Equivalence of the Fractional Fokker-Planck and Subordinated Langevin Equations: The Case of a Time-Dependent Force

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A century after the celebrated Langevin paper [C.R. Seances Acad. Sci. **146**, 530 (1908)] we study a Langevin-type approach to subdiffusion in the presence of time-dependent force fields. Using a subordination technique, we construct rigorously a stochastic Langevin process, whose probability density function is equal to the solution of the fractional Fokker-Planck equation with a time-dependent force. Our model provides physical insight into the nature of the corresponding process through the simulated trajectories. Moreover, the subordinated Langevin equation allows us to study subdiffusive dynamics both analytically and numerically via Monte Carlo methods.

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The seminal works on Brownian diffusion by Einstein [1], Langevin [2], and Smoluchowski [3] have inspired physicists and mathematicians over the last century [4,5]. While the Fokker-Planck-Smoluchowski equation describing the time-evolution of probability density functions (PDFs) was introduced quite early [6], a stochastic theory for proper interpretation of the Langevin equation was developed much later by Itô [7]. Both approaches have been used as basic tools for studying the dynamics of various physical systems driven by Gaussian noise. However, recent interest in complex systems, whose dynamics is not described satisfactorily by the Gaussian diffusion, gave rise to the study of anomalous diffusion processes and, in particular, the distinct class of subdiffusion processes reported in condensed phases [8], ecology [9], and biology [10].

A common description of subdiffusive processes is in terms of the fractional Fokker-Planck equation (FFPE) derived from the continuous-time random walk [11]. The study of subdiffusive dynamics in the presence of purely time-dependent force field, giving rise to a modified FFPE, was proposed in [12]. A similar equation was derived in [13] for the class of dichotomously alternating forces. Formulating the corresponding Langevin equations is essential since the latter provide a detailed description of the underlying physical processes, usually missing in experimental data, leading to subdiffusion and to the FFPE. In a recent paper [14], a model based on the Langevin equation and a subordination technique has been proposed. However, the problem of the equivalence of the two approaches has remained unsolved. In this Letter we fill this gap by introducing a Langevin process and providing a rigorous proof of the equivalence to the FFPE, namely, having the same PDF.

The usual description of subdiffusive dynamics in the presence of a *time-independent* force field $F(x)$ is in terms of the FFPE

$$\frac{\partial w(x,t)}{\partial t} = \left[-\frac{\partial}{\partial x}F(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right]{}_0D_t^{1-\alpha}w(x,t), \qquad (1)$$

where $w(x,0) = \delta(x)$. This equation was first derived in [11], see also [8,15]. Here, the operator ${}_0D_t^{1-\alpha}$, $0 < \alpha < 1$, is the fractional derivative of the Riemann-Liouville type [16], which clearly commutes with the spatial Fokker-Planck operator. Thus, the order of both operators here is irrelevant.

The equivalent Langevin description of the FFPE (1) is in terms of the subordinated process [17] (see also [18–20])

$$Y(t) = X(S_t), \qquad (2)$$

where the parent process $X(\tau)$ is the diffusion process defined as the solution of the Itô stochastic differential equation

$$dX(\tau) = F(X(\tau))d\tau + dB(\tau), \qquad (3)$$

driven by the standard Brownian motion $B(\tau)$. The subordinator S_t, called the inverse α-stable subordinator, is defined as [21,22]

$$S_t = \inf\{\tau : U(\tau) > t\}, \qquad (4)$$

where $U(\tau)$ denotes the α-stable subordinator, i.e., the strictly increasing Lévy motion [23] with Laplace transform $\langle e^{-kU(\tau)}\rangle = e^{-\tau k^\alpha}$. Moreover, $B(\tau)$ and S_t are assumed to be independent. Since the inverse subordinator S_t is non-Markovian, this property is inherited also by the subdiffusion $X(S_t)$.

For the case of a *time-dependent* force $F(t)$, the recently derived version of the fractional Fokker-Planck equation has the form [12]

$$\frac{\partial w(x,t)}{\partial t} = \left[-F(t)\frac{\partial}{\partial x} + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right]{}_0D_t^{1-\alpha} w(x,t), \quad (5)$$

with $w(x,t) = \delta(x)$. When compared to (1), here the fractional operator ${}_0D_t^{1-\alpha}$ does not commute with the Fokker-Planck operator, and it is essential that it appears to the right of $F(t)$, so that it does not act on the time-dependent force. Namely, in the time-dependent case the proper order of the Fokker-Planck operator and the fractional operator ${}_0D_t^{1-\alpha}$ is "first Fokker-Planck and then ${}_0D_t^{1-\alpha}$."

