Competition between subdiffusion and Lévy flights: A Monte Carlo approach

Marcin Magdziarz* and Aleksander Weron
Hugo Steinhaus Center, Institute of Mathematics and Computer Science, Wroclaw University of Technology, Wyb. Wyspianskiego 27, 50-370 Wroclaw, Poland
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In this paper we answer positively a question raised by Metzler and Klafter [Phys. Rep. **339**, 1 (2000)]: can one see a competition between subdiffusion and Lévy flights in the framework of the fractional Fokker-Planck dynamics? Our method of Monte Carlo simulations demonstrates the competition on the level of realizations as well as on the level of probability density functions of the anomalous diffusion process. The simulation algorithm is based on a stochastic representation of the above dynamics.

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I. INTRODUCTION

In the past few years, anomalous diffusion has attracted growing attention, being observed in various fields of physics and related sciences [1]. Anomalous diffusion is characterized through the power law form $\langle(\Delta x)^2\rangle \propto Kt^{\alpha}$ of the mean-square displacement deviating from the well-known property $\langle(\Delta x)^2\rangle \propto Kt$ of Brownian diffusion. According to the value of the anomalous diffusion index α, one distinguishes subdiffusion ($0<\alpha<1$) and superdiffusion ($\alpha>1$) [1]. Brownian diffusion ($\alpha=1$) under the influence of an external force field is typically described by the Fokker-Planck equation [2].

Lévy flights do not possess a finite mean-square displacement. Their physical significance therefore has been questioned, as particles with a finite mass should not execute long jumps instantaneously. However, in recent years, description of physical models in terms of Lévy flights becomes more and more popular. They are used to model a variety of processes, such as bulk-mediated surface diffusion with application to porous glasses and eye lenses, transport in micelle systems or heterogeneous rocks, special problems in reaction dynamics, in single-molecule spectroscopy, and wait-and-switch relaxation (see [1,3,4] and references therein).

The general form of the celebrated fractional Fokker-Planck equation (FFPE), describing the competition between subdiffusion and Lévy flights under the influence of an external potential $V(x)$, is given in [1]:

$$\frac{\partial w(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left(\frac{\partial}{\partial x}\frac{V'(x)}{\eta} + K\nabla^{\mu}\right)w(x,t). \quad (1)$$

Here, the operator

$$ {}_0D_t^{1-\alpha}f(t) = \frac{1}{\Gamma(\alpha)}\frac{d}{dt}\int_0^t (t-s)^{\alpha-1}f(s)ds, \quad (2)$$

$0<\alpha<1$, stands for the fractional derivative of the Riemann-Liouville type and ∇^{μ}, $0<\mu\leq 2$, is the Riesz fractional derivative with the Fourier transform $\mathcal{F}\{\nabla^{\mu}f(x)\} = -|k|^{\mu}\tilde{f}(k)$ [5]. The occurrence of the operator ${}_0D_t^{1-\alpha}$ in Eq. (1) is induced by the heavy-tailed waiting times between successive jumps of the particle, whereas ∇^{μ} is related to the heavy-tailed distributions of the jumps in the underlying continuous-time random walk (CTRW) scheme. Equation (1) was first derived in [6] from a generalized master equation. The constant K is the anomalous diffusion coefficient, whereas η denotes the generalized friction constant. For $\mu=2$, we obtain the FFPE describing subdiffusion in accordance with the mean-squared displacement [1,7], while for $\alpha=1$, Eq. (1) reduces to the Markovian Lévy flight [3]. The case $\mu=2$, $\alpha=1$ corresponds to the standard Fokker-Planck equation.

Many physical transport problems occur under the influence of an external field. A framework for the treatment of anomalous diffusion problems under the influence of an external force 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] and nonexponential relaxation patterns [8]. The FFPE can be rigorously derived from the generalized master equation or the continuous-time random walk models as shown in [6,9]. The numerical simulation of the anomalous transport in a tilted periodic potential within the framework of the FFPE through the underlying CTRW was presented recently in [10]. A related problem for the fractional Fokker-Planck dynamics for Lévy flights in the context of resonant activation was numerically studied in [11,12].

