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Fractional Klein–Kramers dynamics for subdiffusion and Itô formula

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Abstract. Subdiffusion in the presence of an external force field has been recently described in phase space by the fractional Klein–Kramers equation. In this paper using a subordination method, we identify a two-dimensional stochastic process (position, velocity) whose probability density function is a solution of the fractional Klein–Kramers equation. The structure of this process agrees with the two-stage scenario underlying the anomalous diffusion mechanism, in which trapping events are superimposed on the Langevin dynamics. Applying an extension of the celebrated Itô formula for subdiffusion we found that the velocity process can be represented explicitly by a corresponding fractional Ornstein–Uhlenbeck process. A basic feature arising in the context of this stochastic representation is the random change of time of the system made by subordination. For the position and velocity processes we present a computer visualization of their sample paths and we derive an explicit expression for the two-point correlation function of the velocity process. The obtained stochastic representation is crucial in constructing an algorithm to simulate sample paths of the anomalous diffusion, which in turn allows us to detect and examine many relevant properties of the system under consideration.

Keywords: driven diffusive systems (theory), stochastic particle dynamics (theory)
Fractional Klein–Kramers dynamics for subdiffusion and Itô formula

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1. Introduction

An anomalous process $Z(t)$ is characterized through its nonlinear in time mean-squared displacement (MSD): $\langle (Z(t) - \langle Z(t) \rangle)^2 \rangle \propto K t^a$, where $K$ is a diffusion coefficient. If $0 < a < 1$ then we have subdiffusion and if $a > 1$ we have superdiffusion. There exist two approaches to describe and investigate subdiffusion processes in the framework of continuous time random walk (CTRW). The first one is the fractional Fokker–Planck equation (FFPE) [1]–[3], and the second one is the subordinated Langevin equation [4]–[8]. Our approach is based on subordinated Langevin equations without using FFPEs. Such an approach allows us to analyze statistical properties of the trajectories and gives the complete description of the stochastic process [9,10].

Many physical transport phenomena take place under the influence of an external field. A framework for the treatment of anomalous diffusion problems under the influence of an external field is developed in terms of the FFPE. It provides a useful approach for the description of transport dynamics in complex systems which are governed by anomalous diffusion [1,2] and non-exponential relaxation patterns [11]–[13]. The FFPE can be rigorously derived from the generalized master equation on the CTRW models as shown in [1].

The CTRW is a successful model for normal and anomalous diffusion in a variety of physical systems [2]. It provides a firm statistical foundation for the FFPE and it is a simple model for the investigation of such intriguing phenomena of non-equilibrium statistical physics as weak ergodicity breaking [14], ageing phenomena [15], and inertial particles diffusing in a potential [16].

Unlike Markovian diffusion processes, which are fully characterized by their transition probabilities, non-Markovian anomalous diffusion requires the full hierarchy of multi-point distribution functions for its complete characterization [17]. So, in consequence, multi-point correlation functions are necessary tools to distinguish between CTRW stochastic dynamics and other non-Markovian models of anomalous diffusion like, for example, fractional Brownian motion [18,19]. We note here that even the simple two-point
correlation function cannot be found from the FFPE since the corresponding process is non-Markovian.

In the classical theory of Brownian transport the phase space dynamics is described by the deterministic Klein–Kramers equations [2]. In the high-friction limit it reduces to the Fokker–Planck–Smoluchowski equation, whereas in the low-friction limit case one obtains the Rayleigh equation describing the relaxation of the velocity probability distribution function (PDF) toward the Maxwell distribution. For a discussion of generalized Klein–Kramers equations based on the generalized Chapman–Kolmogorov equation, see [20]. Classical Brownian transport is characterized by linear in time MSD in the force free limit. However, in various physical systems, it has been found that temporal and spatial correlations cause anomalous transport with corresponding non-Gaussian PDF and nonlinear in time MSD [2].