The derivation of the FFPE (5) was based on the generalized master equation with two balance conditions: the probability conservation in a given state and under transition between different states. In [12] the authors showed that the moments

$$m_n(t) = \int_{-\infty}^{\infty} x^n w(x,t) dx$$

of the solution $w(x,t)$ of Eq. (5) satisfy the following recursive relation:

$$\frac{dm_n(t)}{dt} = nF(t)_0D_t^{1-\alpha} m_{n-1}(t) + \frac{n(n-1)}{2}{}_0D_t^{1-\alpha} m_{n-2}(t) \quad (6)$$

with $m_0(t) = 1$, $m_{-1}(t) = 0$, and $n \in \mathbb{N}$. The analysis of the first two moments $m_1(t)$ and $m_2(t)$ confirmed that the systems described by (5) display two significant physical properties, namely, the death of linear response and the field-induced dispersion [12].

We now address the problem of the equivalent Langevin description of the subdiffusive dynamics (5). In other words, we ask how to define a stochastic process, whose PDF obeys Eq. (5). Clearly, one cannot copy the scheme of the Langevin equations (3) and (4) solving the time-independent case. The reason is that for such a model the force field F would vary in the random time S_t and not in real time t, which cannot be physically accepted [14]. The solution of this problem can be obtained by the proper application of the subordination method. Let us introduce the following subordinated Langevin equation:

$$\hat{Y}(t) = \hat{X}(S_t). \quad (7)$$

Here, the process $\hat{X}(\tau)$ is the solution of the following stochastic differential equation:

$$d\hat{X}(\tau) = F(U(\tau))d\tau + dB(\tau), \quad (8)$$

where $U(\tau)$ is the strictly increasing α-stable Lévy motion and S_t is its inverse defined by Eq. (4) [14]. Equations (2) and (3) for time-independent fields and Eqs. (7) and (8) for time-dependent fields constitute the Langevin equation equivalent to the corresponding FFPEs, Eq. (1) and (5).

Before proving that the PDF of $\hat{Y}(t)$ is the solution of (5), let us discuss the structure of (8). When compared to the definition (3), the crucial factor here is the process $U(\tau)$, which enters Eq. (8) based on the physical requirement that the *deterministic* time-dependent force $F(t)$ should not be modified by the subordinator S_t. Indeed, after subordinating the process $\hat{X}(\tau)$ by S_t, the actual force is given by $F(U(S_t))$. Since in every jump moment we have $U(S_t) = t$ (see [24,25]), the particle is biased by the force $F(U(S_t)) = F(t)$. Namely, the force in $\hat{Y}(t)$ varies in real time t and is not modified randomly by the subordinator S_t. Note that the similar situation was reported in [13] for the case of FFPE (5), where the fractional operator ${}_0D_t^{1-\alpha}$ appeared to the right of $F(t)$, in order not to modify the force.

An important advantage of the current Langevin approach is the fact that it can be easily extended to the general case of the space-time-dependent force $F(x,t)$. One only needs to replace the force $F(U(\tau))$ in Eq. (8) with the force $F(x, U(\tau))$. The Langevin representation (7) provides information about all the trajectories, which from the mathematical point of view is the complete description of the stochastic process.

Now, let us show that the PDF of $\hat{Y}(t)$ is the solution of (5). Because of the space limitation, only the key steps of the proof are presented. It should be noted that the methods and results in the case of time-dependent force vastly differ from the space-dependent case. Our method is based on the analysis of the moments. First, let us note that the process $\hat{Y}(t)$ can be represented as

$$\hat{Y}(t) = \int_0^t F(t_1)dS_{t_1} + B(S_t). \quad (9)$$

Thus, it consists essentially of two contributions: the stochastic integral depending on the external time-dependent force, and the force-free pure subdiffusive part. Denote the moments $a_n(t) = \langle [B(S_t)]^n \rangle$ and $b_n(t) = \langle [\int_0^t F(t_1)dS_{t_1}]^n \rangle$. Since the Fourier transform of $B(S_t)$ is given by the Mittag-Leffler function $\langle e^{ikB(s_t)} \rangle = E_\alpha(-k^2 t^\alpha)$ [8], the moments $a_n(t)$ satisfy the relation

$$\frac{da_n(t)}{dt} = \frac{n(n-1)}{2}{}_0D_t^{1-\alpha} a_{n-2}(t). \quad (10)$$

Taking advantage of the change of variable formula, we obtain

$$\left(\int_0^t F(t_1)dS_{t_1}\right)^n = n! \int_0^t \int_0^{t_1} \dots \times \int_0^{t_{n-1}} F(t_1)\dots F(t_n) dS_{t_n} \dots dS_{t_1}.$$