In this paper, we derive the stochastic representation of the solution $w(x,t)$ of the FFPE (1)—i.e., we show that $w(x,t)$ is equal to the probability distribution function (PDF) $p(x,t)$ of the subordinated process

$$Y(t) = X(S_t). \quad (3)$$

Here the parent process $X(\tau)$ is defined as the solution of the stochastic differential equation (SDE)

$$dX(\tau) = -V'(X(\tau))\eta^{-1}d\tau + K^{1/\mu}dL_{\mu}(\tau) \quad (4)$$

driven by symmetric μ-stable Lévy motion $L_{\mu}(\tau)$ with the Fourier transform $\langle e^{ikL_{\mu}(\tau)}\rangle = e^{-\tau|k|^{\mu}}$ [13]. Observe that $L_{\mu}(\tau)$ is indexed by the internal time τ, which is not physical time. However, the subordination $X(S_t)$ changes the time scale from the internal time τ to physical time t. The subordinator

*Electronic address: marcin.magdziarz@pwr.wroc.pl

S_t, which is assumed to be independent of $L_\mu(\tau)$, is defined as

$$S_t = \inf\{\tau : U(\tau) > t\}. \quad (5)$$

Here, $U(\tau)$ denotes a strictly increasing α-stable Lévy motion [13]—i.e., an α-stable process with Laplace transform

$$\langle e^{-kU(\tau)}\rangle = e^{-\tau k^\alpha}, \quad (6)$$

where $0<\alpha<1$. Some interesting physical properties of the inverse-time α-stable subordinator S_t have been discussed in the papers [14–18]. Note that the role of the subordinator S_t in the stochastic representation (3) is analogous to the role of the fractional Riemann-Liouville derivative (2) in the FFPE (1), since S_t appears in a natural way as the limit process of the CTRW scheme with heavy-tailed waiting-time distributions between successive jumps of a particle. The process S_t is strictly increasing and it tends to infinity for $t\to\infty$. Moreover, S_t is α self-similar [19], which implies that in the case of constant potential, $V(x)=\text{const}$, the subordinated process $X(S_t)$ is α/μ self-similar.

II. STOCHASTIC REPRESENTATION

In a recent paper [20], the authors have derived the stochastic representation of the FFPE (1) only for the subdiffusive case, $\mu=2$. In what follows, we extend these considerations to the general case $0<\mu\leqslant 2$ and provide computer tools to study the competition between subdiffusion and Lévy flights.

Now, we show that the PDF $p(x,t)$ of the subordinated process $X(S_t)$ defined in (3) and the solution of Eq. (1) coincide. First, let us note that, from the total probability formula, we get

$$p(x,t) = \int_0^\infty f(x,\tau)g(\tau,t)d\tau.$$

Here, by $f(x,\tau)$ and $g(\tau,t)$ we denote the PDFs of $X(\tau)$ and S_t, respectively. The above formula in the Laplace space yields

$$\hat{p}(x,k) = \int_0^\infty e^{-kt}p(x,t)dt = \int_0^\infty f(x,\tau)\hat{g}(\tau,k)d\tau. \quad (7)$$

Next, since the process $X(\tau)$ is given by the SDE (4), its PDF $f(x,\tau)$ obeys the Lévy-flight-type FFPE [3]

$$\frac{\partial f(x,\tau)}{\partial \tau} = \left(\frac{\partial}{\partial x}\frac{V'(x)}{\eta} + K\nabla^\mu\right)f(x,\tau). \quad (8)$$

By taking the Laplace transform of both sides of the last equation, we obtain

$$k\hat{f}(x,k) - f(x,0) = \frac{\partial}{\partial x}\frac{V'(x)}{\eta}\hat{f}(x,k) + K\nabla^\mu\hat{f}(x,k). \quad (9)$$

Now, let us find the relationship between the PDFs $f(x,\tau)$ and $g(\tau,t)$. Since $U(\tau)$ from definition (5) is $1/\alpha$ self-similar, its PDF obeys the scaling relation

$$u(t,\tau) = \frac{1}{\tau^{1/\alpha}}u\left(\frac{t}{\tau^{1/\alpha}},1\right).$$

