Fractional Fokker-Planck equation with tempered α-stable waiting times: Langevin picture and computer simulation

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In this paper we introduce a Langevin-type model of subdiffusion with tempered α-stable waiting times. We consider the case of space-dependent external force fields. The model displays subdiffusive behavior for small times and it converges to standard Gaussian diffusion for large time scales. We derive general properties of tempered anomalous diffusion from the theory of tempered α-stable processes, in particular we find the form of the fractional Fokker-Planck equation corresponding to the tempered subdiffusion. We also construct an algorithm of simulation of sample paths of the introduced process. We apply the algorithm to approximate solutions of the fractional Fokker-Planck equation and to study statistical properties of the tempered subdiffusion via Monte Carlo methods.

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I. INTRODUCTION

A complete description of subdiffusive dynamics under the influence of an external space-dependent force field is given in terms of the celebrated fractional Fokker-Planck equation (FFPE) [1,2],

$$\frac{\partial w(x,t)}{\partial t} = {_0}D_t^{1-\alpha} \left[-\frac{\partial}{\partial x} F(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2} \right] w(x,t), \qquad (1)$$

where $w(x,0) = \delta(x)$. Here, the operator ${_0}D_t^{1-\alpha}$ (with $0 < \alpha < 1$) is the fractional Riemann-Liouville derivative and $F(x)$ is the external force. The above equation was derived in the framework of continuous-time random walk (CTRW) with heavy-tailed α-stable waiting times. A further generalization of Eq. (1) accounting for a broad jump distance statistics, which led to space-time FFPE, was discussed in detail in [2]. However, FFPE (1) is suitable for describing time evolution of the probability density function (PDF) of a limited class of anomalous diffusion processes, for which the subdiffusion exponent α does not change in time.

In a more general setting, one has to take into account the case of nonunique diffusion exponent. In many physical systems we observe a transition from the initial subdiffusive character of motion ($\alpha < 1$) to the standard linear in time mean-squared displacement for long times ($\alpha = 1$). The coexistence of subdiffusion and normal diffusion was empirically confirmed in a number of systems, i.e., in a random motion of bright points associated with magnetic fields at the solar photosphere [3]. The transition from anomalous to normal diffusion was also observed in the motion of molecules diffusing in living cells [4,5]. Other important applications related to finance [6], turbulence [7], and geophysics [8] should also be mentioned.

To model such dualism of physical systems, a modification of the CTRW scenario leading to FFPE (1) is necessary.

In particular, an appropriate truncation of heavy-tailed α-stable waiting times is needed in order to eventually cancel the anomalous character of motion. In the physical literature, the first step in this direction was done by Mantegna and Stanley [9]. Their idea of cutting of the heavy tails was further developed by Koponen [10], who proposed smoothly truncated stable distributions. Recently, Rosinski [11] introduced a class of tempered α-stable distributions. The modification that he proposed was done on the level of the Lévy measure, which resulted in many desired properties of the introduced laws. In particular, tempered α-stable distributions are infinitely divisible, so that there is an underlying stochastic process with stationary independent increments, which can be discretized for simulation at any scale, with a corresponding semigroup and generator that leads to a useful governing equation. Moreover, tempered distributions have finite moments of all orders; on the other hand they resemble stable laws in many aspects (see [11] for the details).

In this paper, we use tempered α-stable distributions to model processes exhibiting transition from anomalous to normal motion under the influence of external space-dependent force fields. The force-free case was already introduced in [12], without developing the associated governing equation. That was done in [8]. The aspect of relaxation responses induced by tempered α-stable laws was discussed in detail in [13]. Some related investigations devoted to the problem of nonunique subdiffusion exponent can be found in [14,15]. The problem of modeling subdiffusion with time-dependent force fields in the general case of infinitely divisible waiting times (and in particular the tempered α-stable waiting times) was solved in [16–18].

