Numerical approach to the fractional Klein-Kramers equation

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Subdiffusion in the presence of an external force field can be described in phase space by the fractional Klein-Kramers equation. In this paper, we explore the stochastic structure of this equation. Using a subordination method, we define a random process whose probability density function is a solution of the fractional Klein-Kramers equation. The structure of the introduced process agrees with the two-stage scenario underlying the anomalous diffusion mechanism, in which trapping events are superimposed on the Langevin dynamics. We develop an efficient computer algorithm for visualization of fractional Klein-Kramers dynamics and present some simulation results based on Monte Carlo techniques.

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I. INTRODUCTION

In the classical theory of Brownian transport the phase space dynamics is described by the deterministic Klein-Kramers equation [1–5]. In the high-friction limit it reduces to the Fokker-Planck-Smoluchowski equation, whereas in the low-friction-limit case one obtains the Rayleigh equation describing the relaxation of the velocity probability density function (PDF) toward the Maxwell distribution. Classical Brownian transport is characterized by linear-in-time mean-squared displacement in the force-free limit. However, in various physical systems, it has been found that temporal and spatial correlations cause anomalous transport with a corresponding non-Gaussian PDF and nonlinear-in-time mean-squared displacement. In [6,7], Metzler and Klafter introduced the fractional Klein-Kramers equation (FKKE)

$$\frac{\partial W(x,v,t)}{\partial t} = {}_0D_t^{1-\alpha}\left[-\gamma v\frac{\partial}{\partial x}+\gamma\frac{\partial}{\partial v}\left(\eta v-\frac{F(x)}{m}\right)+\gamma\eta\frac{k_BT}{m}\frac{\partial^2}{\partial v^2}\right]W(x,v,t) \tag{1}$$

describing both the velocity v and coordinate x of a particle with mass m exhibiting subdiffusion in an external force field $F(x)=-\Phi'(x)$. Here, η denotes the friction constant, k_BT is the Boltzmann temperature, and the factor γ is the ratio of the intertrapping time scale and the internal waiting scale [6]. The operator

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

$0<\alpha<1$, stands for the fractional derivative of the Riemann-Liouville type [8], and it introduces memory effects to the system. The stationary solution of the FKKE (1) is given by the Gibbs-Boltzmann equilibrium distribution $W_{st}(x,v)=N\exp\{-\beta E\}$, where $\beta=(k_BT)^{-1}$, $E=mv^2/2+\Phi(x)$, and N is the appropriate normalizing constant. For $\alpha=1$ we recover the standard Klein-Kramers equation. Superdiffusive transport in the framework of the Klein-Kramers equation is described in detail in [9], whereas the case in which the fractional derivative term acts only on the dissipative part of the standard Klein-Kramers operator can be found in [10,11]. Additionally, the Lévy-flight approach to the Klein-Kramers dynamics is discussed in [12].

The Klein-Kramers equation is fundamental in modeling of particle escape over a barrier and many other physical processes. Similarly, the FKKE plays a crucial role in investigating the variety of systems characterized by slow dynamics. Equation (1) describes the multiple-trapping scenario, in which the trapping events are superimposed on the Langevin dynamics. In this scenario, the test particle moves according to Brownian diffusion; however it is successively immobilized in traps. The particle is released after some waiting time drawn from the heavy-tailed probability density function $w(t)\sim ct^{-1-\alpha}$. It is assumed here that, following a trapping event, the particle is released with the same position and velocity that it had prior to the immobilization. The immobilization-releasing scenario is in fact a combination of the Langevin dynamics and trapping periods in a sequential manner.

The paper is structured as follows. In Sec. II, by the subordination method, we recognize the explicit form of the two-dimensional stochastic process standing behind Eq. (1). In Sec. III we propose an efficient computer algorithm for visualization of the fractional Klein-Kramers dynamics. We show that our algorithm and Monte Carlo methods provide tools for investigations of the FKKE. We end the paper with a short summary and conclusions in Sec. IV.