Using the property $\Pr(S_t<\tau)=\Pr(U(\tau)\geqslant t)$, we obtain after some standard calculations

$$g(\tau,t) = -\frac{\partial}{\partial \tau}\int_0^t u(y,\tau)dy = \frac{t}{\alpha\tau}u(t,\tau).$$

Consequently, by taking advantage of (6), we calculate the Laplace transform

$$\hat{g}(\tau,k) = \int_0^\infty e^{-kt}\frac{t}{\alpha\tau}u(t,\tau)dt = -\frac{1}{\alpha\tau}\frac{\partial}{\partial k}\int_0^\infty e^{-kt}u(t,\tau)dt = k^{\alpha-1}e^{-\tau k^\alpha}.$$

Using the above result in combination with (7), we get

$$\hat{p}(x,k) = \int_0^\infty f(x,\tau)k^{\alpha-1}e^{-\tau k^\alpha}d\tau = k^{\alpha-1}\hat{f}(x,k^\alpha). \quad (10)$$

The last formula, applied to (9), after the change of variables $k\to k^\alpha$, gives

$$k\hat{p}(x,k) - p(x,0) = k^{1-\alpha}\left(\frac{\partial}{\partial x}\frac{V'(x)}{\eta}\hat{p}(x,k) + K\nabla^\mu\hat{p}(x,k)\right). \quad (11)$$

Note that, since $S_0=0$, the initial conditions of $X(\tau)$ and $X(S_t)$ coincide; thus $f(x,0)=p(x,0)$. Finally, inverting the Laplace transform in the last equation, we obtain

$$\frac{\partial p(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left(\frac{\partial}{\partial x}\frac{V'(x)}{\eta} + K\nabla^\mu\right)p(x,t).$$

Thus, we have proved that the PDF $p(x,t)$ of $X(S_t)$ is the solution of the FFPE (1).

The obtained stochastic representation of the FFPE shows that the temporal fractional derivative ${}_0D_t^{1-\alpha}$ in Eq. (1) causes the change of the operational time of the system represented by the occurrence of the inverse-time α-stable subordinator S_t. The process S_t is responsible for the subdiffusive behavior of the system (long rests of the particle), whereas the parent process $X(\tau)$ introduces the Lévy-flight-type behavior (long jumps of the particle). The subordinated process $X(S_t)$ combines both these characteristics, resulting in competition between subdiffusion and Lévy flights (Fig. 1).

As a by-product of our considerations, from Eq. (10), we obtain the following scaling relation in the Laplace space between the two PDFs$-w(x,t)$ and $f(x,t)$ being solutions of Eq. (1) and Eq. (8), respectively:

$$\hat{w}(x,k) = k^{\alpha-1}\hat{f}(x,k^\alpha).$$

Let us note that the same functional relation has been derived in [7,14] and used in [20] in the proof of the stochastic representation for the pure subdiffusive case. Since such a relation has not been known for the case considered here of subdiffusion with Lévy flights, our proof of the stochastic

