# Stochastic processes crossing from ballistic to fractional diffusion with memory: Exact results

Valery Ilyin,[1] Itamar Procaccia,[1] and Anatoly Zagorodny[2]

[1]*Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel*
[2]*Bogolyubov Institute for Theoretical Physics, 252143 Kiev, Ukraine*
(Received 19 November 2009; published 25 March 2010)

We address the now classical problem of a diffusion process that crosses over from a ballistic behavior at short times to a fractional diffusion (subdiffusion or superdiffusion) at longer times. Using the standard non-Markovian diffusion equation we demonstrate how to choose the memory kernel to exactly respect the two different asymptotics of the diffusion process. Having done so we solve for the probability distribution function (pdf) as a continuous function which evolves inside a ballistically expanding domain. This general solution agrees for long times with the pdf obtained within the continuous random-walk approach, but it is much superior to this solution at shorter times where the effect of the ballistic regime is crucial.

## I. INTRODUCTION

Since the classical work of Hurst [1] on the stochastic discharge of reservoirs and rivers, nature has offered us a large number of examples of diffusion processes which are "anomalous" in the sense that an observable $X$ diffuses in time such that its variance grows according to

$$\langle \Delta X^2 \rangle(t) \sim D_\alpha t^\alpha \quad \text{for } t \gg t_c, \tag{1}$$

where $\alpha \neq 1$, angular brackets mean an average over repeated experiments and $D_\alpha$ is a coefficient with the appropriate dimensionality. This long-time behavior with $\alpha \neq 1$ is generic when the diffusion steps are correlated, with persistence for $\alpha > 1$ and antipersistence for $\alpha < 1$ [2]. The list of systems displaying such behavior is extensive and growing. Some subdiffusive examples: charge-carrier transport in amorphous semiconductors [3], NMR diffusiometry in percolative [4] and porous systems [5], reptation dynamics in polymeric systems [6], transport on fractal geometries [7], diffusion of scalar tracer in convection [8], etc. Superdiffusive examples include special domains of rotating flow [9], collective slip diffusion on solid surfaces [10], Richardson turbulent diffusion [11], bulk-surface exchange controlled dynamics in porous glasses [12], quantum optics [13], etc. This multitude of examples created an urgent need to formulate novel stochastic theories to compute the probability distribution function (pdf) that is associated with anomalous diffusive processes of this type [14]. However, all these past approaches considered only the long-time behavior Eq. (1) and disregarded the important fact that in many cases the short-time behavior is different, being

$$\langle \Delta X^2 \rangle(t) \sim D_2 t^2 \quad \text{for } t \ll t_c. \tag{2}$$

This short-time behavior is known as "ballistic" and is generic for a wide class of processes. In this Rapid Communication we show how to find the pdf of a process that satisfies Eqs. (1) and (2) simultaneously in the asymptotic limits. The presence of Eq. (2) at short times influences the solution in a fundamental way that cannot be neglected.

The correlations between stochastic steps mean that the diffusion process is not Markovian but rather has memory. Thus the pdf of the observable $X$, $f(X,t)$ is expected to satisfy a diffusion equation with memory [15],

$$\frac{\partial f(X,t)}{\partial t} = \int_0^t dt' K(t-t')\nabla^2 f(X,t), \tag{3}$$

with $K(t)$ being the memory kernel and $\nabla^2$ as the Laplace operator. In this Rapid Communication we study the class of processes which satisfy Eqs. (2) and (3) with $\alpha < 2$.

First of all we find an expression for the kernel $K(t)$ which is unique for a given law of mean-square displacement. Second we consider the kernel which contains both ballistic contribution Eq. (2) *and* long-time behavior (1). For this case we find an exact equation and a solution for Eq. (3). Lastly a simple interpolation formula for the kernel is inserted to the exact equation which is then solved for the pdf of $X$ without any need for the fractional dynamics approach [14]. Some interesting characteristics of the solution are described below.