2. Definitions and notation

A large class of subdiffusive processes $Y_\alpha(t)$ can be constructed as follows [7, 8]:

$$Y_\alpha(t) = X(S_\alpha(t)), \quad t \in [0, T],$$

where $\{X(\tau)\}_{\tau \geq 0}$ is a Brownian diffusion (with internal time $\tau$) given by

$$dX(\tau) = F(X(\tau))\eta^{-1}d\tau + (2K)^{1/2}dB(\tau), \quad X(0) = X_0,$$

where $F(x)$ is a force. Moreover, $\eta$ is the generalized friction constant and the constant $K$ denotes the anomalous diffusion coefficient. Subordinator $S_\alpha(t)$ is independent on $X(\tau)$. It is called the inverse $\alpha$-stable subordinator since it is defined in the following way [21, 22]:

$$S_\alpha(t) = \inf\{\tau > 0 : U_\alpha(\tau) > t\},$$

where $\{U_\alpha(\tau)\}_{\tau \geq 0}, \alpha \in (0, 1)$, denotes a strictly increasing $\alpha$-stable Lévy motion [23], with Laplace transform $\langle e^{-kU_\alpha(\tau)} \rangle = e^{-k^{\alpha}}$. The role of the inverse $\alpha$-stable subordinator $S_\alpha(t)$ is parallel to the role played by the Riemann–Liouville operator $\frac{d}{dt}D_t^{1-\alpha}$ in the FFPEs, see [2, 5, 7, 8].

Let us note that so called time-change operation (subordination) $\tau \to S_\alpha(\tau)$ transforms a Brownian diffusion $X(\tau)$ with the MSD $\langle X^2(\tau) \rangle \propto \tau$ into the subdiffusive process $Y_\alpha(t)$ with $\langle Y_\alpha^2(t) \rangle \propto t^{\alpha}, 0 < \alpha < 1$.

From (1) it follows that subdiffusion is a combination of two independent processes: the first process $X(\tau)$ is the Brownian diffusion and the second one introduces the trapping events and is represented by $S_\alpha(t)$, therefore properties of $S_\alpha(t)$ are relevant for understanding subdiffusion.

The inverse $\alpha$-stable subordinator $S_\alpha(t)$ starts from zero, is nondecreasing, and it has continuous sample paths. Those properties follows directly from definition (3) of $S_\alpha(t)$ and allow us to understand and treat the inverse $\alpha$-stable subordinator as a random time. From $1/\alpha$-selfsimilarity of $U_\alpha(\tau)$ it follows that in each point $t \geq 0$, $S_\alpha(t)$ has the same distribution as $(t/U_\alpha(1))^{\alpha}$ and moreover $S_\alpha(t)$ is $\alpha$-selfsimilar, i.e. for each $c > 0$, $S_\alpha(ct) \overset{d}{=} c^\alpha S_\alpha(t)$. Furthermore, almost all sample paths of $S_\alpha(t)$ have finite variation on each bounded interval, trajectories of $S_\alpha(t)$ are continuous but simultaneously singular (meaning that $(d/dt)S_\alpha(t) = 0$ almost everywhere), [24]. Moreover, $S_\alpha(t)$ is
a non-Markovian process and its increments are neither independent nor stationary. Moments of \( S_\alpha(t) \) \((p \in [1, \infty]\)) are given in terms of the gamma function. In particular \( \langle S_\alpha(t) \rangle = t^\alpha/\Gamma(\alpha + 1) \) and \( \langle S_\alpha^2(t) \rangle = 2t^{2\alpha}/\Gamma(2\alpha + 1) \). For each \( k \geq 0 \) and \( t \geq 0 \), the Laplace transform of \( S_\alpha(t) \) is given by

\[
\langle e^{-kS_\alpha(t)} \rangle = E_\alpha(-kt^\alpha),
\]

where \( E_\alpha(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(na + 1)} \) is the Mittag-Leffler function [25].

The subordinated Langevin equation describing subdiffusive process \( Y_\alpha(t) \) can be written in the form

\[
dY_\alpha(t) = F(Y_\alpha(t)) \eta^{-1} dS_\alpha(t) + (2K)^{1/2} dB(S_\alpha(t)), \quad Y_\alpha(0) = X_0.
\]

Unfortunately, the solution of this stochastic differential equation (SDE) is non-Markovian. Nevertheless, it was pointed out in [4, 5] that such SDEs have clear and strict physical meaning: among others, the subordination does not break the fluctuation-dissipation relation and the Boltzmann H-theorem.