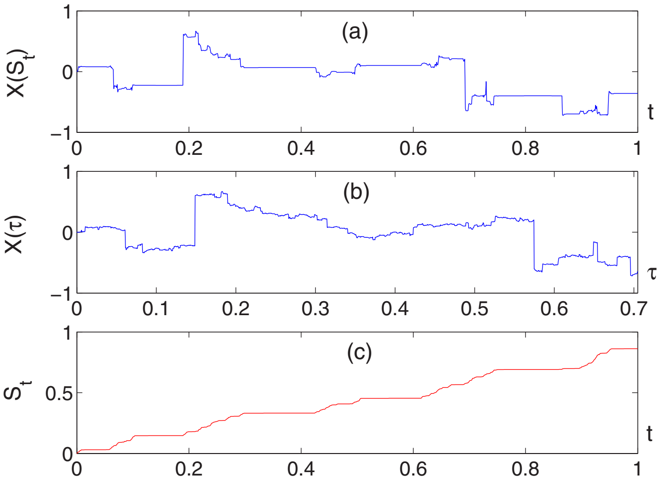

FIG. 1. (Color online) Sample realizations of (a) the anomalous diffusion $X(S_t)$, (b) the μ-stable parent process $X(\tau)$, and (c) the inverse-time α-stable subordinator S_t, in the presence of a constant potential $V(x)=\text{const}$. The parameters are $\alpha=0.7$, $\mu=1.3$, $K=1$, and $\eta=1$. The constant intervals of $X(S_t)$ indicate the heavy-tailed waiting times, while the long jumps of the process confirm the heavy-tailed distributions of transfers. The interplay between long rests and long jumps is distinct.

representation of Eq. (1) is considerably different from the one given in [20].

III. SIMULATION ALGORITHM

In this section, we construct a method of approximating sample paths of the process whose dynamics is described by the FFPE (1). Our method is based on the derived stochastic representation (3): every trajectory is obtained as a subordination of two independent trajectories of the processes $X(\tau)$ and S_t.

Suppose, we want to approximate the process $X(S_t)$ on the lattice $\{t_i=i\Delta t: i=0,1,\ldots,N\}$, where $\Delta t=T/N$ and T is the time horizon. The proposed algorithm consists of two steps.

(I) Our first aim is to approximate the values $S_{t_0},S_{t_1},\ldots,S_{t_N}$ of the subordinator S_t. Therefore, we begin by approximating a realization of the strictly increasing α-stable Lévy motion $U(\tau)$ on the mesh $\tau_j=j\Delta\tau$, $j=0,1,\ldots,M$ (it is recommended to choose $\Delta\tau<\Delta t$). Using the standard method of summing increments of the process $U(\tau)$ we get

$$U(\tau_0)=0,$$

$$U(\tau_j)=U(\tau_{j-1})+\Delta\tau^{1/\alpha}\xi_j, \qquad (12)$$

where ξ_j are the i.i.d. totally skewed positive α-stable random variables. The procedure of generating realizations of ξ_j is the following [21–23]:

$$\xi_j=c_1\frac{\sin[\alpha(V+c_2)]}{[\cos(V)]^{1/\alpha}}\left(\frac{\cos[V-\alpha(V+c_2)]}{W}\right)^{(1-\alpha)/\alpha},$$

where $c_1=[\cos(\pi\alpha/2)]^{-1/\alpha}$, $c_2=\pi/2$, the random variable V is uniformly distributed on $(-\pi/2,\pi/2)$, and W has exponential distribution with mean 1. The iteration (12) ends when $U(\tau)$ crosses the level T, i.e., when for some $j_0=M$ we get $U(\tau_{M-1})\leqslant T<U(\tau_M)$. Since $U(\tau)$ is strictly increasing, such M always exists.

Now, for every element t_i of the lattice $\{t_i=i\Delta t: i=0,1,\ldots,N\}$, we find the element τ_j such that $U(\tau_{j-1})<t_i\leqslant U(\tau_j)$, and finally, from definition (5), we get that in such a case

$$S_{t_i}=\tau_j.$$

Since $U(\tau)$ is strictly increasing, the above method of finding the values S_{t_i}, $i=0,1,\ldots,N$, can be implemented efficiently [20].

(II) In the second step, we find the approximated values $X(S_{t_0}),X(S_{t_1}),\ldots,X(S_{t_N})$ of the subordinated process $X(S_t)$. Recall that from (I) we have at our disposal the approximations $S_{t_0},S_{t_1},\ldots,S_{t_N}$. First, we approximate the solution $X(\tau)$ of the SDE (4) on the lattice $\{\bar{\tau}_k=k\Delta\bar{\tau}: k=0,1,\ldots,L\}$ (it is recommended to choose $\Delta\bar{\tau}<\Delta t$). Here, the number L is equal to the first integer that exceeds the value $S_{t_N}/\Delta\bar{\tau}$. Employing the Euler scheme for stable processes [13,22] we obtain