## II. DETERMINATION OF THE KERNEL $K(t)$

To determine the kernel in Eq. (3) we use a result obtained in [16]. Consider the auxiliary equation

$$\frac{\partial P(X,t)}{\partial t} = \nabla^2 P(X,t). \tag{4}$$

Define the Laplace transform of the solution of Eq. (4) as

$$\widetilde{P}(X,s) \equiv \int_0^t dt e^{-st} P(X,t), \tag{5}$$

it was shown in [16] that the solution of Eq. (3) with the same initial conditions can be written as

$$\widetilde{f}(X,s) = \frac{1}{\widetilde{K}(s)} \widetilde{P}\left(X, \frac{s}{\widetilde{K}(s)}\right), \tag{6}$$

where here and below the tilde above the symbol means the Laplace transform. The development that we propose here is to replace in Eq. (6) the Laplace transform $\widetilde{K}(s)$ with the Laplace transform of the mean-square displacement. This is done by first realizing (by computing the variance and integrating by parts) that

$$\frac{\partial \langle X^2 \rangle(t)}{\partial t} = 2 \int_0^t dt' K(t - t'), \qquad (7)$$

or, equivalently,

$$\widetilde{K}(s) = \frac{s^2 \widetilde{\langle X^2 \rangle}(s)}{2} = \frac{s}{2} \frac{\partial \widetilde{\langle X^2 \rangle}(t)}{\partial t} + \frac{s}{2} \frac{\partial \widetilde{\langle X^2 \rangle}(t)}{\partial t} - \frac{\partial \langle X^2 \rangle(t)}{2 \, \partial t}. \quad (8)$$

The second line was written in order to find the time representation of $K(t)$ which is the inverse Laplace transform,

$$K(t) = \frac{1}{2} \left( \delta(t) \frac{\partial}{\partial t} \langle X^2 \rangle(t) + \frac{\partial^2}{\partial t^2} \langle X^2 \rangle(t) \right) = \frac{1}{2} \frac{\partial}{\partial t} \left( H(t) \frac{\partial \langle X^2 \rangle(t)}{\partial t} \right), \qquad (9)$$

where $H(t)$ is the Heaviside function. Obviously, using the first line of Eq. (8) in Eq. (6) the solution is entirely determined by whatever law is given for the variance, together with initial conditions.

For ordinary diffusion the variance is defined by Eq. (1) with $\alpha = 1$ and $t_c = 0$. It follows from Eq. (9) that the kernel is $K(t) \sim \delta(t)$ and Eq. (3) is reduced to Markovian Eq. (4); this process does not possess any memory. More complicated examples are considered below.

### III. EXAMPLE I: FRACTIONAL DIFFERENTIAL EQUATIONS

In recent literature the problem of a diffusion process which is consistent with Eq. (1) only for all times (i.e., $t_c = 0$) is investigated using the formalism of fractional differential equations (see, e.g., [14]). In this formalism Eq. (3) is replaced by the fractional equation

$$\frac{\partial f(X,t)}{\partial t} = D_\alpha \, _0\mathbf{D}_t^{1-\alpha} \frac{\partial^2 f(X,t)}{\partial x^2}, \qquad (10)$$

where the Rieman-Liouville operator $_0\mathbf{D}_t^{1-\alpha}$ is defined by

$$_0\mathbf{D}_t^{1-\alpha} \, \phi(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t dt' \frac{\phi(x,t')}{(t - t')^{1-\alpha}}, \qquad (11)$$

where $\Gamma(\alpha)$ is the gamma function. It is easy to see that this equation follows from Eq. (3) with the kernel evaluated by Eq. (9) with variance (1). We reiterate however that this equation is consistent with Eq. (1) for all times $t \geq 0$. This of course is a problem since this formalism cannot agree with the ballistic short-time behavior which is generic in many systems.