II. UNDERLYING STOCHASTIC PROCESS

In what follows, we explore the stochastic structure of Eq. (1). We show that the PDF $P(x,v,t)$ of the two-dimensional stochastic process

$$\mathbf{Y}(t) = (X(S_t), V(S_t)) \tag{3}$$

is a solution of the FKKE (1). Here, the process $(X(\tau),V(\tau))$ is defined as the solution of the following two-dimensional Itô stochastic differential equation:

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$$dV(\tau) = \gamma\left(-\eta V(\tau) + \frac{F(X(\tau))}{m}\right)d\tau + \sqrt{2\gamma\eta\frac{k_BT}{m}}dB(\tau),$$

$$dX(\tau) = \gamma V(\tau)d\tau, \tag{4}$$

driven by the standard Brownian motion $B(\tau)$ with mean 0 and $\langle B^2(\tau)\rangle = \tau$. The subordinator S_t, which is assumed to be independent of $B(\tau)$, is defined as

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

It is called the inverse-time α-stable subordinator. Here, $U(\tau)$ is the strictly increasing α-stable Lévy motion [13], i.e., the α-stable process with Laplace transform $\langle e^{-kU(\tau)}\rangle = e^{-\tau k^\alpha}$, where $0 < \alpha < 1$. Many interesting physical properties of S_t have been discussed in the papers [14–18]. Let us stress that the role of S_t is analogous to the role of the fractional operator ${}_0D_t^{1-\alpha}$ in Eq. (1). It originates from the multiple-trapping events in the underlying continuous-time random walk scenario, while the Brownian diffusion Eqs. (4) describe the motion of the particle between consecutive trapping events. The subordination of $(X(\tau), V(\tau))$ to S_t via Eq. (3) results in a combination of the Langevin dynamics and trapping periods.

Taking advantage of the total probability formula, we get the result that the PDF $P(x,v,t)$ of process (3) is given by

$$P(x,v,t) = \int_0^\infty f(x,v,\tau)s(\tau,t)d\tau.$$

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

$$\hat{P}(x,v,k) = \int_0^\infty f(x,,v,\tau)\hat{s}(\tau,k)d\tau. \tag{6}$$

Next, we find the expression for $\hat{s}(\tau,k)$. It is easy to verify [17] that the relation

$$s(\tau,t) = \frac{t}{\alpha\tau}u(t,\tau)$$

holds, where by $u(t,\tau)$ we denote the PDF of the process $U(\tau)$ from definition (5). Consequently, we can calculate the Laplace transform

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

Using the above result in combination with (6), we get

$$\hat{P}(x,v,k) = \int_0^\infty f(x,v,\tau)k^{\alpha-1}e^{-\tau k^\alpha}d\tau = k^{\alpha-1}\hat{f}(x,v,k^\alpha). \tag{7}$$

Now, since the process $(X(\tau), V(\tau))$ is given by (4), its PDF $f(x,v,\tau)$ obeys the equation

$$\frac{\partial f(x,v,\tau)}{\partial t} = \left[-\gamma v\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial v}\left(\eta v - \frac{F(x)}{m}\right) + \gamma\eta\frac{k_BT}{m}\frac{\partial^2}{\partial v^2}\right]f(x,v,\tau).$$

Equivalently, in the Laplace space we have

$$k\hat{f}(x,v,k) - f(x,v,0) = \left[-\gamma v\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial v}\left(\eta v - \frac{F(x)}{m}\right) + \gamma\eta\frac{k_BT}{m}\frac{\partial^2}{\partial v^2}\right]\hat{f}(x,v,k). \tag{8}$$

Finally, the above formula after the change of variables $k \to k^\alpha$ and in combination with (7) gives

$$k\hat{P}(x,v,k) - P(x,v,0) = k^{1-\alpha}\left[-\gamma v\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial v}\left(\eta v - \frac{F(x)}{m}\right) + \gamma\eta\frac{k_BT}{m}\frac{\partial^2}{\partial v^2}\right]\hat{P}(x,v,k). \tag{9}$$

