Subdiffusive Klein-Kramers Model and Itô Formula.

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In this paper we analyze possible extensions of the celebrated Itô formula for subdiffusion. Namely, we show that for any subdiffusive process \( Y_\alpha(t) \) which is a diffusion limit of continuous time random walks, its image \( f(Y_\alpha(t), t) \) by a smooth function \( f \) is given again by a stochastic differential equation of the Langvin type. Obtained two generalizations of the classical Itô formula provide useful tools for solving the subdiffusive Klein-Kramers equation and directly lead to two different subdiffusive Ornstein-Uhlenbeck processes. For the second model the Galilean invariance holds. For the first model we found the approximated velocity process with desired invariance. For both Ornstein-Uhlenbeck processes the explicit stochastic representations and first two moments are derived.

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I. INTRODUCTION

The anomalous processes are characterized through the non-linear in time mean-squared displacement (MSD) [1, 2]:

\[
\langle (X_\tau - \langle X_\tau \rangle)^2 \rangle \propto K \tau^\alpha
\]

where \( K \) is a diffusion coefficient. If \( 0 < \alpha < 1 \) then we have subdiffusion and if \( \alpha > 1 \) we have superdiffusion. There exist two approaches to describe and investigate subdiffusion processes in the framework of CTRW. The first one is the Fractional Fokker-Planck Equation (FFPE) [1–3], and the second one is the subordinated Langevin equation [4, 5]. Our approach is based on the subordinated Langevin equations without using FFPEs. Such an approach allows to analyze statistical properties of the trajectories and gives the complete description of the stochastic process [6, 7]. Thereby it provides deeper insight into the physical nature of the subdiffusion.

The subdiffusive process \( Y_\alpha(t) \) is defined as follows [4, 5]:

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

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

\[
dX(\tau) = F(X(\tau)) \eta^{-1} d\tau + (2K)^{\frac{1}{2}} dB(\tau),
\]

\[
X(0) = X_0,
\]

where \( F(x) = -V'(x) \) (\( F(x) \) is a force and \( V(x) \) is an external potential). 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 [8, 9]:

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

where \( \{U_\alpha(\tau)\}_{\tau \geq 0}, \alpha \in (0, 1), \) denotes a strictly increasing \( \alpha \)-stable Lévy motion [10], with Laplace transform \( \langle e^{-\xi U_\alpha(\tau)} \rangle = e^{-\tau \xi^\alpha} \). The role of the inverse \( \alpha \)-stable subordinator \( S_\alpha(t) \) is parallel to the role played by the Riemann-Liouville operator \( \alpha \mathcal{D}^{1-\alpha}_t \) in the FFPEs, see [2, 4, 5]. For more details see Appendix A.

The classical Itô formula is a main tool for solving Stochastic Differential Equations (SDEs) (in particular SDEs of type (3) for process \( X(\tau) \)) as well as in a derivation of the Feynman-Kac formula which establishes a link between Partial Differential Equations (PDEs) and stochastic processes (given by some SDEs including Brownian diffusion), [11, 12]. In this paper we show how to describe subdiffusive process \( Y_\alpha(t) \) by using SDEs of the Langevin type. We derive two generalizations of the Itô formula for subdiffusion in Appendix B. The main idea employed here is the fact that the subdiffusion process (2) is a semimartingale, [13]. Next, we show how to use the Itô formula to solve subordinated SDEs and to get the explicit representation of process \( Y_\alpha(t) \).

In section II and III we apply the Itô formula for studying properties of two different subdiffusive Klein-Kramers models. The velocity processes in form of two types subdiffusive Ornstein-Uhlenbeck processes are obtained. The subordinated technique is employed here and it is an efficient way to investigate different versions of the Klein-Kramers model, see [14].

First, in section II, we use the Itô formula in order to investigate the subdiffusive particle’s motion under external force-field, and next the subdiffusive particle’s free motion. We focus on the subdiffusive Klein-Kramers model introduced and discussed in [15, 16] and [17]. We show that, for this model, there does not exist any stochastic process describing the velocity of the subdiffusive particle for which the Galilean invariance holds. In section III we propose another subdiffusive modification of the Klein-Kramers model for which the Galilean invariance holds and the displacement process \( x(t) \) still remains subdiffusive in sense of MSD. The proposed model is based on a SDE of the Langevin type with subdiffusive noise. We show how to solve it (in the free-force case) taking advantage of the Itô formula (B7) for subdiffusion for function dependent on real time \( t \). Moreover, we derive the explicit formulas for the subdiffusive displacement and the

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velocity processes and we calculate their first and second moments.