The paper is structured as follows. In Sec. II we give a brief description of tempered α-stable processes and their inverses. We introduce a model called tempered subdiffusion, which is capable of describing transition between anomalous and normal motions in the presence of external force. The model is defined by the use of the subordination method. We show that the PDF of the introduced model obeys a generalized FFPE, in which the fractional derivative is replaced with some other integro-differential operator. We

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prove that the stationary distribution follows the classical Boltzmann-Gibbs law. Taking advantage of the Langevin picture of tempered subdiffusion, we present in Sec. III an efficient algorithm of simulating its sample paths. An application of Monte Carlo methods allows us to approximate solutions of the generalized FFPE and to detect some relevant statistical properties of tempered dynamics.

II. TEMPERED SUBDIFFUSION AND THE CORRESPONDING FFPE

FFPE (1) is a very convenient tool to study anomalous transport in the presence of external force fields. Recall that the Langevin picture of Eq. (1) is given in terms of the subordinated process [19–21],

$$Z(t) = X(S(t)).$$

Here, the process $X(\tau)$ is given by the Itô stochastic differential equation (SDE),

$$dX(\tau) = F(X(\tau))d\tau + dB(\tau),\qquad(2)$$

driven by the standard Brownian motion $B(\tau)$. Moreover, $S(t)$ is the inverse α-stable subordinator defined as $S(t) = \inf\{\tau: U(\tau) > t\}$, where $U(\tau)$ is the strictly increasing α-stable Lévy motion [22]. The diffusion process $X(\tau)$ governs the spatial properties of motion, whereas the inverse subordinator $S(t)$ introduces the mechanism of heavy-tailed traps (periods in which the particle stays motionless). The trapping events slow down dramatically the overall motion, which results in the sublinear in time mean-squared displacement of the test particle. Consequently, to attain the transition from subdiffusion to normal diffusion (i.e., to eventually cancel the effects of the trapping periods on the particle motion), an appropriate modification of the waiting-time distributions is necessary. Following the idea presented in [12,13], we modify the heavy-tailed distribution of waiting times in Eq. (1), by replacing it with tempered α-stable laws.

The tempered α-stable random variable $T_{\alpha,\lambda} > 0$ is conveniently defined via its Laplace transform

$$E(e^{-uT_{\alpha,\lambda}}) = e^{-[(u+\lambda)^\alpha - \lambda^\alpha]},$$

where the constant $\lambda > 0$ is the tempering parameter and $0 < \alpha < 1$ is the stability parameter. Note that for $\lambda \searrow 0$, we recover the Laplace transform of one-sided stable distribution. It is worth mentioning that the PDF of $T_{\alpha,\lambda}$ has the form $ce^{-\lambda x}f_\alpha(x)$, where $f_\alpha(x)$ is the PDF of one-sided stable distribution and $c > 0$ is the normalizing constant [11]. Therefore, moments of all orders of $T_{\alpha,\lambda}$ are finite, which makes the tempered α-stable distributions particularly attractive for physical applications.

Given an infinitely divisible tempered α-stable random variable $T_{\alpha,\lambda}$, we can extend our definition by taking time into account and introduce the corresponding tempered α-stable Lévy process $T_{\alpha,\lambda}(\tau)$ via its Laplace transform,

$$E(e^{-uT_{\alpha,\lambda}(\tau)}) = e^{-\tau[(u+\lambda)^\alpha - \lambda^\alpha]}.$$

Consequently, we define the inverse tempered α-stable subordinator by

$$S_{\alpha,\lambda}(t) = \inf\{\tau > 0: T_{\alpha,\lambda}(\tau) > t\},\quad t \geq 0,$$

The process $S_{\alpha,\lambda}(t)$ is a new operational time of the system. Finally, the model of tempered subdiffusion is defined as the subordinated Langevin process,

$$Y(t) = X(S_{\alpha,\lambda}(t)),\qquad(3)$$

where the process $X(\tau)$ is the solution of the Itô SDE (2). Similarly to the pure subdiffusion case, $X(\tau)$ is responsible for the jumps of the particle, whereas $S_{\alpha,\lambda}(t)$ governs the trapping events, which now follow the tempered α-stable law. It turns out that by adapting $S_{\alpha,\lambda}(t)$ as a new clock of the system, we are able to recover the desired transition from anomalous to normal diffusion. Indeed, one can show [23] that $S_{\alpha,\lambda}(t) \propto t$ as $t \to \infty$. Thus, for large time scale the process Y behaves as the standard diffusion X. Moreover, as shown in [12] for the force-free case, the second moment of tempered subdiffusion satisfies $\langle Y^2(t) \rangle \propto t^\alpha$ for small enough t. This is typical for subdiffusive dynamics.