The classical Itô formula is a main tool for solving SDEs (in particular SDEs of type (2) for process \( X(\tau) \)). However, we will need here the following extension for the subdiffusion process given by the SDE (5). Let \( f \) be a smooth function, then \( \{f(Y_\alpha(t), S_\alpha(t))\}_{t \in [0,T]} \) is the solution of the subordinated SDE:

\[
df (Y_\alpha(t), S_\alpha(t)) = f_y (Y_\alpha(t), S_\alpha(t)) F(Y_\alpha(t)) \eta^{-1} dS_\alpha(t) + (f_x (Y_\alpha(t), S_\alpha(t)) + K f_{yy} (Y_\alpha(t), S_\alpha(t))) dS_\alpha(t) + f_y (Y_\alpha(t), S_\alpha(t)) (2K)^{1/2} dB(S_\alpha(t)).
\]

The above result follows from the two-dimensional Itô formula for semimartingales \( S_\alpha(t) \) and \( Y_\alpha(t) \) [26]. See also [27].

### 3. Fractional Klein–Kramers equation

The generalization of the classical Fokker–Planck equation to the phase space, i.e. taking account of both the position and the velocity of the particles whose mass cannot be neglected, was put forward by Klein [28] and was rederived by Kramers [29]. See also [30] for historical comments.

In the literature, different fractional generalizations of the classical Klein–Kramers equation were introduced based on FFPEs [2, 6, 20]. We focus here on the fractional Klein–Kramers equation introduced and discussed in [31–33]:

\[
\frac{\partial W(x, v, t)}{\partial t} = \gamma_0 D_t^{1-\alpha} \left[ -v \frac{\partial}{\partial x} + \frac{\partial}{\partial v} \left( \eta v - \frac{F(x)}{m} \right) + \eta k_B T \frac{\partial^2}{\partial v^2} \right] W(x, v, t),
\]

where \( m \) is a mass of the particle, \( \eta \) is the friction constant (proportional to velocity), \( k_B T \) is the Boltzmann temperature and the factor \( \gamma_0 \) is the ratio of the intertrapping time scale and the internal waiting scale whose units are \( [\gamma_0] = s^{-\alpha} \) [32]. Moreover, \( D_t^{1-\alpha} \) is the Riemann–Liouville fractional integral operator [25]. The above FFPE describes an evolution in time of the PDF \( W(x, v, t) \) in phase space, for both the velocity \( v \) and position \( x \) of a subdiffusive particle in an external force field \( F(x) \). The numerical methods and approach by the subordinated Langevin equations for the FKKE (7) can be found in [33].
The Klein–Kramers equation is fundamental in modeling of particle escape over a barrier, first passage time and many other physical processes. Similarly, FKKE plays a crucial role in investigating the variety of systems characterized by slow dynamics. Equation (7) describes the multiple trapping scenario, in which the trapping events are superimposed on the Langevin dynamics. In this scenario, the test particle moves according to Brownian diffusion. However it is successively immobilized in traps. The particle is released after some waiting time drawn from the heavy-tailed density function $w(t) \propto t^{-1-\alpha}$ determined by the subordinator $S_\alpha(t)$. It is assumed here that, following a trapping event, the particle is released with the same position and velocity that it had prior to the immobilization [2,33].

The Langevin picture of the classical Klein–Kramers equation for the particle’s movement under external potential is the following:

$$\frac{dx}{d\tau} = v(\tau) \, d\tau, \quad x(0) = x_0, \quad (8)$$

$$\frac{dv}{d\tau} = \left( -\eta v(\tau) + \frac{F(x(\tau))}{m} \right) \, d\tau + \sqrt{2\eta k_B T \over m} \, dB(\tau), \quad v(0) = v_0, \quad (9)$$

where $F(x)$ is an external force. Now, let us consider the fractional analogue of the classical model for the particle’s motion under an external force field.