II. SUBDIFFUSIVE KLEIN-KRAMERS MODEL

In the literature, there were introduced different subdiffusive (fractional) generalizations of the classical Klein-Kramers model based on FFPEs [2, 14–16, 18–20]. We focus here on the subdiffusive Klein-Kramers model introduced and discussed in [15, 16] and [17]:

$$\frac{\partial W(x, v, t)}{\partial t} = \gamma_0 D_1^{1-\alpha} \left[ -v \frac{\partial}{\partial x} + \frac{\partial}{\partial v} \left( \eta v - \frac{F(x)}{m} \right) \right] +$$

$$+ \frac{k_B T}{m} \frac{\partial^2}{\partial v^2} W(x, v, t),$$

(5)

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 $[\gamma_0] = s^{-\alpha}$ [16]. The above FFPE describes an evolution in time of the PDF $W(x, v, t)$ in phase space, for both the velocity $v$ and coordinate $x$ of a subdiffusive particle in an external force field $F(x) = -V'(x)$. The numerical methods and approach by the subordinated Langevin equations for the FKKE (5) can be found in [17].

First, we show that there does not exist a rigorously defined stochastic process which can be interpreted as the velocity of the subdiffusive particle for which the Galilean invariance holds. So, the relationship between displacement and the velocity $\dot{x}(t) = v(t)$ does not hold.

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

$$x(u) = x(0) + \int_0^u \gamma_0 v(\tau) d\tau, \quad x(0) = x_0,$$

$$dv(\tau) = \gamma_0 \left( -\eta v(\tau) + \frac{F(x(\tau))}{m} \right) d\tau + \sqrt{2\gamma_0 \eta k_B T \frac{m}{m}} dB(\tau),$$

$$v(0) = v_0,$$  
(6)

where $F(x) = -V'(x)$ is an external force and $\gamma_0$ is an additional factor needed to define subdiffusive Klein-Kramers model (see [15–17]). Now, let us consider the subdiffusive analogon of the classical model for the particle’s motion under external force-field.

Subdiffusive behavior (with characteristic stops) is understood in sense of the MSD $\langle x^2(u) \rangle \propto u^\alpha$, $0 < \alpha < 1$, so the displacement process $x(u)$ should be subordinated by $S_\alpha(t)$.

The subdiffusive model of the particle’s motion under external potential is defined here by: $Y_\alpha(t) = x_0 + \int_0^t \gamma_\alpha v(\tau) d\tau$, where $Y_\alpha(t) = x(S_\alpha(t))$ is the subdiffusive displacement with characteristics stops and $x(u)$ and $v(\tau)$ are given by the system of SDEs (6).

Using the relation for subordinated integrals we get that:

$$Y_\alpha(t) = x_0 + \int_0^t \gamma_\alpha v(S_\alpha(u)) dS_\alpha(u).$$  
(7)

Moreover, in case of system of Eqs. (6), we conclude that for subdiffusive movement of the particle it should be used the following system of subordinated SDEs:

$$dY_\alpha(t) = \gamma_\alpha v(S_\alpha(t)) dS_\alpha(t), \quad Y_\alpha(0) = x_0$$

$$dv(S_\alpha(t)) = \gamma_\alpha \left(-\eta v(S_\alpha(t)) + \frac{F(Y_\alpha(t))}{m}\right) dS_\alpha(t) +$$

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

(8)

Actually, it was proved in [17], that PDF $W(y, v, t)$ of the two-dimensional stochastic process $Z_\alpha(t) = (Y_\alpha(t), v(S_\alpha(t)))$ satisfying SDEs (8) is the solution of the FKKE (5).

In this place, let us note that the relationship between the mean position $\langle Y_\alpha(t) \rangle$ and the mean velocity $\langle v(S_\alpha(t)) \rangle$ is the following [15–17]: $(d/dt)\langle Y_\alpha(t) \rangle = \gamma_\alpha D_1^{1-\alpha} \gamma_\alpha \langle v(S_\alpha(t)) \rangle$.

So, the Galilean invariance is violated in the mean sense.

After this discussions a more general question is the following: does there exist any well-defined stochastic process $v_\alpha^*(t)$ (some modification of $v(S_\alpha(t))$) which can be interpreted as a “normal” velocity of the subdiffusive particle in considered here model (8) for which the Galilean invariance holds? As we show in a moment, the answer is no!