In what follows, we prove that the PDF of the tempered subdiffusion $Y(t)$ satisfies the following generalized FFPE:

$$\frac{\partial w(x,t)}{\partial t} = \Phi_t\left[-\frac{\partial}{\partial x}F(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right]w(x,t),\qquad(4)$$

where $w(x,0) = \delta(x)$. Here, Φ_t is the integro-differential operator defined as

$$\Phi_t f(t) = \frac{d}{dt}\int_0^t M(t-y)f(y)dy,$$

where the memory kernel $M(t)$ is defined via its Laplace transform,

$$\hat{M}(u) = \int_0^\infty e^{-ut}M(t)dt = \frac{1}{(u+\lambda)^\alpha - \lambda^\alpha}.$$

Observe that for $\lambda \searrow 0$, the integro-differential operator Φ_t is proportional to the fractional Riemann-Liouville derivative, and we recover FFPE (1). Moreover, when $M(t) = 1$, formula (4) reduces to the classical Fokker-Planck equation.

The operator Φ_t is closely related to the tempered fractional derivative discussed in [8,24]. Specifically, if you apply the operator Φ_t^{-1} to the both sides of Eq. (4) then $\Phi_t^{-1}(\frac{\partial}{\partial t})$ is the tempered fractional derivative, which was originally developed in [25].

Since the process $X(\tau)$ is given by the Itô SDE (2), its PDF $f(x,\tau)$ obeys the ordinary Fokker-Planck equation

$$\frac{\partial f(x,\tau)}{\partial \tau} = \left[-\frac{\partial}{\partial x}F(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right]f(x,\tau).\qquad(5)$$

For convenience let us introduce the notation

$$L_{FP} = \left[-\frac{\partial}{\partial x}F(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right].\qquad(6)$$

The Laplace image of Eq. (5) with respect to the variable τ has the following form:

$$u\hat{f}(x,u) - f(x,0) = L_{FP}\hat{f}(x,u). \tag{7}$$

Similarly, Eq. (4) in the Laplace space u yields

$$u\hat{w}(x,u) - w(x,0) = L_{FP}\frac{u}{(u+\lambda)^\alpha - \lambda^\alpha}\hat{w}(x,u). \tag{8}$$

Next, let us denote the PDFs of $T_{\alpha,\lambda}(\tau)$ and $S_{\alpha,\lambda}(t)$ by $h(t,\tau)$ and $g(\tau,t)$, respectively. Using the property $\mathbb{P}(S_{\alpha,\lambda}(t) \le \tau) = \mathbb{P}(T_{\alpha,\lambda}(\tau) \ge t)$, we obtain

$$g(\tau,t) = -\frac{\partial}{\partial\tau}\int_{-\infty}^{t} h(t',\tau)dt'. \tag{9}$$

Consequently, the Laplace transform of $g(\tau,t)$ with respect to t is equal to

$$\hat{g}(\tau,u) = \frac{(u+\lambda)^\alpha - \lambda^\alpha}{u}e^{-\tau[(u+\lambda)^\alpha - \lambda^\alpha]}. \tag{10}$$