### IV. EXAMPLE II: BALLISTIC BEHAVIOR

For $X$ one dimensional the solution of Eq. (4) with the initial condition $P(X, t=0) = \delta(X)$ is given by

$$\widetilde{P}(X,s) = \frac{1}{2\sqrt{s}} \exp(-|X|\sqrt{s}). \qquad (12)$$

Substituting in Eq. (6) we find that

$$\widetilde{f}(X,s) = \frac{1}{\sqrt{2s^3 \widetilde{\langle X^2 \rangle}(s)}} \exp\left( -|X| \sqrt{\frac{2}{s\widetilde{\langle X^2 \rangle}(s)}} \right). \quad (13)$$

For systems with the pure ballistic behavior (e.g., dilute gas) the variance can be written as $\langle X^2 \rangle_t = \langle u^2 \rangle t^2$, where $\langle u^2 \rangle$ is the mean-square average of the particle velocities. The Laplace transform of this expression is given by $\widetilde{\langle X^2 \rangle}(s) = 2\langle u^2 \rangle / s^3$ and the Laplace transform of the pdf is defined by

$$\widetilde{f}(X,s) = \frac{1}{2\sqrt{\langle u^2 \rangle}} \exp\left( -|X| \frac{s}{\sqrt{\langle u^2 \rangle}} \right). \qquad (14)$$

The inverse transform reads as

$$f(X,t) = \frac{1}{2} \delta(|X| - \sqrt{\langle u^2 \rangle} t). \qquad (15)$$

This solution corresponds to a deterministic evolution; there is a complete memory of the initial conditions in the absence of interparticle interactions, $K(t) = \langle u^2 \rangle$.

### V. GENERAL CASE

In the general case the mean-square displacement satisfied some law $\langle X^2 \rangle(t)$ which is supposed to be known at all times, with possible asymptotic behavior as shown in Eqs. (1) and (2)). To find the appropriate general solution we will split $\widetilde{f}(X,s)$ into two parts, $\widetilde{f}_I(X,s)$ and $\widetilde{f}_{II}(X,s)$, such that the first part is constructed to agree with the existence of a ballistic regime. Suppose that in that regime, at short time, the mean-square displacement can be expanded in a Taylor series

$$\langle X^2 \rangle(t) = \sum_{i=0}^{\infty} a_i t^{\mu_i - 1} = a_0 t^2 + a_1 t^3 + a_2 t^4 + \cdots, \quad (16)$$

where $\mu_0 = 3$, $\mu_1 = 4$, etc. Then the Laplace transform $\widetilde{\langle X^2 \rangle}(s)$ can be written for $s \to \infty$ as [17]

$$\widetilde{\langle X^2 \rangle}(s) = \sum_{i=0}^{\infty} a_i \Gamma(\mu_i) \frac{1}{s^{\mu_i}} = 2a_0 \frac{1}{s^3} + 6a_1 \frac{1}{s^4} + 24a_2 \frac{1}{s^5} + \cdots. \qquad (17)$$

Substituting Eq. (17) up to $\mathrm{O}(s^{-4})$ in Eq. (13) yields

$$\widetilde{f}_I(X,s)_{s \to \infty} = \frac{1}{2\sqrt{a_0}} \exp\left[ -\frac{|X|}{\sqrt{a_0}} \left( s - \frac{3a_1}{2a_0} \right) \right]. \qquad (18)$$

The inverse Laplace transform of this result reads as

$$f_I(X,t) = \frac{1}{2} \exp\left( \frac{3a_1}{2a_0} t \right) \delta(|X| - \sqrt{a_0} t). \qquad (19)$$

Not surprisingly, this partial solution corresponds to a deterministic propagation. Note that in order to avoid exponential divergence in time we must have $a_1 < 0$ in expansion (16).

Having found $\widetilde{f}_I(X,s)$ we can now write $\widetilde{f}_{II}(X,s)$ simply as

$$\widetilde{f}_{II}(X,s) = \widetilde{f}(X,s) - \widetilde{f}_I(X,s). \qquad (20)$$
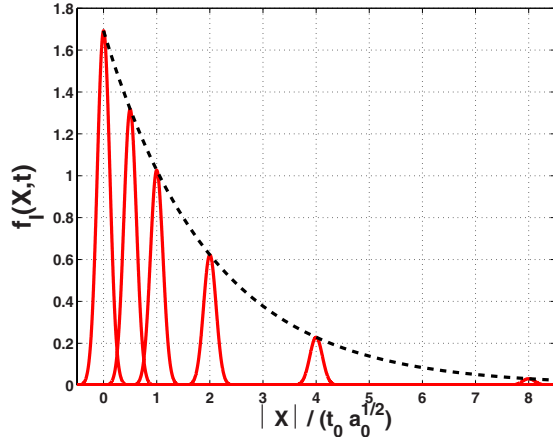
Calculating this difference explicitly we find