Let us assume that there exists stochastic process (denoted by $v_\alpha^*(t)$) which can be interpreted as the velocity of the subdiffusive particle and the Galilean invariance holds. Under such an assumption, the relationship $Y_\alpha(t) = v_\alpha^*(t)$ between subdiffusive displacement process $Y_\alpha(t)$ and the process $v_\alpha^*(t)$ holds. So, to get an explicit stochastic representation of the process $v_\alpha^*(t)$ we need the following representation of $Y_\alpha(t)$:

$$Y_\alpha(t) = x_0 + \int_0^t \gamma_\alpha v(S_\alpha(u)) \xi_\alpha(u) \, du,$$  
(9)

where $\xi_\alpha(u)$ is a stochastic process related to $S_\alpha(u)$, see (7). From the definition of the above Riemann-Stieltjes integral it is only possible when $\xi_\alpha(t) = S'_\alpha(t)$ (where $S'_\alpha(t)$ denotes derivative of $S_\alpha(t)$). But from Appendix A, $S'_\alpha(t)$ is equal to 0 almost everywhere, so $dS_\alpha(t) \neq S'_\alpha(t) dt$ and hence the formula (9) is meaningless. Therefore, there does not exist a
rigorously defined stochastic process $v_\alpha^*(t)$, which can be understood as a velocity of the subdiffusive particle, for which the Galilean invariance holds.

Nevertheless, it is possible to define some approximation of the velocity process for which the Galilean invariance holds. A natural method to avoid difficulties with $S'_\alpha(t)$ is to use approximation of derivative (see Fig.1):

$$S'_\alpha(t) \approx \frac{S_\alpha(t + \delta t) - S_\alpha(t)}{\delta t} = S^{(\delta t)}_\alpha(t), \quad \text{(10)}$$

for some fixed, appropriately small parameter $\delta t > 0$.

![Figure 1](image1.png)

**FIG. 1:** (Color on line) Sample realizations of (a) inverse $\alpha$-stable subordinator $S_\alpha(t)$, (b) process $S^{(\delta t)}_\alpha(t)$. The parameters are: $\alpha = 0.9$, $\delta t = 0.005$ and time period $[0, 10]$.

Let us consider process $Y_\alpha(t)$ for $t \in [0, T]$ ($T$ is a fixed time). Let $0 = u_0 < u_1 < \ldots < u_n = T$ be partition of the interval $[0, T]$ such that $u_i = i\delta t$, $i = 0, 1, \ldots, n$, where $\delta t = T/n$. Then $Y_\alpha(t)$ can be approximated on interval $[0, T]$ by the process $Y^{(\delta t)}_\alpha(t)$ defined as (the integral is approximated by sum, compare with formula (9)):

$$Y^{(\delta t)}_\alpha(u_i) = x_0 + \sum_{k=1}^{i} v(S_\alpha(u_{k-1}))(S_\alpha(u_k) - S_\alpha(u_{k-1})) =$$

$$= x_0 + \sum_{k=1}^{i} \left[ v(S_\alpha(u_{k-1}))S^{(\delta t)}_\alpha(u_{k-1}) \right](u_k - u_{k-1}), \quad \text{(11)}$$

where $i = 0, \ldots, n$. Such an approach is natural from the practical applications point of view, because for computer simulations we always use a discrete approximation of the continuous processes defined on finite interval of time. Now, we can conclude that the velocity process (actually its approximation) in subdiffusive model, which has the natural physical interpretation (i.e., Galilean invariance holds) should be defined as:

$$v^{(\delta t)}_\alpha(t) = \gamma_\alpha v(S_\alpha(t))S^{(\delta t)}_\alpha(t). \quad \text{(12)}$$

The relationship between processes $Y^{(\delta t)}_\alpha(t)$ and $v^{(\delta t)}_\alpha(t)$ for $t \in [0, T]$, is exactly the same as in (9), that is $Y^{(\delta t)}_\alpha(t) = x_0 + \int_{0}^{t} v^{(\delta t)}_\alpha(u)\, du$.

Notice, that the approximated velocity process $v^{(\delta t)}_\alpha(t)$ consists of two processes: first process $v^{(\delta t)}_\alpha(t)$ causes that if particle is immobilized in trap (stays motionless) then its velocity is equal to 0, while the second process $\gamma_\alpha v(S_\alpha(t))$ describes the usual velocity of the particle and it is subdiffusive. On the one hand, see Fig.2, approximated velocity process $v^{(\delta t)}_\alpha(t)$ behaves similarly to $v(S_\alpha(t))$, but on the other hand process $v^{(\delta t)}_\alpha(t)$ is more complicated and irregular than $v(S_\alpha(t))$ and this is its disadvantage. Furthermore, there does not exist any FFPE describing the PDF of the process $v^{(\delta t)}_\alpha(t)$, because it is not continuous.