Using the total probability formula and the independence of $X(\tau)$ and $S_{\alpha,\lambda}(t)$, we get that the PDF $p(x,t)$ of $X(S_{\alpha,\lambda}(t))$ is given by

$$p(x,t) = \int_0^\infty f(x,\tau)g(\tau,t)d\tau. \tag{11}$$

Thus, using the above formula together with Eq. (10), we obtain

$$\hat{p}(x,u) = \int_0^\infty e^{-ut}p(x,t)dt = \int_0^\infty f(x,\tau)\hat{g}(\tau,u)d\tau$$

$$= \int_0^\infty f(x,\tau)\frac{(u+\lambda)^\alpha - \lambda^\alpha}{u}e^{-\tau[(u+\lambda)^\alpha - \lambda^\alpha]}d\tau$$

$$= \frac{(u+\lambda)^\alpha - \lambda^\alpha}{u}\hat{f}(x,(u+\lambda)^\alpha - \lambda^\alpha). \tag{12}$$

Now by the change of variables $u \rightarrow [(u+\lambda)^\alpha - \lambda^\alpha]$ in Eq. (7) we obtain

$$[(u+\lambda)^\alpha - \lambda^\alpha]\hat{f}(x,(u+\lambda)^\alpha - \lambda^\alpha) - f(x,0)$$

$$= L_{FP}\hat{f}(x,(u+\lambda)^\alpha - \lambda^\alpha). \tag{13}$$

Finally, from Eq. (12) and fact that $f(x,0) = p(x,0)$ we infer that in the Laplace space $\hat{p}(x,u)$ satisfies the equation

$$u\hat{p}(x,u) - p(x,0) = L_{FP}\frac{u}{(u+\lambda)^\alpha - \lambda^\alpha}\hat{p}(x,u). \tag{14}$$

Comparing the above with Eq. (8) we have

$$w(x,t) = p(x,t). \tag{15}$$

Thus, we have shown that the solution $w(x,t)$ of the generalized FFPE (4) describes the dynamics of the PDF of the subordinated process $X(S_{\alpha,\lambda}(t))$.

Using the same arguments as in [2], we can show that the stationary solution $w_{st}(x)$ of Eq. (4) coincides with the Boltzmann-Gibbs distribution. Let us write the right-hand side of Eq. (4) as

$$\frac{\partial w(x,t)}{\partial t} = \Phi_t\frac{\partial S(x,t)}{\partial x}, \tag{16}$$

where

$$S(x,t) = \left[-F(x) + \frac{1}{2}\frac{\partial}{\partial x}\right]w(x,t) \tag{17}$$

is the probability current. Denote by $V(x)$ the external potential. Consequently, $F(x) = -V'(x)$. If $w(x,t)$ reaches its stationary state (i.e., it does not depend on time), then $S(x,t)$ must be a constant. Therefore, if $S_{st}(x) = 0$ at any point x, it must be equal to zero everywhere. Thus, the stationary solution of Eq. (4) satisfies

$$\left[V'(x) + \frac{1}{2}\frac{\partial}{\partial x}\right]w_{st}(x) = 0, \tag{18}$$

from which we can easily obtain the Boltzmann-Gibbs distribution

$$w_{st}(x) = A\exp[-2V(x)], \tag{19}$$

where A is the appropriate normalization constant.

III. NUMERICAL APPROXIMATION OF SAMPLE PATHS

Let us now show how to simulate sample paths of the tempered subdiffusion process $Y(t) = X(S_{\alpha,\lambda}(t))$. Our method uses explicitly the fact that $Y(t)$ is defined via subordination. Every sample path of $Y(t)$ is obtained as a superposition of independently generated trajectories of $X(\tau)$ and $S_{\alpha,\lambda}(t)$. Now, suppose that we want to simulate $Y(t)$ on the interval $[0,T]$, where T is the time horizon. The proposed algorithm consists of two steps:

(I) In the first step we approximate the trajectory of the inverse subordinator $S_{\alpha,\lambda}(t)$. We use the following approximation process:

$$S_{\alpha,\lambda,\Delta t}(t) = [\min\{n \in \mathbb{N}: T_{\alpha,\lambda}(n\Delta t) > t\} - 1]\Delta t, \tag{20}$$

where Δt is the step length and $t \in [0,T]$. One can show [18] that the approximation process $S_{\alpha,\lambda,\Delta t}(t)$ satisfies

$$\sup_{t\in[0,T]}|S_{\alpha,\lambda,\Delta t}(t) - S_{\alpha,\lambda}(t)| \le \Delta t.$$