$$X(\bar{\tau}_0)=0,$$

$$X(\bar{\tau}_k)=X(\bar{\tau}_{k-1})-\frac{V'(X(\bar{\tau}_{k-1}))}{\eta}\Delta\bar{\tau}+K^{1/\mu}(\Delta\bar{\tau})^{1/\mu}\bar{\xi}_k, \qquad (13)$$

for $k=1,2,\ldots,L$. Here $\bar{\xi}_k$ are i.i.d. random variables with standard symmetric μ-stable distribution. The method of computer simulating realizations of the random variables $\bar{\xi}_k$ is the following [21–23]:

$$\bar{\xi}_k=\frac{\sin(\mu\bar{V})}{[\cos(\bar{V})]^{1/\mu}}\left(\frac{\cos(\bar{V}-\mu\bar{V})}{\bar{W}}\right)^{(1-\mu)/\mu},$$

$k=1,2,\ldots,L$. Here, the random variable $\bar{V}$ is uniformly distributed on $(-\pi/2,\pi/2)$ and $\bar{W}$ has exponential distribution with mean 1. $\bar{V}$ and $\bar{W}$ are assumed to be independent of each other and independent of the random variables V and W from the first step of the algorithm. Finally, we obtain the approximate values $X(S_{t_0}),X(S_{t_1}),\ldots,X(S_{t_N})$ by finding for every t_i from the lattice $\{t_i=i\Delta t: i=0,1,\ldots,N\}$ such an index k that the condition $\bar{\tau}_k\leqslant S_{t_i}\leqslant\bar{\tau}_{k+1}$ holds true. Then we get

$$X(S_{t_i})=X(\bar{\tau}_k), \qquad (14)$$

$i=0,1,\ldots,N$. It is not recommended to use linear interpolation at this point, since the realizations of $X(\tau)$ are not continuous for $0<\mu<2$. By choosing the approximation of $X(S_{t_i})$ as in Eq. (14), we assure that the processes $X(\tau)$ and $X(S_t)$ have jumps of the same length (Fig. 1).

The algorithm introduced allows us to simulate sample paths of the anomalous diffusion $X(S_t)$ for an arbitrary potential and for the whole range of parameters $0<\alpha<1$ and $0<\mu\leqslant 2$. Figures 1–3 visualize the interplay between subdiffusion and Lévy flights in the system under consideration. The constant parts of the sample path indicate the heavy-

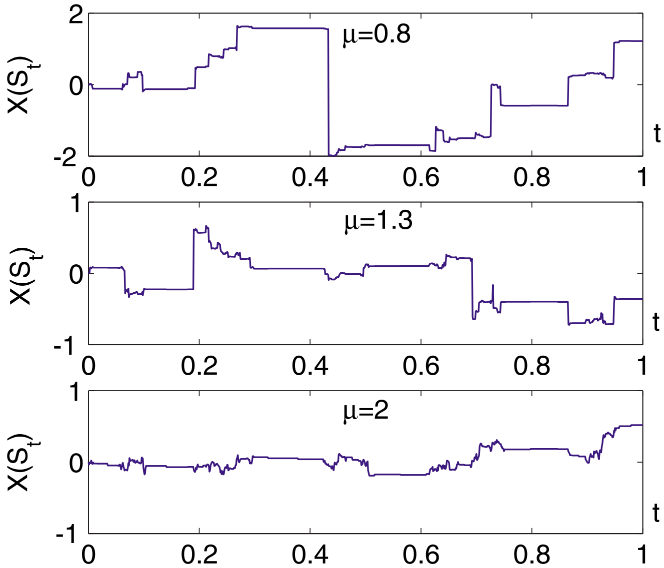

FIG. 2. (Color online) Comparison of three sample realizations of anomalous diffusion $X(S_t)$ for different parameters $\mu=0.8$, $\mu=1.3$, and $\mu=2$, respectively. The parameters $\alpha=0.7$, $K=1$, $\eta=1$, $V(x)=\text{const}$, and the realization of the inverse-time α-stable subordinator S_t are the same as in Fig. 1. Observe that the constant intervals of $X(S_t)$ are repeated, while the long jumps of the process characterized by μ are different. The smaller μ, the longer the jumps. Only for $\mu=2$ are there no jumps. This demonstrates a competition between the subdiffusive parameter α and the Lévy flight parameter μ.