Now, we apply the Itô formula for subdiffusion (see Appendix B) to find the explicit representation of the process $v(S_\alpha(t))$. In case of constant force $F(x) = F$ the explicit solution of the subordinated SDE (8) can be obtained by using the Itô formula for subdiffusion (B5) with random time dependent function $f(x, S_\alpha(t)) = xe^{\gamma_\alpha \eta S_\alpha(t)}$. Indeed:

$$d(v(S_\alpha(t))e^{\gamma_\alpha \eta S_\alpha(t)}) = Fe^{\gamma_\alpha \eta S_\alpha(t)}dS_\alpha(t) +$$
Now, after integrating both sides of Eq. (13) we get an explicit representation of \( v(S_\alpha(t)) \):

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

Notice, that if we known the explicit representation of process \( v(S_\alpha(t)) \), one can easily compute its moments. For example in case of the free particle’s movement \( F(x) = 0 \), Eq. (8) takes a simpler form:

\[
\frac{dv}{dt}(S_\alpha(t)) = -\gamma_\alpha \gamma S_\alpha(t) dS_\alpha(t) + \sqrt{\frac{2 \gamma_\alpha \eta k_B T}{m}} dB(S_\alpha(t)),
\]

\[ v(0) = v_0. \]  

This is the Ornstein-Uhlenbeck type subordinated SDE [21], see also [22]. One can get the explicit formula for \( v(S_\alpha(t)) \) putting \( F = 0 \) into Eq. (14) and obtain:

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

The corresponding FPPE (The fractional Rayleigh equation) describing the PDF \( P(v, t) \) of the process \( v(S_\alpha(t)) \), given by (16), has the following form [2, 15, 16, 18, 19]:

\[
\frac{\partial P(v, t)}{\partial t} = \eta_\alpha \gamma_0 D_1^{1-\alpha} \left[ \frac{\partial}{\partial v} v + \frac{k_B T}{m} \frac{\partial^2}{\partial v^2} \right] P(v, t).
\]  

The first moment of the Ornstein-Uhlenbeck process (16) is the following:

\[
\left\langle v(S_\alpha(t)) \right\rangle = \langle v_0 \rangle e^{-\gamma_\alpha \eta S_\alpha(t)} + \frac{1}{\gamma_\alpha \eta} \left\langle e^{-\gamma_\alpha \eta S_\alpha(t)} \right\rangle + \frac{k_B T}{m} \int_0^t \left\langle e^{-\gamma_\alpha \eta S_\alpha(t) - S_\alpha(u)} \right\rangle dB(S_\alpha(u)) = \langle v_0 \rangle E_\alpha (-\gamma_\alpha \eta t^\alpha),
\]

because \( \langle B(S_\alpha(u)) \rangle = 0 \) and \( \left\langle e^{-\gamma_\alpha \eta S_\alpha(t)} \right\rangle \) is the Laplace transform of \( S_\alpha(t) \) (see Appendix A). While the second moment of \( v(S_\alpha(t)) \) can be calculated as follows:

\[
\left\langle v^2(S_\alpha(t)) \right\rangle = \langle v_0^2 \rangle \left\langle e^{-2\gamma_\alpha \eta S_\alpha(t)} \right\rangle + \frac{k_B T}{m} \int_0^t \left\langle e^{-2\gamma_\alpha \eta S_\alpha(t) - S_\alpha(u)} \right\rangle dB(S_\alpha(u)) = \langle v_0^2 \rangle E_\alpha (-2\gamma_\alpha \eta t^\alpha) + \frac{k_B T}{m} \int_0^t \left\langle e^{-2\gamma_\alpha \eta S_\alpha(t) - S_\alpha(u)} \right\rangle dB(S_\alpha(u)).
\]  

In above calculations we use the formula for square of sum, Itô isometry (because \( [B(S_\alpha(u))] = S_\alpha(u) \)), fact that \( \langle B(S_\alpha(u)) \rangle = 0 \) and the Laplace transform of \( S_\alpha(t) \). Let us note that above results are the same as those obtained in [16, 18, 19], where moments were computed by using the FPPE.