Therefore, the smaller Δt we choose, the better approximation we obtain. In view of Eq. (20), to simulate numerically the process $S_{\alpha,\lambda,\Delta t}(t)$, one only needs to generate the values $T_{\alpha,\lambda}(n\Delta t)$, where $n = 1,2,\ldots$. This can be done by the standard method of summing up the independent and stationary increments of the Lévy process $T_{\alpha,\lambda}(t)$,

$$T_{\alpha,\lambda}(0) = 0, \tag{21}$$

$$T_{\alpha,\lambda}(n\Delta t) = T_{\alpha,\lambda}([n-1]\Delta t) + Z_i, \tag{22}$$

where Z_i are independent tempered α-stable random variables, each with the same Laplace transform $E(e^{-uZ_i}) = e^{-\Delta t[(u+\lambda)^\alpha - \lambda^\alpha]}$. The algorithm of generating Z_i has been recently proposed in [24]. For completeness of the presentation, we give it in the Appendix. We underline that the
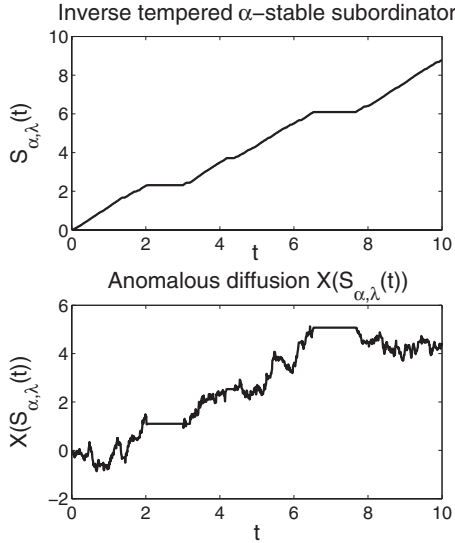
FIG. 1. An exemplary sample path of the inverse tempered α-stable subordinator $S_{\alpha,\lambda}(t)$ (top panel) and the tempered subdiffusion process $Y(t)=X(S_{\alpha,\lambda}(t))$ (bottom panel). The parameters are $\alpha=0.95$, $\lambda=0.01$, $F(x)=0$.

proposed method here of approximating sample paths of $S_{\alpha,\lambda}(t)$ is very efficient since the approximation process $S_{\alpha,\lambda,\Delta t}(t)$ is actually a simple continuous-time random walk with each jump equal to Δt and ith waiting time equal to Z_i.

(II) In the second step our aim is to approximate the diffusion process $X(\tau)$ given by SDE (2). Note that the approximation process $S_{\alpha,\lambda,\Delta t}(t)$ considered in the previous step takes only the values of the form $k\Delta t$ (with $k=0,1,\ldots,N$), where N is the appropriate last index satisfying $N\Delta t=S_{\alpha,\lambda,\Delta t}(T)$. Therefore, we have to approximate the diffusion process $X(\tau)$ only in the time points $\tau_k=k\Delta t$, where $k=0,1,\ldots,N$. This is done by the classical Euler scheme [22],

$$X(0) = 0,$$

$$X(\tau_k) = X(\tau_{k-1}) + F(X(\tau_{k-1}))\Delta t + \Delta t^{1/2}\xi_k, \qquad (23)$$

where $k=1,2,\ldots,N$. Here, ξ_k are independent random variables, each distributed according to the standard normal distribution $\xi_k \sim N(0,1)$.

Concluding, from the first step of the algorithm we get the approximated trajectory of $S_{\alpha,\lambda}(t)$. From the second step we obtain the trajectory of $X(\tau)$. Finally, by putting them together, we obtain the trajectory of the tempered subdiffusion $X(S_{\alpha,\lambda}(t))$.