tailed waiting times, while the long jumps of the particle confirm the heavy-tailed distributions of transfers in the underlying CTRW scheme. The subdiffusive behavior of the

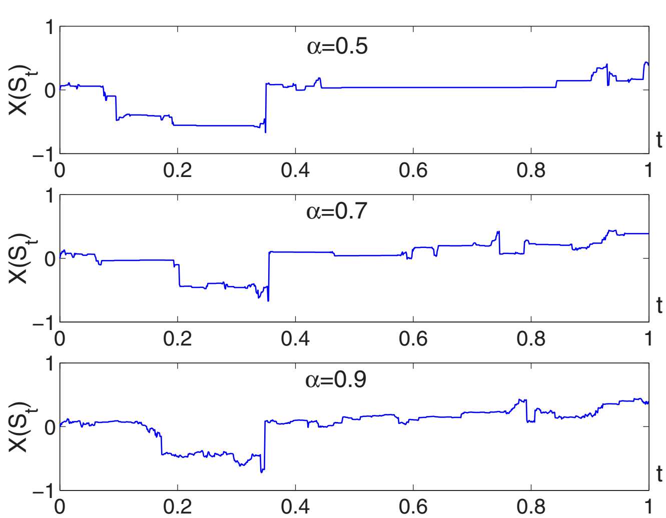

FIG. 3. (Color online) Comparison of sample realizations of anomalous diffusion $X(S_t)$ for three different subordinators S_t with indices $\alpha=0.5$, $\alpha=0.7$, and $\alpha=0.9$, respectively, and the same realization of $X(\tau)$. The other parameters are $\mu=1.3$, $K=1$, $\eta=1$, and $V(x)=\text{const}$. The height of jumps of $X(S_t)$ is repeated, while the waiting times (constant intervals) depend on α. The smaller α, the longer the waiting times. This demonstrates a competition between the subdiffusive parameter α and the Lévy flight parameter μ.

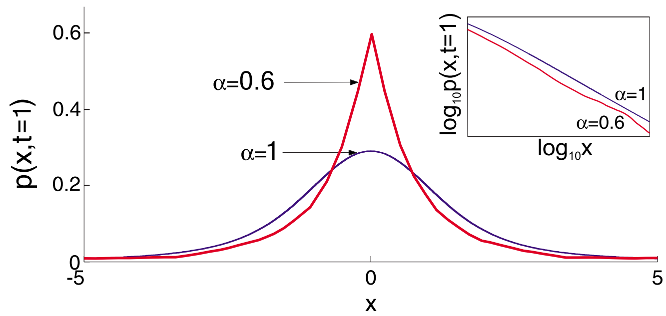

FIG. 4. (Color online) Comparison of the PDFs of the process $X(S_t)$ for two different parameters α with fixed parameter $\mu=1.4$. In the case $\alpha=0.6$ we observe the cusp shape of the PDF, whereas for $\alpha=1$ (pure Lévy flight) the PDF is smooth at $x=0$. The log-log scale window confirms that in both cases the tails decay as a power law. The parameters are $V(x)=\text{const}$, $K=1$, and $\eta=1$.

system is caused by the inverse-time α-stable subordinator, whereas the Lévy-flight-type behavior is inherited from the parent process $X(\tau)$ described by the SDE (4).

IV. MONTE CARLO APPROACH

Since the solution of the FFPE (1) in a numerically treatable form is not known, one can use Monte Carlo methods basing on our algorithm to approximate this solution. In Figs. 4 and 5 we present exemplary PDFs $p(x,t)$ obtained with the help of the Rozenblatt-Parzen kernel density estimator. The estimator was constructed on the basis of 10^4 simulated realizations. The cusp shape of the PDFs, caused by the influence of the subordinator S_t, can be observed for $\alpha<1$. For $\alpha=1$ the operator ${}_0D_t^{1-\alpha}$ in Eq. (1) disappears and we obtain standard Lévy flight with the corresponding PDF smooth at $x=0$. The log-log scale windows in Figs. 4 and 5 indicate that the tails of the PDFs for $\mu<2$ decay as a power law,