### III. KLEIN-KRAMERS MODEL WITH SUBDIFFUSIVE NOISE

In this section we analyze the version of the Klein-Kramers model with subdiffusive noise \( B(S_\alpha(t)) \). Let us consider the following system of SDEs:

\[
x_\alpha(t) = x_\alpha(0) + \int_0^t v_\alpha(\tau) d\tau, \quad x_\alpha(0) = x_0,
\]

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

\[ v_\alpha(0) = v_0. \]  

The main difference between models (8) and (20) is that in SDEs (20) occurs deterministic differential \( dt \) instead of \( dS_\alpha(t) \) as in (8). So this is the SDE of type (B7). Therefore, to investigate version (20) of the Klein-Kramers model we can apply the Itô formula for subdiffusion (B7) with function dependent on real time. Moreover, let us note that in considered
here Klein-Kramers model it is obvious that \( \dot{x}_\alpha(t) = v_\alpha(t) \), thus the Galilean invariance holds.

To simplify calculations let us consider Eqs. (20) with \( F(x) = 0 \). Under such an assumption, the velocity process with subdiffusive noise satisfy the following SDE:

\[
dv_\alpha(t) = -\eta v_\alpha(t) dt + \sqrt{2\gamma_\alpha \eta k_B T/m} dB(S_\alpha(t)),
\]

\[
v_\alpha(0) = v_0.
\]

This is the Ornstein-Uhlenbeck type SDE (compare with (15)). Taking the function \( f(x, t) = xe^{\eta t} \), we get:

\[
d(v_\alpha(t)e^{\eta t}) = \sqrt{2\gamma_\alpha \eta k_B T/m} e^{\eta t} dB(S_\alpha(t)).
\]

From here:

\[
v_\alpha(t) = e^{-\eta t}(v_0 + \sqrt{2\gamma_\alpha \eta k_B T/m} \int_0^t e^{\eta u} dB(S_\alpha(u))).
\]

Notice, that random factor dependent on \( B(S_\alpha(u)) \) in Eq. (23) decays on some random intervals of time corresponding to constant periods of the inverse \( \alpha \)-stable subordinator \( S_\alpha(t) \).

The velocity process is a purely deterministic and equal to \( v_\alpha(t) = v_0 e^{-\eta t} \) on constant periods of \( S_\alpha(t) \) and the displacement process is equal to \( x_\alpha(t) = x_0 + \int_0^t v_\alpha(u) du = x_0 + \frac{\eta}{\alpha}(1 - e^{-\eta t}) \). For this reason these are called semi-deterministic processes.

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

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

while the second moment of \( v_\alpha(t) \) can be computed in the following way:

\[
\langle v_\alpha^2(t) \rangle = \langle v_0^2 \rangle e^{-2\eta t} +
\]

\[
+ \left\langle \left( e^{-\eta t} \sqrt{2\gamma_\alpha \eta k_B T/m} \int_0^t e^{\eta u} dB(S_\alpha(u)) \right)^2 \right\rangle +
\]

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

\[
e^{-2\eta t} \left( \langle v_0^2 \rangle + 2\gamma_\alpha \eta k_B T/m \int_0^t e^{2\eta u} dS_\alpha(u) \right).
\]

In above calculations we applied the same tools as in computations of the second moment (formula (19)) in previous section. Now, taking advantage of the following formula for the first moment for integral of the inverse subordinator [28]:

\[
\left\langle \int_0^t F(u) dS_\alpha(u) \right\rangle = \frac{1}{\Gamma(\alpha)} \int_0^t u^{-\alpha} F(u) du,
\]

thereby we get finally:

\[
\langle v_\alpha^2(t) \rangle = e^{-2\eta t} \left( \langle v_0^2 \rangle + \frac{2\gamma_\alpha \eta k_B T/m \Gamma(\alpha)}{\Gamma(\alpha)} \int_0^t e^{2\eta u} dS_\alpha(u) \right).
\]

Simulated paths of the velocity \( v_\alpha(t) \) and the displacement \( x_\alpha(t) = x_0 + \int_0^t v_\alpha(u) du \) processes are presented in Fig.3 and clearly they have a semi-deterministic character.

**IV. CONCLUSIONS**

In this work we concentrate on the subdiffusive processes. Our approach is based on the subordinated Langevin equations without using FFPEs. We have derived two different Itô formulas for Brownian subdiffusions (Appendix B) which can be used to investigate subdiffusive Klein-Kramers models and for solution of subordinated SDEs. We have also discussed properties of the inverse-time \( \alpha \)-stable subordinator \( S_\alpha(t) \) (internal time clock, Appendix A) playing the parallel role to the Riemann-Liouville operator \( _0D^\delta_t \) in the FFPEs framework.
As an application of the Itô formulas we have derived here the subdiffusive and so called semi-deterministic Ornstein-Uhlenbeck processes, see Fig.2 and Fig.3, respectively. The basic difference between two versions of Klein-Kramers models investigated in sections II and III is that on constant periods of the inverse $\alpha$-stable subordinator $S_\alpha(t)$ the semi-deterministic versions of stochastic processes describing the displacement and the velocity are a purely deterministic but not constant (compare Fig.2 and Fig.3).