The above algorithm allows us to simulate sample paths of the process $X(S_{\alpha,\lambda}(t))$ for arbitrary external forces $F(x)$ and with no restriction to the parameters $\alpha \in (0,1)$ and $\lambda > 0$. In Fig. 1 we see the typical trajectories of the inverse subordinator and tempered subdiffusion in the force-free case. The constant intervals in both trajectories represent the trapping events distributed according to the tempered α-stable laws. Figure 2 depicts quantile lines corresponding to the process $X(S_{\alpha,\lambda}(t))$, which give essential statistical information about the evolution in time of the trajectories. The
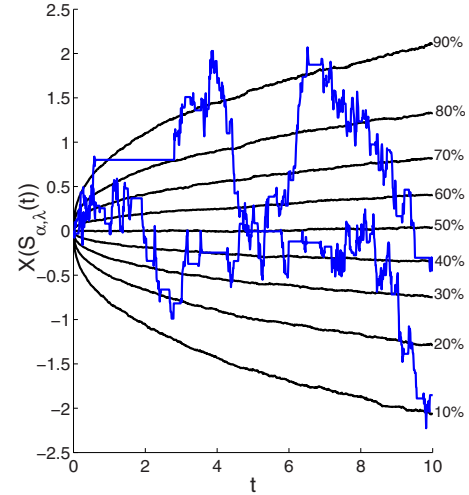

FIG. 2. (Color online) Estimated quantile lines (black lines) with the two sample paths (blue lines) of the anomalous diffusion $X(S_{\alpha,\lambda}(t))$. The parameters are as in Fig. 1.

quantile lines were estimated via Monte Carlo methods on the basis of 10^4 simulated trajectories. Recall that a p-quantile line, $p \in (0,1)$, of a stochastic process $Y(t)$ is a function $q_p(t)$ given by the relationship $\mathbb{P}(Y(t) \leq q_p(t))=p$.

Monte Carlo methods can be employed to estimate solutions of the generalized FFPE (4). In Fig. 3 we can see the estimated PDFs of the process $X(S_{\alpha,\lambda}(t))$ in the double-well potential $V(x)=(x^4/4-8x^2)/20$. These PDFs are also solutions of Eq. (4) with $F(x)=-V'(x)=-(x^3-16x)/20$.

Figure 4 shows the quantile lines for the case of tempered subdiffusion in the double-well potential. The lines become parallel, which indicates that the process reaches its equilibrium. In Fig. 5 we compared the theoretical and estimate stationary PDFs. We see almost perfect agreement between both functions. The PDF estimation was performed using
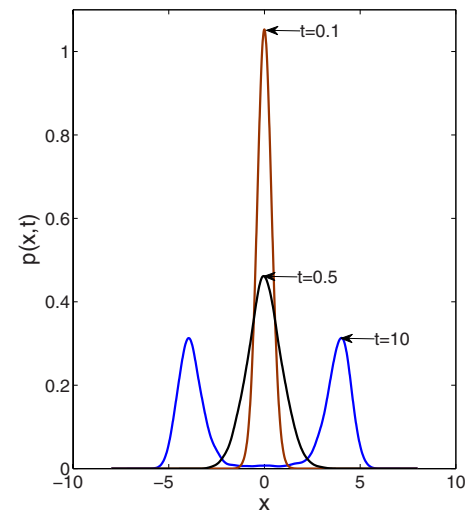

FIG. 3. (Color online) Evolution in time of the PDF of the anomalous diffusion $Y(t)=X(S_{\alpha,\lambda}(t))$. The parameters are $\alpha=0.95$, $\lambda=0.01$, and $F(x)=-V'(x)=-(x^3-16x)/20$. The results were obtained via Monte Carlo methods on the basis of 10^4 simulated trajectories.
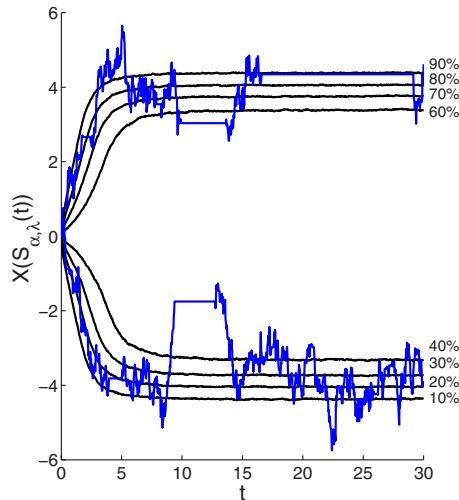
FIG. 4. (Color online) Estimated quantile lines with the two sample paths of the anomalous diffusion $X(S_{\alpha,\lambda}(t))$. As the quantile lines become parallel, they indicate that the process is asymptotically stationary. Parameters are as in Fig. 3.