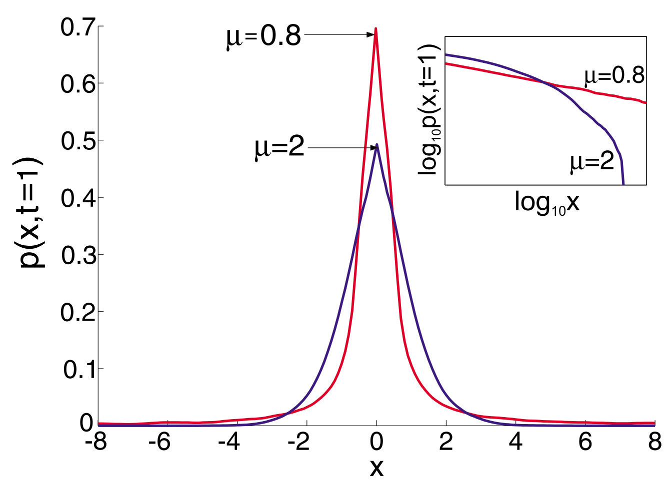

FIG. 5. (Color online) Comparison of the PDFs of the process $X(S_t)$ for two different parameters μ with fixed $\alpha=0.7$. The cusp shape of both PDFs is induced by the subordinator S_t. However, the tails of the PDF for $\mu=0.8$ decay as a power law, whereas for $\mu=2$ (subdiffusion) the decay is much faster (see the log-log scale window). The parameters are $V(x)=\text{const}$, $K=1$, and $\eta=1$.

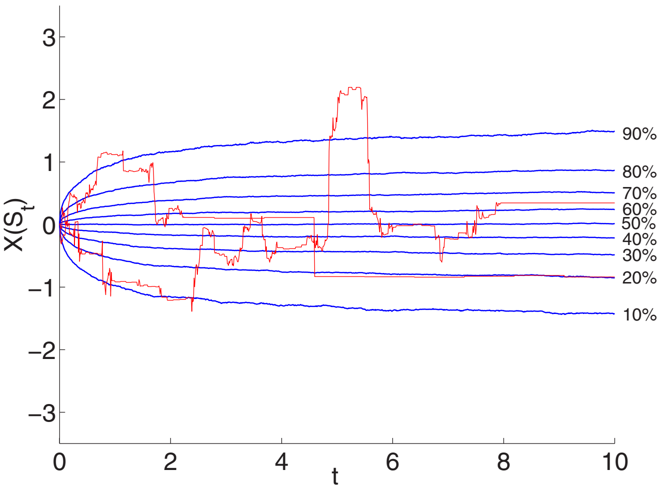

FIG. 6. (Color online) Estimated quantile lines and two sample trajectories of the process $X(S_t)$ in the presence of the harmonic potential $V(x)=x^2/2$. The parameters are $\alpha=0.7$, $\mu=1.5$, $K=1$, and $\eta=1$. The shape of the quantile lines (asymptotically parallel lines) confirms that the process reaches its stationary solution as $t\to\infty$.