Taking advantage of an explicit representation of subdiffusive Ornstein-Uhlenbeck processes (16) and (23), we have computed their moments. The obtained results for process (16), are the same as in [16, 18, 19], by using FFPEs.

The explicit stochastic representation of physical processes given by the SDEs allows to understand properties of subdiffusion, to calculate moments and their asymptotic behavior as well as to apply Monte Carlo methods. For example, another advantage of our approach is a possibility to analyze sample paths of subdiffusive processes and not only their probability distribution function (PDF) as it is in the FFPEs framework. Such an approach gives the complete mathematical description of the subdiffusive processes.

We demonstrate that the subordinated Langevin picture of subdiffusion and the Itô formula provide convenient tools and allow to study deeper subdiffusive dynamics.

V. ACKNOWLEDGMENTS

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Appendix A: SUBORDINATORS

From (2) 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 and we discuss them here.

The inverse $\alpha$-stable subordinator $S_\alpha(t)$ starts from zero, is nondecreasing, and it has continuous sample paths. Those properties follow directly from definition (4) of $S_\alpha(t)$ and allow 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 $c > 0$, $S_\alpha(ct) \sim c^\alpha S_\alpha(t)$. 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 (it means that $S'_\alpha(t) = 0$ almost everywhere), [26]. Moreover, $S_\alpha(t)$ does not have Markov property and its increments are neither independent nor stationary. Moments of $S_\alpha(t)$ are given by ($p \in [1, \infty]$):

$$\langle S^p_\alpha(t) \rangle = \frac{\Gamma(p+1)t^p\alpha}{\Gamma(p\alpha+1)},$$  \hspace{1cm} (A1)

where $\Gamma(x) = \int_0^\infty x^{a-1}e^{-x}dx$ is the Gamma function. In particular $\langle S_\alpha(t) \rangle = \frac{t^\alpha}{\Gamma(\alpha+1)}$, and $Var(S_\alpha(t)) = \frac{2\Gamma(2\alpha)}{\Gamma(2\alpha+1)} - \left(\frac{t^\alpha}{\Gamma(\alpha+1)}\right)^2$. Taking advantage of the Chebyshev inequality and the formula for the first moment of $S_\alpha(t)$, we get for each $t \geq 0$:

$$P(S_\alpha(t) \geq t) \leq \frac{1}{t^{1-\alpha}\Gamma(\alpha+1)}.$$  \hspace{1cm} (A2)

Also for each $k \geq 0$ and $t \geq 0$, the Laplace transform of $S_\alpha(t)$ is given by $\langle e^{-kS_\alpha(t)} \rangle = E_\alpha(-ke^\alpha)$, where

$$E_\alpha(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(n\alpha+1)}$$

is the Mittag-Leffler function [25]. It was showed in [5] that for all $0 < u \leq t < \infty$:

$$\langle S_\alpha(u)S_\alpha(t) \rangle = \frac{u^{2\alpha}}{\Gamma(2\alpha+1)} + \frac{\alpha}{\Gamma^2(\alpha+1)} \int_0^u (t-s)^{\alpha} s^{\alpha-1}ds.$$  \hspace{1cm} (A3)

Hence, the covariance function for $S_\alpha(t)$ is given by:

$$Cov(S_\alpha(u), S_\alpha(t)) =$$

$$= \frac{u^{2\alpha}}{\Gamma(2\alpha+1)} + \frac{\alpha}{\Gamma^2(\alpha+1)} \int_0^u (t-s)^{\alpha} s^{\alpha-1}ds - \frac{(ut)^\alpha}{\Gamma^2(\alpha+1)}.$$  \hspace{1cm} (A4)

The most important conclusions from presented here properties of the inverse $\alpha$-stable subordinator is that $S_\alpha(t)$ can be interpreted as a random time (the inner time clock) and moreover we can define Stieltjes integral for it, because $S_\alpha(t)$ has finite variation.

The properties of subordinated Brownian motion $B(S_\alpha(t))$ were discussed in detail in [26]. Let us note that the solution of SDE (3) exists and is unique only if coefficients satisfy the space-variable Lipschitz condition and the spatial growth condition [11, 12]. The subdiffusion with a purely time dependent force $F(t)$ was discussed in [3, 27]. In turn, subdiffusion driven by the space-time-dependent force $F(x,t)$ was considered in [5].