Rozenblatt-Parzen kernel estimator from the sample of 10^4 simulated trajectories.

IV. CONCLUSIONS

In this paper we have extended the model of tempered subdiffusion proposed in [12,13] to the case of space-dependent force fields. Our model is a combination of two independent stochastic mechanisms: the first one is a classical diffusion process $X(\tau)$ governing the spatial properties (jumps) of the test particle and the second mechanism of trapping events (tempered α-stable waiting times) is represented by the inverse subordinator $S_{\alpha,\lambda}(t)$. We have derived the generalized FFPE, which describes the dynamics of the PDF of the subordinated process $X(S_{\alpha,\lambda}(t))$. In the special case, $\lambda=0$, we recover the typical equation of subdiffusion (1). The proposed Langevin approach here to tempered subdiffusion allowed us to construct a numerical algorithm of simulating sample paths of the introduced process. The algorithm can be applied to examine many relevant properties of the system via Monte Carlo methods. In particular, one can approximate solutions of the generalized FFPE with arbitrary space-dependent forces $F(x)$. One can also verify numerically various physical properties of the tempered subdiffusion, in a similar way as it was done for the typical subdiffusion [26–29]. We believe that our investigations will
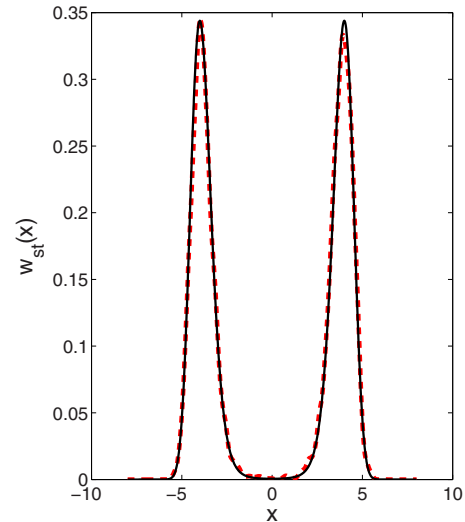

FIG. 5. (Color online) Comparison of the analytical (black solid line) and estimated (red dotted line) stationary PDFs of the tempered subdiffusion in the double-well potential. We observe almost perfect agreement between both lines. Parameters are as in Fig. 3.

provide another insight into the physical and biological systems, in which the transition between anomalous and normal diffusions occurs.

APPENDIX

For completeness, we present the method of simulating tempered α-stable random variables. The method has been recently introduced in [24]. Suppose that we want to generate the tempered random variable $Z > 0$ with the Laplace transform $E(e^{-uZ}) = e^{-\Delta t[(u+\lambda)^\alpha - \lambda^\alpha]}$. The method is the following:

(I) Generate exponential random variable E with mean λ^{-1}.

(II) Generate totally skewed α-stable random variable S using the following formula [30]:

$$S = \Delta t^{1/\alpha} \frac{\sin\left[\alpha\left(U + \frac{\pi}{2}\right)\right]}{\cos(U)^{1/\alpha}} \left(\frac{\cos\left[U - \alpha\left(U + \frac{\pi}{2}\right)\right]}{W}\right)^{(1-\alpha)/\alpha}.$$
(A1)

Here, U is uniformly distributed on $[-\pi/2, \pi/2]$, and W has an exponential distribution with mean 1.

(III) If $E > S$ put $Z = S$; otherwise go to step (I).

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