Moreover, employing the theory of point processes [26], we get for the expected value

$$\langle dS_{t_n} \dots dS_{t_1} \rangle = \prod_{i=1}^n u(dt_i - t_{i+1}),$$

where $u(t) = \langle S_t \rangle = \frac{t^\alpha}{\Gamma(\alpha+1)}$ and $t_{n+1} = 0$. Therefore, the moments $b_n(t)$ obey the relation

$$\frac{db_n(t)}{dt} = nF(t)_0D_t^{1-\alpha}b_{n-1}(t). \quad (11)$$

By the same method, we show that the moments $c_{k,n}(t) = \langle[B(S_t)]^k[\int_0^t F(t_1)dS_{t_1}]^n\rangle$

$$\frac{dc_{k,n}(t)}{dt} = nF(t)_0D_t^{1-\alpha}c_{k,n}(t) + \frac{k(k-1)}{2}{}_0D_t^{1-\alpha}c_{k-2,n}(t). \quad (12)$$

Finally, using Newton's binomial expansion and the results (10)–(12), we obtain that the moments $r_n(t) = \langle\hat{Y}^n(t)\rangle$ satisfy the recursive relation

$$\frac{dr_n(t)}{dt} = nF(t)_0D_t^{1-\alpha}r_{n-1}(t) + \frac{n(n-1)}{2}{}_0D_t^{1-\alpha}r_{n-2}(t) \quad (13)$$

with $r_0(t) = 1$, $r_{-1}(t) = 0$, and $n \in \mathbb{N}$. Therefore, by (6) and (13), the moments of the process $\hat{Y}(t)$ coincide with the moments of the solution $w(x, t)$ of FFPE (5). Since the Fourier transform of $\hat{Y}(t)$ is analytical, it is determined by the moments [27]. Thus, the distribution of $\hat{Y}(t)$ must coincide with the distribution $w(x, t)$. We conclude that the PDF of $\hat{Y}(t)$ solves (5).

The above result gives a justification of the Langevin description of subdiffusive dynamics in the presence of time-dependent force fields. It allows us to investigate the properties of the trajectories using both analytical and numerical tools. In particular, one can simulate sample paths of $\hat{Y}(t)$ and study their behavior using Monte Carlo methods. The natural approximation of the subordinator S_t [see definition (4)] has the form

$$S_t^{(\delta)} = (\min\{n \in \mathbb{N}: U(\delta n) > t\} - 1)\delta, \quad (14)$$

where $\delta > 0$ is the step length. The "-1" term in the above expression comes from the fact that we want the process $S_t^{(\delta)}$ to start at the origin. Consequently, the strongly convergent approximation of the process $\hat{Y}(t)$ is given by

$$\hat{Y}^{(\delta)}(t) = \int_0^t F(u)dS_u^{(\delta)} + B(S_t^{(\delta)}). \quad (15)$$

To simulate the process $S_t^{(\delta)}$, one only needs to generate the random variables $U(\delta n)$, $n = 1, 2, \ldots$. This is accomplished by the following recursive algorithm:

$$U(0) = 0, \quad U(\delta n) = U(\delta(n-1)) + \delta^{1/\alpha}\xi_n,$$

where ξ_n, $n = 1, 2, \ldots$, are the i.i.d. totally skewed positive α-stable random variables. The procedure of generating realizations of ξ_n is the following [23]:

$$\xi_n = \frac{\sin(\alpha(V + c_1))}{[\cos(V)]^{1/\alpha}}\left(\frac{\cos(V - \alpha(V + c_1))}{W}\right)^{(1-\alpha)/\alpha},$$

where $c_1 = \pi/2$, the random variable V is uniformly distributed on $(-\pi/2, \pi/2)$ and W has exponential distribution with mean one.

As for the process $\hat{Y}^{(\delta)}(t)$, the integral in (15) can be written as

$$\int_0^t F(u)dS_u^{(\delta)} = \delta\sum_{n=1}^N F(U(\delta n)),$$

where N is an integer number such that $U(\delta N) < t \leq U(\delta(N+1))$. The last sum can easily be calculated numerically; therefore, the above formula allows us to simulate sample paths of $\hat{Y}^{(\delta)}(t)$. Note that the numerical method of simulating the trajectories of Brownian motion as well as α-stable Lévy motion is well known (see, e.g., [23]).

Figure 1 shows typical trajectories and nine quantile lines of the process $\hat{Y}^{(\delta)}(t)$ for the case $F(t) = \sin t$. Results were obtained using the above described simulation algorithm. The flat periods in each trajectory are typical for subdiffusion and represent long rests between consecutive jumps of the particle. The shape of the quantile lines is typical for the sinusoidal force.