FIG. 1. (Color online) The time evolution of the function $f_I(X,t)$ defined by Eq. (19) for time intervals $t/t_0 = 0.5$, 1, 2, 4, and 8 (the time scale $t_0 = a_0/(3a_1)$). The $\delta$ function is graphically represented by narrow Gaussians.

$$\widetilde{f}_{II}(X,s) = \frac{1}{2}\left[\sqrt{\frac{2}{s^3 \widetilde{\langle X^2 \rangle}(s)}}\right]\exp\left\{-|X|\left[\sqrt{\frac{2}{s\widetilde{\langle X^2 \rangle}(s)}}\right.\right.$$

$$\left.\left. - \frac{s}{\sqrt{a_0}}\right]\right\} - \frac{1}{\sqrt{a_0}}\exp\left[\frac{3a_1}{2a_0^{3/2}}|X|)\right]\exp\left(-\frac{|X|}{\sqrt{a_0}}s\right)$$

$$\equiv \widetilde{F}(X,s)\exp\left(-\frac{|X|}{\sqrt{a_0}}s\right). \tag{21}$$

The inverse Laplace transform of Eq. (21) is given by

$$f_{II}(X,t) = F(X, t - |X|/\sqrt{a_0})H(\sqrt{a_0}t - |X|). \tag{22}$$

The importance of this result is that the explicit Heaviside function is taking upon itself the discontinuity in the solution $f_{II}(X,t)$. The exact value of the function $F(X, t - |X|/\sqrt{a_0})$ at the point $|X| = \sqrt{a_0}t$ can be calculated using the initial value theorem and is given by

$$F(X,0) = -\left\{\frac{3}{4}\frac{a_1}{a_0^{3/2}} + \frac{1}{2\sqrt{a_0}}\left[\frac{27}{8}\left(\frac{a_1}{a_0}\right)^2 - 6\frac{a_2}{a_0}\right]t\right\}$$

$$\times \exp\left(-\frac{3}{2}\frac{a_1}{a_0}t\right). \tag{23}$$

Summing together results (19) and (22) in the time domain we get a general solution of the non-Markovian problem with a short-time ballistic behavior in the form

$$f(X,t) = \frac{1}{2}\exp\left(\frac{3a_1}{2a_0}t\right)\delta(|X| - \sqrt{a_0}t)$$

$$+ F\left(X, t - \frac{|X|}{\sqrt{a_0}}\right)H(\sqrt{a_0}t - |X|). \tag{24}$$

This is the main result of the present Rapid Communication. The diffusion repartition of the probability distribution function occurs inside the spatial diffusion domain which increases in a deterministic way. The first term in Eq. (24) corresponds to the propagating $\delta$ function which is inherited
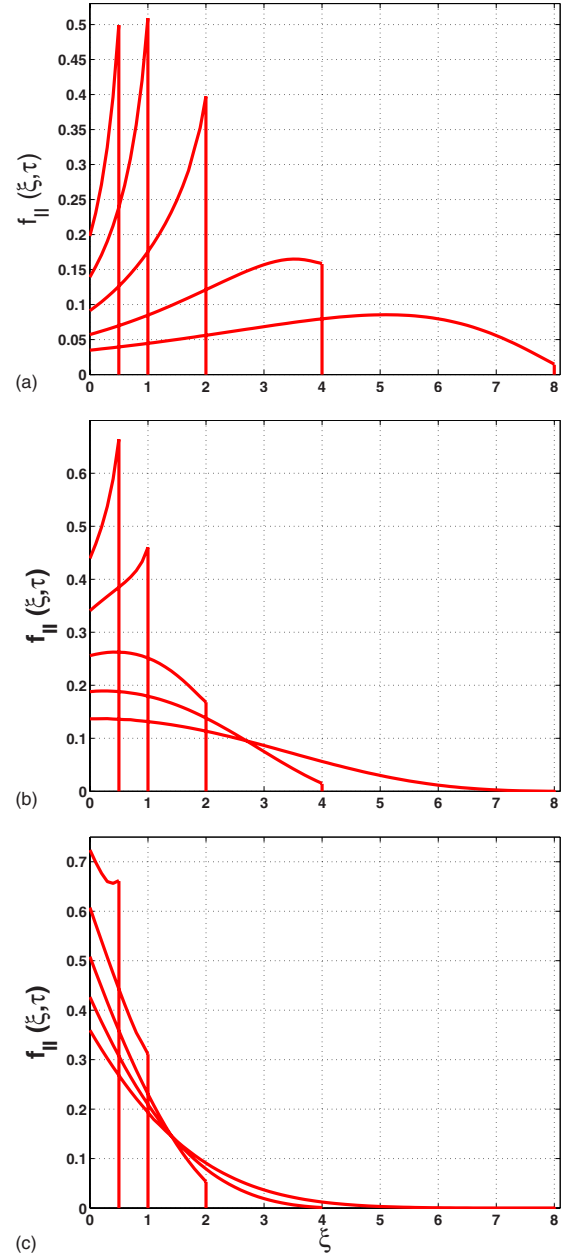