Inverting the Laplace transform, we obtain

$$\frac{\partial P(x,v,t)}{\partial t} = {}_0D_t^{1-\alpha}\left[-\gamma v\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial v}\left(\eta v - \frac{F(x)}{m}\right) + \gamma\eta\frac{k_BT}{m}\frac{\partial^2}{\partial v^2}\right]P(x,v,t). \tag{10}$$

Thus, we have proved that the PDF $P(x,v,t)$ of the process $(X(S_t), V(S_t))$ is a solution of the FKKE (1). Comparing the structure of the process (3) with the continuous-time random walk scenario underlying the FKKE, we observe that the subordinator S_t is responsible for the subdiffusive behavior of the particle (trapping events), whereas the Brownian diffusion (4) governs the motion of the particle between the trapping periods. A similar mechanism has been observed in the case of the fractional Fokker-Planck equation [19–21].

III. NUMERICAL APPROACH

The previously derived stochastic representation of the FKKE determines a simple algorithm for approximating sample paths of the anomalous diffusion process corresponding to (1). In our method, every trajectory of $(X(S_t), V(S_t))$ is obtained as a superposition of sample paths of $(X(\tau), V(\tau))$ and S_t. A similar approach to the numerical approximation of the fractional Fokker-Planck dynamics was presented in recent papers [20,21]. A different method based on the continuous-time random walk scenario can be found in [22].

The proposed method of approximating sample paths of $(X(S_t), V(S_t))$ on the lattice $\{t_i = i\Delta t; i = 0,1,\ldots,N\}$, where $\Delta t = T/N$ and T is the time horizon, consists of two steps.

(I) In the first step we approximate the values $S_{t_0}, S_{t_1}, \ldots, S_{t_N}$ of the subordinator S_t. This part of the algorithm is identical to the one introduced in [20]; however, for completeness it is repeated here. We begin with 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 recom-

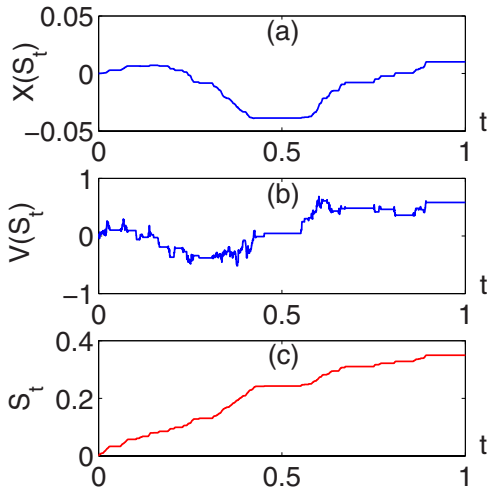

FIG. 1. (Color online) Sample realizations of (a) the position process $X(S_t)$, (b) the velocity process $V(S_t)$, and (c) the subordinator S_t. The constant intervals of the subordinator S_t, representing the trapping periods of the test particle, transfer to the processes $X(S_t)$ and $V(S_t)$. Clearly, after a trapping event the particle is released with the same position and velocity. The parameters are $\alpha=0.8$, $m=k_BT=\eta=1$, and $F(x)=0$.

mended to choose $\Delta\tau<\Delta t$). Using the standard method of summing increments of the process $U(\tau)$, we get

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

$$U(\tau_j)=U(\tau_{j-1})+\Delta\tau^{1/\alpha}\xi_j, \tag{11}$$

where ξ_j are the independent, identically distributed (i.i.d.) totally skewed positive α-stable random variables. The procedure of generating realizations of ξ_j is the following [23–25]:

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

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 (11) ends when $U(\tau)$ crosses the level T, i.e., when for some $j_0=:M$ we get $U(\tau_{M-1})\le T<U(\tau_M)$. 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 $U(\tau_{j-1})<t_i\le U(\tau_j)$, and finally, from definition (5), we get that in such a case