Appendix B: The Itô formula for subdiffusion

We describe here two different generalizations of the classical Itô formula for subdiffusion. The first generalization of the Itô formula for function dependent on random time $S_\alpha(t)$ is useful for solving subordinated SDEs. The second one, for function dependent on real time $t$, allows to represent the image of a subdiffusive processes by any smooth function i.e. $f(Y_\alpha(t), t)$.

At the beginning let us recall the concept of continuous semimartingales. It is a process $\{X(\tau)\}_{\tau \geq 0}$ which has the
Doob-Meyer decomposition [23, 24, 29]: \( X(\tau) = X(0) + A(\tau) + M(\tau) \) a.s., where \( M(0) = A(0) = 0, M(\tau) \) is a continuous local martingale and \( A(\tau) \) is a continuous stochastic process of finite variation. The useful property of a continuous semimartingale is that it has a finite quadratic variation \([X]_{\tau} = [M]_{\tau}, \) see [23, 24]. In turn the quadratic covariation of two continuous semimartingales \( X(\tau) = X(0) + A^{(x)}(\tau) + M^{(x)}(\tau) \) and \( Y(\tau) = Y(0) + A^{(y)}(\tau) + M^{(y)}(\tau) \) is defined as \([X, Y]_{\tau} = [M^{(x)}, M^{(y)}]_{\tau}\). Moreover, the image of a continuous semimartingale by any smooth function \( f(X(\tau), \tau) \) is again a continuous semimartingale and furthermore subordinated (time-changed) continuous semimartingale \( Y_{\alpha}(t) = X(S_{\alpha}(t)) \) is also a continuous semimartingale.

The continuous semimartingales play a crucial role in mathematics [23, 24] and also in physics [13, 26]. In particular, in the investigation of subdiffusions. Why? Because a large class of subdiffusions can be obtained by subordination of Brownian diffusion (Eq. (2)) if and only if they are continuous semimartingales, [13]. The most important tool to investigate both of the classical diffusive processes and continuous semimartingales is the celebrated Itô formula, [11, 12, 23, 24]. For jump-diffusion case see [30].

The Itô formula for semimartingales gives the explicit form of SDE for image of a continuous semimartingale \( \{X(\tau)\}_{\tau \geq 0} \) by any smooth function \( f \). Namely, a new process \( f(X(\tau), \tau) \) satisfies the following SDE [23, 24]:

\[
df f(X(\tau), \tau) = f_x(X(\tau), \tau) d\tau + f_x(X(\tau), \tau) dX(\tau) + \frac{1}{2} f_{xx}(X(\tau), \tau) d[X]_{\tau}.
\]

For example, since processes of form (3) are continuous semimartingales, the Itô formula for them takes the following form [12]:

\[
d f f(X(\tau), \tau) = f_x(X(\tau), \tau) dX(\tau) +\left( f_x(X(\tau), \tau) + K f_{xx}(X(\tau), \tau) \right) d\tau,
\]

because \([X]_{\tau} = 2K d\tau\).

Now, we show how to represent subdiffusion defined by Eq. (2) and (3) using only one subordinated Langevin equation. The advantage of such a representation is that we need only one equation to describe subdiffusion. The idea of modeling subdiffusion by subordinated SDE was also presented in [31]. So, if \( \{Y_{\alpha}(t)\}_{t \in [0, T]} \) is defined by Eq. (2), where \( \{X(\tau)\}_{\tau \geq 0} \) is the solution of the SDE (3), then \( \{Y_{\alpha}(t)\}_{t \in [0, T]} \) is the solution of the following subordinated SDE:

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

\( Y_{\alpha}(0) = X_0 \). \hspace{1cm} (B3)

The above convenient representation of subdiffusion process \( Y_{\alpha}(t) \) follows from the following integral identity:

\[
Y_{\alpha}(t) = \int_0^t F(X(\tau)) \eta^{-1} d\tau + \left( 2K \right)^{\frac{1}{2}} dB(\tau) = \int_0^t F(Y_{\alpha}(u)) \eta^{-1} dS_{\alpha}(u) + (2K)^{\frac{1}{2}} dB(S_{\alpha}(u)). \hspace{1cm} (B4)
\]

Observe, that in Eq. (B3) occur two new types of the stochastic differentials, for the inverse \( \alpha \)-stable subordinator \( S_{\alpha}(t) \), defined in (4) and for the subordinated Brownian motion \( B(S_{\alpha}(t)) \). Only when we take the deterministic subordinator \( S_{1}(t) = t \) (i.e., \( \alpha = 1 \)), then we obtain the classical SDE for Brownian diffusion. The subordinated SDE (B3) will play a crucial role in our further considerations. Now, we introduce two generalizations of the Itô formula, which can be very useful to investigate subdiffusive processes. The first subdiffusive Itô formula for function dependent on random time \( S_{\alpha}(t) \) allows to solve subordinated SDE (B3).