Subdiffusive behavior (with characteristic stops) is understood in the sense of the MSD $(Y^2(t)) \propto t^\alpha$, $0 < \alpha < 1$, so subordination of the position process $x(u)$ by $S_\alpha(t)$ leads directly to the new subdiffusive position process $x_\alpha(t)$. Thus, the construction of the subdiffusive model for the particle’s motion under external force is the following:

$$x_\alpha(t) = x_0 + \int_0^{S_\alpha(t)} \gamma_\alpha v(\tau) \, d\tau,$$

where $x_\alpha(t) = x(S_\alpha(t))$ is the subdiffusive position with characteristics stops, $\gamma_\alpha$ is an additional factor needed to define the fractional dynamics and $x(u), v(\tau)$ are given by the system of SDEs (8) and (9). Using the property of subordinated integrals and a notation $v(S_\alpha(u)) = v_\alpha(u)$, we obtain that

$$x_\alpha(t) = x_0 + \int_0^t \gamma_\alpha v(S_\alpha(u)) \, dS_\alpha(u) = x_0 + \int_0^t \gamma_\alpha v_\alpha(u) \, dS_\alpha(u). \quad (10)$$

Moreover, in the case of the system of equations (8) and (9), we conclude that for subdiffusive movement of the particle it should be replaced by the following system of subordinated SDEs:

$$\frac{dx_\alpha}{d\tau} = \gamma_\alpha v_\alpha(t) \, dS_\alpha(t), \quad x_\alpha(0) = x_0, \quad (11)$$

$$\frac{dv_\alpha}{d\tau} = \gamma_\alpha \left( -\eta v_\alpha(t) + \frac{F(x_\alpha(t))}{m} \right) \, dS_\alpha(t) + \sqrt{2\gamma_\alpha \eta k_B T \over m} \, dB(S_\alpha(t)), \quad v(0) = v_0. \quad (12)$$

Actually, it was proved in [33] that the PDF $W(y,v,t)$ of the two-dimensional stochastic process $Z_\alpha(t) = (x_\alpha(t), v_\alpha(t))$ satisfying SDEs (11) and (12) is the solution of the FKKE (7).

Generally, the analytical solution $(x_\alpha(t), v_\alpha(t))$ of SDEs (11) and (12) is hard to determine and it depends strongly on the force field $F(x)$. However, taking advantage of the Itô formula (6), in many cases it is possible to find the explicit form of the solution. Then, one can obtain all probabilistic properties of both processes, i.e. the corresponding multi-point correlation functions, moments and asymptotic distributions.
For example, in the case of constant force \( F(x) = F \) the explicit solution of the velocity SDE (12) can be obtained by using the Itô formula for subdiffusion (6) with random time dependent function \( f(x, S_\alpha(t)) = x \langle e^{\gamma x} S_\alpha(t) \rangle \). Indeed

\[
d(v_\alpha(t)e^{\gamma \eta S_\alpha(t)}) = \frac{F}{m} e^{\gamma \eta S_\alpha(t)} \, dS_\alpha(t) + \sqrt{2\alpha \eta \frac{k_B T}{m} e^{\gamma \eta S_\alpha(t)}} \, dB(S_\alpha(t)),
\]

(13) since \( f_s(x, S_\alpha(t)) = -\gamma \eta x f_\xi(x, S_\alpha(t)) = 0 \). Now, after integrating both sides of equation (13) we get an explicit representation of \( v_\alpha(t) \):

\[
v_\alpha(t) = v_0 e^{-\gamma \eta S_\alpha(t)} + \frac{F}{\gamma \eta m} (1 - e^{-\gamma \eta S_\alpha(t)})
+ \sqrt{2\alpha \eta \frac{k_B T}{m} \int_0^t e^{-\gamma \eta (S_\alpha(t) - S_\alpha(u))} \, dB(S_\alpha(u))}.
\]

(14)

In the case of the free particle’s movement \( F(x) = 0 \), equation (12) takes a simpler form:

\[
dv_\alpha(t) = -\gamma \eta v_\alpha(t) \, dS_\alpha(t) + \sqrt{2\alpha \eta \frac{k_B T}{m} \, dB(S_\alpha(t)),} \quad v(0) = v_0.
\]

(15)

This is the Ornstein–Uhlenbeck type [34] subordinated SDE, see also [35]. One can get the explicit formula for \( v_\alpha(t) \) putting \( F = 0 \) into equation (14) and obtain

\[
v_\alpha(t) = e^{-\gamma \eta S_\alpha(t)} \left( v_0 + \sqrt{2\alpha \eta \frac{k_B T}{m} \int_0^t e^{\gamma \eta S_\alpha(u)} \, dB(S_\alpha(u))} \right).
\]

(16)

