)^n}{\Gamma(1+(2-\alpha)n)}\,, \tag{15}$$

which leads to a damped, oscillatory behaviour. The oscillations mirror the moving humps, similar to the purely oscillatory mode behaviour $P_w(k_0,t) = \cos(-\sqrt{K_2 k_0^2}t)$ of the travelling wave solution $P_w(x,t)$.

Let us finally address the Pólya returning probability to the origin. According to eq. (7), the probability to find the particle at the origin decays in the course of time like

$$P(0,t) = \left(2\Gamma(\alpha/2)\sqrt{K_{2-\alpha}}t^{1-\alpha/2}\right)^{-1}, \tag{16}$$

where $1-\alpha/2 \in (1/2,1)$. The Pólya returning probability, accordingly, decays faster in time than for the Brownian case, reflecting the joint effect of the depletion close to the origin and the hump motion carrying away a major portion of the probability. This effect is connected to the faster spreading expressed in eq. (3), through $P(0,t) \propto \langle x^2(t)\rangle^{-1/2}$.

The most prominent features of the fractional dynamics model eq. (1) of SSD processes are the non-locality in time being manifest in the presence of the fractional operator (2), as well as the propagating humps exhibited by the pdf, eq. (4). The latter mark the turnover between an initial increase of the pdf towards the final exponential (compressed Gaussian) behaviour. The SSD fractional dynamics model thus combines elements of the time-local diffusion equations with position- or time-dependent diffusion coefficients, and the Lévy walk model.

The basic criterion in distinguishing the different models describing SSD is, as is known from the Richardson case, the pdf. In that concern, the SSD fractional propagator with its distinct propagating humps is contrasting the (stretched) Gaussian shape found for the modified, local diffusion equations [1, 2, 15], and the Lévy walk process whose pdf gradually approaches a Lévy distribution the edges of which spread like $|x| = vt$ [6]. It is worth remarking that even if the humps cannot be monitored in a given experimental window, the very shape of the compressed Gaussian in the present model is distinguishable from the (stretched) Gaussian character prevailing in the models with position- and time-dependent diffusion coefficient, as well as from the stable pdf observed for the Lévy walk models.

Fractional dynamics has been studied extensively in the subdiffusive domain, in the absence and presence of external fields, and in both position and phase space [9, 10]. In the present study we have promoted a complementary fractional model for SSD in the force-free case. Whereas for slow diffusion ($0 < \kappa < 1$), the fractional diffusion model is equivalent to continuous time random walk models with a self-similar waiting time distribution, the pdf in the fractional wave equation (1) differs from the evolving Lévy stable form of the pdf in the Lévy walk model. The former combines a modified Gaussian decay of the pdf obtained from generalised diffusion equations with the temporal power law memory prevalent in continuous time random walk models. In the SSD domain, fractional dynamics for fast single-particle diffusion thus mirrors certain features which are believed to prevail in the Richardson pair diffusion.

For slow diffusion in external force fields, a position space and phase space framework in terms of fractional Fokker-Planck-Smoluchowski and fractional Klein-Kramers equations has been established [8, 10, 13]. A fractional equation for SSD transport in the presence of an external potential has been suggested in ref. [12]. However, it has not been proved whether the corresponding solution is a proper pdf. This problem will be addressed in a forthcoming work.

Possible applications of our fractional SSD model include front or wave propagation in complex systems where the presence of disorder gives rise to the increasingly blurred humps, as well as their sub-ballistic spreading.

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