Since the analytical solutions of FFPE (5) are not known, one can take advantage of the corresponding Langevin picture to find their approximations with no restrictions to the force $F(t)$. Figure 2 presents such approximated solutions for the case $F(t) = \sin t$, obtained by the Monte Carlo method. The solutions were estimated from the sample of 104 simulated trajectories of the process $\hat{Y}^{(\delta)}(t)$ with the help of the Rozenblatt-Parzen kernel estimator [23]. Since no direct calculation of the solution $w(x, t)$ from the FFPE (5) is available, the simulation results are not a corroboration of the theoretical results, but rather an example of the usefulness and power of our approach.

Concluding, in this Letter we have rigorously derived the Langevin picture of subdiffusive dynamics described by FFPE (5) with time-dependent force. Our model is

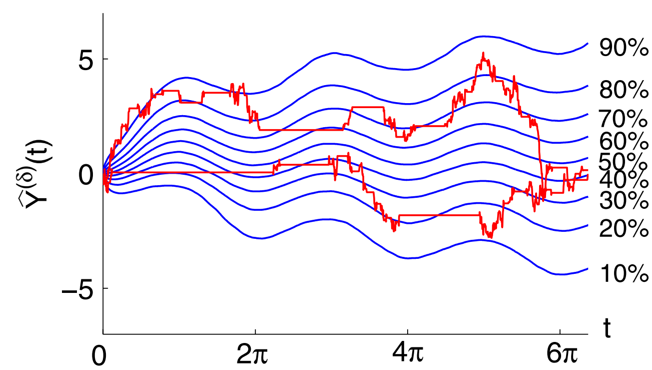

FIG. 1 (color online). Two sample paths and nine quantile lines (10%, 20%, ..., 90%), see [17], of the process $\hat{Y}^{(\delta)}(t)$ for $F(t) = \sin t$, $\alpha = 0.8$, and $\delta = 0.01$, obtained with the help of the introduced simulation algorithm. The flat periods of the process are typical for subdiffusion and represent the heavy-tailed rests of the particle. The shape of the quantile lines corresponds to the sinusoidal time-dependent force with the period 2π.

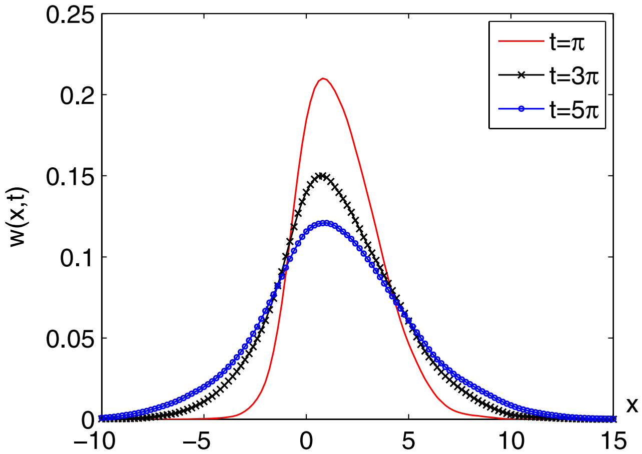

FIG. 2 (color online). Approximated solutions $w(x, t)$ of the fractional Fokker-Planck equation (5) with $F(t) = \sin t$, $\alpha = 0.8$, and $\delta = 0.01$, obtained by Monte Carlo method. The solutions were estimated from the sample of 10^4 simulated trajectories of the process $\hat{Y}^{(\delta)}(t)$ with the help of the Rozenblatt-Parzen density estimator.

based on the combination of standard diffusion with the proper use of subordination. To fulfill the physical requirement that the deterministic time-dependent force should not be changed by the subordination, we have modified the diffusion equation accordingly. As a result we have obtained a physical model equivalent to the time-dependent FFPE. In contrast to [13], this solves the problem concerning the validity of subordination method for time-dependent forces. By the appropriate construction of the parent process (8) we subordinate the process without changing the force. Therefore, F varies in the real time t. The presented approach gives a deep physical insight into the trajectories, providing the complete mathematical description of the non-Markovian stochastic process. This allows us to examine the properties of subdiffusion both analytically and numerically. Moreover, approximate solutions of FFPE (5) for any form of the force are at hand. We have described in detail the method of simulating sample paths of the introduced process. We have presented some numerical results obtained via Monte Carlo methods. In particular, we have estimated solutions of the time-dependent FFPE for the case of a sinusoidal force. Extensions of the Langevin model to the more general classes of noise (e.g., Lévy noises) are straightforward [14].

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