4. Correlation function for the fractional Klein–Kramers dynamics

Using (16) we can analyze many probabilistic characteristics of the velocity process. The first moment of the Ornstein–Uhlenbeck process (16) can be calculated in the following way:

\[
\langle v_\alpha(t) \rangle = \langle v_0 \rangle \langle e^{-\gamma \eta S_\alpha(t)} \rangle + \left\langle \sqrt{2\alpha \eta \frac{k_B T}{m} \int_0^t e^{-\gamma \eta (S_\alpha(t) - S_\alpha(u))} \, dB(S_\alpha(u))} \right\rangle
\]

\[
= \langle v_0 \rangle E_\alpha (-\gamma \eta t^\alpha),
\]

(17)

because \( \langle B(S_\alpha(u)) \rangle = 0 \) and \( \langle e^{-\gamma \eta S_\alpha(t)} \rangle \) is the Laplace transform of \( S_\alpha(t) \) expressed in the form of the Mittag-Leffler function (4).

The covariance function \( \text{Cov}(v_\alpha(t), v_\alpha(u)) \) of the velocity process can be calculated as follows:

\[
\text{Cov}(v_\alpha(t), v_\alpha(u)) = \langle v_\alpha(t)v_\alpha(u) \rangle - \langle v_\alpha(t) \rangle \langle v_\alpha(u) \rangle
\]

\[
= 2\gamma \eta \frac{k_B T}{m} \left( \int_0^t e^{-\gamma \eta (S_\alpha(t) - S_\alpha(\tau))} \, dB(S_\alpha(\tau)) \int_0^u e^{-\gamma \eta (S_\alpha(u) - S_\alpha(\tau))} \, dB(S_\alpha(\tau)) \right)
\]

\[
+ \langle v_0^2 \rangle \left( e^{-\gamma \eta (S_\alpha(t) + S_\alpha(u))} \right) - \langle v_0 \rangle^2 E_\alpha (-\gamma \eta t^\alpha) E_\alpha (-\gamma \eta u^\alpha)
\]

\[
= 2\gamma \eta \frac{k_B T}{m} \left( \int_0^{\min\{t,u\}} e^{-\gamma \eta (S_\alpha(t) + S_\alpha(u) - 2S_\alpha(\tau))} \, dS_\alpha(\tau) \right)
\]

\[
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\[ + \langle v_0^2 \rangle \left( e^{-\frac{\gamma t}{m} (S_0(t) + S_0(u))} \right) - \langle v_0 \rangle^2 E_{\alpha} \left( \frac{\gamma t^\alpha}{m} \right) E_{\alpha} \left( -\frac{\gamma t^\alpha}{m} \right) \]

\[ = \frac{k_B T}{m} \left( \left( e^{-\frac{\gamma t}{m} (S_0(t) + S_0(u)) - 2\alpha (\min(t,u))} \right) - \left( e^{-\frac{\gamma t}{m} (S_0(t) + S_0(u))} \right) \right) \]

\[ + \langle v_0^2 \rangle \left( e^{-\frac{\gamma t}{m} (S_0(t) + S_0(u))} \right) - \langle v_0 \rangle^2 E_{\alpha} \left( \frac{\gamma t^\alpha}{m} \right) E_{\alpha} \left( -\frac{\gamma t^\alpha}{m} \right) \].  

(18)

In the above calculations we use the generalized Itô isometry (see [26]), the fact that \( \langle B(S_0(u)) \rangle = 0 \) and the Laplace transform of \( S_0(t) \). Now, the variance and correlation functions of the velocity process can be easily computed using the relations \( \text{Var}(v_\alpha(t)) = \text{Cov}(v_\alpha(t), v_\alpha(t)) \) and \( \text{Corr}(v_\alpha(t), v_\alpha(u)) = \text{Cov}(v_\alpha(t), v_\alpha(u))/\sqrt{\text{Var}(v_\alpha(t))\text{Var}(v_\alpha(u))} \). For instance

\[ \text{Var}(v_\alpha(t)) = \frac{k_B T}{m} \left( \langle v_0^2 \rangle - \frac{k_B T}{m} \right) E_{\alpha} \left( -\frac{2\gamma t^\alpha}{m} \right) - \langle v_0 \rangle^2 E_{\alpha} \left( -\frac{\gamma t^\alpha}{m} \right). \]

Observe that the above obtained first and second moments are the same as those presented earlier in [32,36,37], where tedious computations were done by using the FFPE methodology. Our approach here is different, since it is based on the subordinated Langevin equation and the Itô formula which allow us to derive a two-point correlation function. This is a main difference from the earlier works.