1. The case of random time dependent function

Let \( \{X(\tau)\}_{\tau \geq 0} \) be the solution of the SDE (3) and \( f \) be a smooth function, then \( \{f(Y_{\alpha}(t), S_{\alpha}(t))\}_{t \in [0, T]} \) is the solution of the subordinated SDE:

\[
df f(Y_{\alpha}(t), S_{\alpha}(t)) = f_g(Y_{\alpha}(t), S_{\alpha}(t)) \frac{F(Y_{\alpha}(t))}{\eta} dS_{\alpha}(t) + \left( f_h(Y_{\alpha}(t), S_{\alpha}(t)) + K f_{yy}(Y_{\alpha}(t), S_{\alpha}(t)) \right) dS_{\alpha}(t) + f_g(Y_{\alpha}(t), S_{\alpha}(t)) (2K)^{\frac{1}{2}} dB(S_{\alpha}(t)). \hspace{1cm} (B5)
\]

The above formula follows from the 2-dimensional Itô formula for semimartingales \( S_{\alpha}(t) \) and \( Y_{\alpha}(t) \) (see [22] and [24]), which gives the following SDE:

\[
df f(Y_{\alpha}(t), S_{\alpha}(t)) = f_s(Y_{\alpha}(t), S_{\alpha}(t)) dS_{\alpha}(t) + f_g(Y_{\alpha}(t), S_{\alpha}(t)) dY_{\alpha}(t) + \frac{1}{2} f_{yy}(Y_{\alpha}(t), S_{\alpha}(t)) d[Y_{\alpha}]_{t} + f_g(Y_{\alpha}(t), S_{\alpha}(t)) (2K)^{\frac{1}{2}} dB(S_{\alpha}(t)). \hspace{1cm} (B6)
\]

Taking advantage of the facts that \( |S_{\alpha}|_{t} = 0 \) (it is a continuous semimartingale so its Doob-Meyer decomposition does not consist a local martingale because it is equal to 0, therefore it is the process with finite quadratic variation), \( d[Y_{\alpha}]_{t} = 2K dS_{\alpha}(t) \) [32], \( |S_{\alpha}|_{t} = |M_{S_{\alpha}}|_{t} = 0 \) (where \( M_{S_{\alpha}} \) is a unique local martingale in the Doob-Meyer decomposition of a continuous semimartingale \( Y_{\alpha}(t) \)) and after putting the differential \( dY_{\alpha}(t) \) given by (B3) into (B6), we get the SDE (B5).

Let us notice that when we take the deterministic subordinator \( S_{1}(t) = t \) (i.e., \( \alpha = 1 \)), then formula (B5) reduces to the classical Itô formula for Brownian diffusion.
2. The case of real time dependent function

Now let us consider the image of subdiffusion (2) and (3) by a smooth function \( f(x,t) \), where \( t \) is an usual physical time. Processes defined as \( \tilde{Y}_\alpha(t) = f(Y_\alpha(t),t) \) (unlike \( f(Y_\alpha(t),S_\alpha(t)) \)) have a natural physical interpretation, because function \( f(x,t) \) depend on real time \( t \) and not on random time \( S_\alpha(t) \).

The Itô formula in such a case is different than in case of function dependent on \( S_\alpha(t) \), although it follows from previous result. Indeed, it suffices only to replace \( S_\alpha(t) \) by \( t \) in subordinated SDE (B6). The subordinated SDE for process \( f(Y_\alpha(t),t) = f(X(S_\alpha(t)),t) \) (where \( \{X(\tau)\}_{\tau \geq 0} \) is the solution of the SDE (3) and \( f \) is a smooth function) takes the following form:

\[
\begin{align*}
\frac{df(Y_\alpha(t),t)}{dt} &= f_t(Y_\alpha(t),t)dt + \\
&+ \left( f_y(Y_\alpha(t),t) \frac{F(Y_\alpha(t))}{\eta} + K f_{yy}(Y_\alpha(t),t) \right) dS_\alpha(t) + \\
&+ f_y(Y_\alpha(t),t)(2K)^{\frac{1}{2}} dB(S_\alpha(t)).
\end{align*}
\]  

(B7)