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

(II) In the second step, our goal is to find the approximated values $(X(S_{t_0}),V(S_{t_0})),(X(S_{t_1}),V(S_{t_1})),\ldots,(X(S_{t_N}),V(S_{t_N}))$ of the process $(X(S_t),V(S_t))$. We start by employing the classical Euler scheme to approximate the solution $(X(\tau),V(\tau))$ of the stochastic differential Eq. (4) on the lattice $\{\bar\tau_k=k\Delta\bar\tau; k=0,1,\ldots,L\}$ (it is also recommended to choose $\Delta\bar\tau<\Delta t$). Here L is equal to the first integer that exceeds the value $S_{t_N}/\Delta\bar\tau$. From the Euler scheme [13] we get

$$X(\bar\tau_0)=V(\bar\tau_0)=0,$$

$$V(\bar\tau_k)=V(\bar\tau_{k-1})+\gamma\left(-\eta V(\bar\tau_{k-1})+\frac{F(X(\bar\tau_{k-1}))}{m}\right)\Delta\bar\tau+\left(2\gamma\eta\frac{k_BT}{m}\Delta\bar\tau\right)^{1/2}\bar\xi_k,$$

$$X(\bar\tau_k)=X(\bar\tau_{k-1})+\gamma V(\bar\tau_{k-1})\Delta\bar\tau, \tag{12}$$

for $k=1,2,\ldots,L$. Here $\bar\xi_k$ are i.i.d. random variables with standard normal distribution, $\bar\xi_k\sim N(0,1)$. Recall that from the first step of the algorithm already we have at our disposal the approximations $S_{t_0},S_{t_1},\ldots,S_{t_N}$. Now, since the realizations of $(X(\tau),V(\tau))$ are continuous functions, and since from the iteration scheme (12) we have at our disposal the values $(X(\bar\tau_0),V(\bar\tau_0)),(X(\bar\tau_1),V(\bar\tau_1)),\ldots,(X(\bar\tau_L),V(\bar\tau_L))$, we use the standard linear interpolation in order to obtain the approximate values $(X(S_{t_0}),V(S_{t_0})),(X(S_{t_1}),V(S_{t_1})),\ldots,(X(S_{t_N}),V(S_{t_N}))$. Thus, for every t_i from the lattice $\{t_i=i\Delta t; i=0,1,\ldots,N\}$, we find such an index k that the condition $\bar\tau_k\le S_{t_i}\le\bar\tau_{k+1}$ holds true, and finally, through linear interpolation, we get that

$$X(S_{t_i})=\frac{X(\bar\tau_{k+1})-X(\bar\tau_k)}{\bar\tau_{k+1}-\bar\tau_k}(S_{t_i}-\bar\tau_k)+X(\bar\tau_k),$$

$$V(S_{t_i})=\frac{V(\bar\tau_{k+1})-V(\bar\tau_k)}{\bar\tau_{k+1}-\bar\tau_k}(S_{t_i}-\bar\tau_k)+V(\bar\tau_k),$$

for $i=0,1,\ldots,N$.

The above algorithm allows us to approximate sample paths of $(X(S_t),V(S_t))$ for the whole range of the fractional parameter $\alpha\in(0,1)$ and for an arbitrary force field $F(x)$. The typical trajectories of the process in the case $F(x)=0$ are presented in Fig. 1. The constant intervals of the subordina-

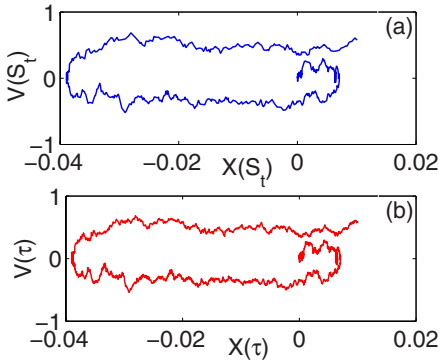

FIG. 2. (Color online) Phase-space diagrams of (a) the sample path $(X(S_t),V(S_t))$, and (b) the corresponding standard diffusion $(X(\tau),V(\tau))$. Both diagrams are identical, which confirms that the motion of the particle between consecutive trapping events is governed by the Langevin dynamics. Parameters as in Fig. 1.