5. Role of subordination in the fractional Klein–Kramers dynamics

In this section we analyze another possible version of the Klein–Kramers dynamics with subdiffusive noise \( B(S_0(t)) \) only. Let us consider the following system of SDEs:

\[ dx_\alpha(t) = v_\alpha(t) \, dt, \quad x_\alpha(0) = x_0, \]

\[ dv_\alpha(t) = \left( -\gamma_\alpha \eta v_\alpha(t) + F(x_\alpha(t)) \right) \, dt + \sqrt{2\gamma_\alpha \eta \frac{k_B T}{m}} \, dB \left( S_0(t) \right), \quad v_\alpha(0) = v_0. \]  

(19)  

(20)

The main difference between equations (11) and (12) and (19) and (20) is that in (20) the deterministic differential \( dt \) occurs instead of \( dS_0(t) \) as in (12). In turn, in the SDE (20) only the Brownian motion is subordinated. As we will show, this change leads to completely different fractional Klein–Kramers dynamics compared with that from the previous section. Compare figures 1 and 2.

Typical trajectories of the stochastic process \( (x_\alpha(t), v_\alpha(t)) \) which are solutions of SDEs (11) and (12) in the case of \( F(x) = 0 \) are presented in figure 1. The constant intervals of the subordinator \( S_0(t) \) representing trapping periods of the test particle transfer directly to the position process \( x_\alpha(t) \) and the velocity process \( v_\alpha(t) \). The initial assumption that a trapped particle is released with the same position and the same velocity that it had prior to the immobility is clearly satisfied. Observe that the violation of the classical Newton type relation \( (d/dt) \langle x(t) \rangle = \langle v(t) \rangle \) is manifested by the fact that the subordinated velocity process \( v_\alpha(t) \) is not equal to zero on the constant intervals of the subordinated position process \( x_\alpha(t) \).

The actual relationship between the mean position and the mean velocity in the fractional Klein–Kramers dynamics is as follows: \( (d/dt) \langle x_\alpha(t) \rangle = \gamma_\alpha v_\alpha(t) \, dB \left( S_0(t) \right) \), see [31,33]. However, what we actually see in figure 1 is by (11) a realization of the more general probabilistic relation, namely \( dx_\alpha(t) = \gamma_\alpha v_\alpha(t) \, dS_0(t) \). This reduces to the Newton type relation only when \( S_0(t) = t \).

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Figure 1. Sample realizations of (a) the subdiffusive position process $x_\alpha(t)$, (b) the velocity process $v_\alpha(t)$ described by equations (11) and (12). The parameters are $\alpha = 0.85$, $F(x) = 0$, $\gamma_\alpha \eta = 0.2$, $m = 2$, $k_B T = 125$, $x_0 = 0$, $v_0 = 10$, $\delta t = 0.005$ and time period $[0,30]$.

This is in contrast with the situation presented in figure 2, where from (19) we have $(d/dt)x_\alpha(t) = \gamma_\alpha v_\alpha(t)$ and the Newton type relation holds for fractional Klein–Kramers dynamics described by equations (19) and (20) in a stronger probabilistic version.

To simplify calculations let us consider equations (19) and (20) with $F(x) = 0$. Under such an assumption, the velocity process with subdiffusive noise satisfies the following SDE:

$$d v_\alpha(t) = -\gamma_\alpha \eta v_\alpha(t) \, dt + \sqrt{2\gamma_\alpha \eta \frac{k_B T}{m}} \, dB(S_\alpha(t)), \quad v_\alpha(0) = v_0. \quad (21)$$

This is the Ornstein–Uhlenbeck type SDE (compare with (15)). Taking the real-time dependent function $f(x,t) = xe^{\gamma_\alpha \eta t}$ and applying the Itô formula (6), we get

$$d(v_\alpha(t)e^{\gamma_\alpha \eta t}) = \sqrt{2\gamma_\alpha \eta \frac{k_B T}{m}} e^{\gamma_\alpha \eta t} dB(S_\alpha(t)). \quad (22)$$

From here

$$v_\alpha(t) = e^{-\gamma_\alpha \eta t} \left( v_0 + \sqrt{2\gamma_\alpha \eta \frac{k_B T}{m}} \int_0^t e^{\gamma_\alpha \eta u} dB(S_\alpha(u)) \right). \quad (23)$$