(a)

(b)

(c)

FIG. 2. (Color online) The continuous part of the pdf [Eq. (22)] for different values of the parameter $\alpha$. Superdiffusion ($\alpha = 3/2$, upper panel), regular diffusion ($\alpha = 1$, middle panel) and subdiffusion ($\alpha = 1/2$, lower panel). Time intervals from the top to the bottom $\tau = 0.5$, 1, 2, 4, and 8. The reader should note that the full solution of the problem is the sum of the two solutions shown in this and the previous figure.

from the initial conditions, and it lives at the edge of the ballistically expanding domain. Schematically the time evolution of this term is shown in Fig. 1, where the $\delta$ function is graphically represented as a narrow Gaussian. The dashed line represents the exponential decay of the integral over the $\delta$ function. The function $F(X, t - \frac{|X|}{\sqrt{a_0}})$ in the time domain is a continuous function and can be evaluated numerically, for example using the direct integration method [18]. Below we demonstrate this calculation with explicit examples.

## VI. INTERPOLATION FOR ALL TIMES

To interpolate Eqs. (1) and (2) we propose the form

$$\langle \Delta X^2 \rangle_t = 2D_\alpha t_0^\alpha \frac{(t/t_0)^2}{[1+(t/t_0)]^{2-\alpha}}, \quad (25)$$

where $0 \le \alpha \le 2$. Here $t_0$ is the crossover characteristic time, at $t \ll t_0$ law (25) describes the ballistic regime and at $t \gg t_0$ the fractional diffusion.

Introduce now dimensionless variables $\langle \xi^2 \rangle_\tau = \langle \Delta X^2 \rangle_t / (2D_\alpha t_0^\alpha)$ and $\tau = t/t_0$. With these variables the last equation reads as

$$\langle \xi^2 \rangle_\tau = \frac{\tau^2}{(1+\tau)^{2-\alpha}}. \quad (26)$$

The Taylor expansion of Eq. (25) is given by

$$\langle \xi^2 \rangle_\tau = \tau^2 - (2-\alpha)\tau^3 + \frac{1}{2}(3-\alpha)(2-\alpha)\tau^4 + \cdots. \quad (27)$$

Substituting these expansion coefficients into Eq. (19) yields the first term in the expression for probability distribution function (24),

$$f_I(x,t) = \frac{1}{2}\exp\left(-\frac{3(2-\alpha)}{2}\tau\right)\delta(|\xi|-\tau). \quad (28)$$

The Laplace transform of Eq. (26) is

$$\widetilde{\langle X^2 \rangle}(s) = \left(\frac{\alpha}{s}-1\right)\frac{1}{s} + \left[(\alpha-1)\left(\frac{\alpha}{s}-2\right)+s\right]\frac{e^s}{s^\alpha}\Gamma(\alpha-1,s), \quad (29)$$

where $\Gamma(a,s)$ is the incomplete gamma function. Note that the case $\alpha=2$ is special, since it annuls the exponent in Eq. (28), leaving as a solution a ballistically propagating $\delta$-function. For all other values of $\alpha < 2$ the inverse Laplace transform of the function $\widetilde{F}(x,s)$ which defines the diffusion

process inside the expanded spatial domain should be evaluated, in general, numerically.