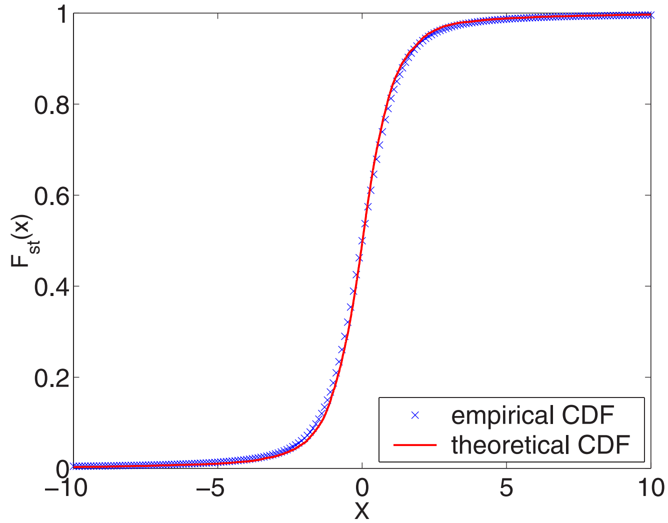

FIG. 7. (Color online) Comparison of the theoretical and estimated CDFs of the stationary solution of Eq. (1) in the presence of the harmonic potential $V(x)=x^2/2$. The empirical CDF was constructed using the Monte Carlo methods. The similarity between both CDFs confirms the correctness of our simulation algorithm. The parameters are $\alpha=0.7$, $\mu=1.5$, $K=1$, and $\eta=1$.

whereas for $\mu=2$ (pure subdiffusion) the decay is much faster.

As already pointed out, in the case of constant potential, $V(x)=\text{const}$, the process $X(S_t)$ is α/μ self-similar. Therefore, the corresponding PDF obeys the scaling relation

$$p(x,t)=\frac{1}{t^{\alpha/\mu}}p\left(\frac{x}{t^{\alpha/\mu}},1\right).$$

Since the PDF $p(x,1)$ decays as a power law for $\mu<2$ (see Figs. 4 and 5), we infer that the stretched Gaussian asymptotic behavior of the PDF $p(x,t)$, typical for the wide range of solutions of the FFPE without Lévy flight component [1,24], is violated in the case $\mu<2$.

The numerical investigations of sample path dynamics prove that for the harmonic potential $V(x)=x^2/2$ the process $X(S_t)$ reaches its stationary solution also for $\mu<2$. The existence of a stationary solution for $\mu=2$ was proved in [1]. As shown in Fig. 6, nine quantile lines (10%, 20%, …, 90%), corresponding to $X(S_t)$, become asymptotically parallel, which confirms that the stationary solution is reached as $t\to\infty$. Recall that a p-quantile line, $p\in(0,1)$, for a stochastic process $Y(t)$ is a function $q_p(t)$ given by the relationship $\Pr[Y(t)\leq q_p(t)]=p$ [13]. Since $S_t\to\infty$ as $t\to\infty$, the stationary solution of Eq. (1) is equal to the stationary solution of the SDE (4). In the case of a harmonic potential $V(x)=x^2/2$, the Fourier transform of the stationary solution $\widetilde{w}_{st}(k)$ is given by

$$\widetilde{w}_{st}(k)=\exp\left(-\frac{\eta K|k|^{\mu}}{\mu}\right).$$

In Fig. 7 we present the theoretical and estimated cumulative distribution functions (CDFs) of the stationary solution. The estimated CDF was constructed with the help of Monte Carlo methods on the basis of 10^4 realizations of $X(S_t)$. We checked that there was a very good agreement between both CDFs, which verifies the correctness of our simulation algorithm.

V. CONCLUSION

We have derived here the stochastic representation of the FFPE describing the competition between subdiffusion and Lévy flights. We have shown that the solution of Eq. (1) is equal to the PDF of the subordinated process $X(S_t)$, where $X(\tau)$ is defined by the SDE (4) and S_t is the inverse-time α-stable subordinator described by Eq. (5). The interplay between long rests and long jumps of the system described by the FFPE (1) is distinct also at the level of the derived stochastic representation. The subdiffusive behavior of the system is caused by the inverse-time α-stable subordinator S_t, whereas the Lévy-flight-type behavior is inherited from the parent process $X(\tau)$ (see Figs. 1–3).

We have used the stochastic representation to construct an efficient computer algorithm of sample path visualization of the anomalous diffusion $X(S_t)$. The algorithm can be applied for arbitrary external potential $V(x)$ and with no restrictions to the parameters $0<\alpha<1$ and $0<\mu\leq 2$. The proposed statistical tools basing on the Monte Carlo techniques allowed us to visualize the competition between subdiffusion and Lévy flights on the level of sample paths (Figs. 2 and 3) as well as on the level of PDFs (Figs. 4 and 5). We expect that the methods presented here will contribute to a better understanding of physical systems displaying both subdiffusive and Lévy-flight-type behavior.

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