Notice that the random factor dependent on $B(S_\alpha(u))$ in equation (23) takes the value zero on some random intervals of time corresponding to constant periods of the inverse $\alpha$-stable subordinator $S_\alpha(t)$. Then, the velocity and the position processes are purely deterministic and are equal to $v_\alpha(t) = v_0 e^{-\gamma_\alpha \eta t}$ and $x_\alpha(t) = x_0 + \int_0^t v_\alpha(u) \, du = x_0 + (v_0 / \gamma_\alpha \eta)(1 - e^{-\gamma_\alpha \eta t})$, respectively on the periods where $S_\alpha(t)$ is constant. It should be emphasized that the processes introduced above with piece-wise deterministic sample paths have already found some applications in risk theory, see [38].

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Figure 2. Sample paths of (a) the position process $x_\alpha(t) = x_0 + \int_0^t v_\alpha(u) \, du$ with subdiffusive noise, (b) the velocity process $v_\alpha(t)$ with subdiffusive noise described by equations (19) and (20). Observe that both $x_\alpha(t)$ and $v_\alpha(t)$ are purely deterministic on random intervals of time: $v_\alpha(t) = v_0 e^{-\gamma_\alpha \eta t}$ and $x_\alpha(t) = x_0 + (v_0/\gamma_\alpha \eta)(1 - e^{-\gamma_\alpha \eta t})$. The parameters are the same as in figure 1.

It is simple to verify that the first moment of $v_\alpha(t)$ has the following form:

$$\langle v_\alpha(t) \rangle = \langle v_0 \rangle e^{-\gamma_\alpha \eta t},$$

while the covariance function is given by

$$\text{Cov}(v_\alpha(t), v_\alpha(u)) = e^{-\gamma_\alpha \eta(t+u)} \left( \text{Var}(v_0) + 2\gamma_\alpha \eta \frac{k_B T}{m \Gamma(\alpha)} \int_0^{\min\{t,u\}} e^{2\gamma_\alpha \eta \tau} \frac{\tau^{1-\alpha}}{\gamma_\alpha \eta + \tau^{1-\alpha}} \, d\tau \right).$$

To get the above formulas we applied the same tools as in the computations of the covariance function (formula (18)) in section 4 and moreover the formula for the first moment for the integral of the inverse subordinator [39]. Simulated paths of the velocity $v_\alpha(t)$ and position $x_\alpha(t) = x_0 + \int_0^t v_\alpha(u) \, du$ processes are presented in figure 2 and clearly they have a piece-wise deterministic character, but are not constant.

6. Summary and conclusions

In this paper, using a subordination method we identify a two-dimensional stochastic process (position, velocity) whose PDF is a solution of the fractional Klein–Kramers equation. The structure of this process agrees with the two-stage scenario underlying the anomalous diffusion mechanism, in which trapping events are superimposed on the Langevin dynamics.

Applying an extension of the celebrated Itô formula for subdiffusion we found that the velocity process can be represented explicitly by a corresponding fractional Ornstein–Uhlenbeck process.
For the position and velocity processes we present a computer visualization of their sample paths (figures 1 and 2) and we derive an explicit expression for the two-point correlation function of the velocity process. The obtained stochastic representation is crucial in constructing an algorithm for simulating sample paths of the anomalous diffusion, which, in turn, allows us to detect and examine many relevant properties of the system under consideration, e.g. modeling of particle escape over a barrier, first passage time and ergodicity breaking.

Since a closed form solution of the fractional Klein–Kramers equation is not known, in order to estimate it one can use a Monte Carlo method based on approximating sample paths of the fractional Ornstein–Uhlenbeck process. An efficient computer algorithm for visualization of the fractional Klein–Kramers dynamics was proposed in [33]. The explicit solutions derived here in the form of Ornstein–Uhlenbeck processes can be used for a simple validation of this methodology.

Let us stress that the single time PDF described by the fractional Klein–Kramers equation gives limited statistical information only. Thus, we would like to underline a need for investigation of multi-point distribution functions in this context, as has been put forward recently [6,17,19]. We hope that our results will contribute to this investigation and to better understanding of the fractional Klein–Kramers dynamics.

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