Results of the calculations following the method of Ref. [18] for the smooth part of the probability distribution function $f_{II}(x,t)$ for different values of the parameter $\alpha$ are shown in Fig. 2. The reader should appreciate the tremendous role of memory. For example, regular diffusion with $\alpha=1$ results in a Gaussian pdf that is peacefully expanding and flattening as time increases. Here, in the mid panel of Fig. 2 we see that the ballistic part which is represented by the advancing and reducing $\delta$ function sends backward the probability that it loses due to the exponential decay seen in Fig. 1. This "back diffusion" leads initially to a qualitatively different looking pdf, with a maximum at the edge of the ballistically expanding domain. At later times the pdf begins to resemble more regular diffusion. The effect strongly depends on $\alpha$ simply due to the appearance of $\alpha$ in the exponent in Eq. (28).

For long times the contribution from $f_I(X,t)$ to the general solution tends to zero and the solutions shown in Fig. 2 agree with the Markovian pdf obtained in the frame of a continuous-time random walk [19]. For the special case $\alpha=0$ Eq. (29) reads as $\widetilde{\langle X^2 \rangle}(s)=1/s+(1-(2+s)e^sE_1(s))$, where $E_1(s)$ is the exponential integral, and the limiting behavior of the general solution from Eq. (24) $f(X,t)_{t \gg |X|/\sqrt{a_0}} \sim F(X,t)$ can be evaluated analytically with the help of the final value theorem $f(X)=\frac{1}{\sqrt{2}}\exp(-\sqrt{2}|X|)$; this result coincides with the pdf from [19] at the same conditions.

In summary, we have shown how to deal with diffusion processes that crossover from a ballistic to a fractional behavior for short and long times respectively, within the time nonlocal approach. General solution (24) demonstrates the effect of the temporal memory in the form of a partition of the probability distribution function inside a spatial domain which increases in a deterministic way. The approach provides a solution that is valid at all times and, in particular, is free from the instantaneous action puzzle.

[1] H. E. Hurst, Trans. Am. Soc. Civ. Eng. **116**, 770 (1951).
[2] B. B. Mandelbrot and J. W. van Ness, SIAM Rev. **10**, 422 (1968).
[3] B. Rinn, W. Dietriech, and P. Maass, Philos. Mag. B **77**, 1283 (1998).
[4] A. Klemm, H.-P. Müller, and R. Kimmich, Physica A **266**, 242 (1999).
[5] F. Klammler and R. Kimmich, Croat. Chem. Acta **65**, 455 (1992).
[6] E. Fischer, R. Kimmich, U. Beginn, M. Möller, and N. Fatkullin, Phys. Rev. E **59**, 4079 (1999).
[7] M. Porto, A. Bunde, S. Havlin, and H. E. Roman, Phys. Rev. E **56**, 1667 (1997).
[8] O. Cardoso and P. Tabeling, Europhys. Lett. **7**, 225 (1988).
[9] E. R. Weeks and H. L. Swinney, Phys. Rev. E **57**, 4915 (1998).
[10] W. D. Luedtke and U. Landman, Phys. Rev. Lett. **82**, 3835 (1999).
[11] L. F. Richardson, Proc. R. Soc. London, Ser. A **110**, 709 (1926).
[12] J. Bodurka, R.-O. Seitter, R. Kimmich, and A. Gutsze, J. Chem. Phys. **107**, 5621 (1997).
[13] S. Schaufler, W. P. Schleich, and V. P. Yakovlev, Phys. Rev. Lett. **83**, 3162 (1999).
[14] R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).
[15] V. M. Kenkre and R. S. Knox, Phys. Rev. B **9**, 5279 (1974).
[16] I. M. Sokolov, Phys. Rev. E **66**, 041101 (2002).
[17] B. van der Pol and H. Bremmer, *Operational Calculus* (Cambridge University Press, Cambrige, 1964).
[18] D. G. Duffy, ACM Trans. Math. Softw. **19**, 333 (1993).
[19] R. C. Ball, S. Havlin, and G. H. Weiss, J. Phys. A **20**, 4055 (1987).