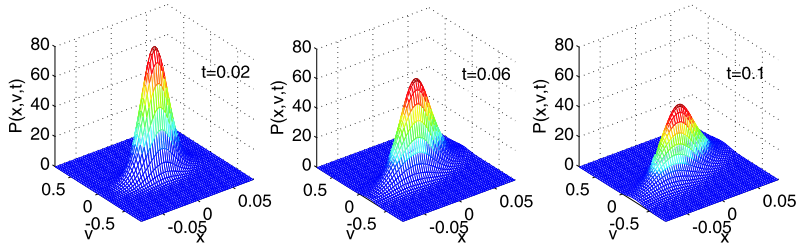

FIG. 3. (Color online) Estimated PDFs $P(x,v,t)$—solutions of the FKKE (1). The estimations were performed on the basis of 10^4 simulated trajectories of the process $(X(S_t),V(S_t))$ using the algorithm introduced in Sec. III. Parameters as in Fig. 1.

tor S_t, representing the trapping periods of the test particle, transfer to the processes $X(S_t)$ and $V(S_t)$. The initial assumption that a trapped particle is released with the same position and velocity that it had prior to the immobilization is evidently satisfied by the sample paths in Fig. 1. However, the consequence of this assumption is the violation of the Newton-type relation $(d/dt)\langle X(t)\rangle=\langle V(t)\rangle$ known from the classical Brownian case. On the level of sample paths of the process, this violation is manifested by the fact that during the trapping periods [constant intervals of $X(S_t)$] the velocity process $V(S_t)$ is not equal to zero. Compare Figs. 1(a) and 1(b). The actual relationship between the mean position and mean velocity in the fractional Klein-Kramers dynamics is the following: $(d/dt)\langle X(S_t)\rangle={}_0D_t^{1-\alpha}\gamma\langle V(S_t)\rangle$. As explained in [6,7], this violation of Newton's law "is only due to the additional waiting time averaging, which camouflages the Newtonian, Langevin-dominated motion events."

In Fig. 2 we present the phase-space diagrams of (a) the sample path $(X(S_t),V(S_t))$, and (b) the corresponding standard diffusion $(X(\tau),V(\tau))$. Both diagrams are identical. This confirms that the motion of a particle between consecutive trapping events is governed by the Langevin dynamics. Note that phase space diagrams neglect the occurrence of trapping periods.

Since a closed-form solution of the FKKE (1) is not known, in order to estimate $P(x,v,t)$ one can use the introduced method of approximating sample paths of $(X(S_t),V(S_t))$. Figure 3 presents the evolution in time of the PDF $P(x,v,t)$ for three different time points in the case $F(x)=0$. The results were obtained using the Rozenblatt-Parzen kernel PDF estimator on the basis of 10^4 simulated sample realizations of the process $(X(S_t),V(S_t))$.

As the numerical investigations show, in the case of the double-well potential $\Phi(x)=x^4/4-2x^2$, the process $(X(S_t),V(S_t))$ reaches its stationary solution. In Fig. 4 we present nine estimated quantile lines $(10\%,20\%,\ldots,90\%)$ corresponding to the processes $X(S_t)$ and $V(S_t)$ obtained with the help of Monte Carlo techniques. In both cases, the quantile lines are asymptotically parallel, which confirms that the stationary solution is reached as $t\to\infty$. The shape of the quantile lines of $X(S_t)$ is typical for double-well potentials. We observe two stable states at $x=\pm 2$. 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]. In Fig. 5 we show both estimated and theoretical stationary solutions of the FKKE. The estimated PDF was constructed on the basis of 10^4 realizations of $(X(S_t),V(S_t))$ with $t=30$. We see that there is a very good agreement between the two PDFs. This confirms the correctness of the algorithm used for approximating sample paths. It is worth emphasizing that analogous statistical methods and simulation techniques can be applied to investigate the fractional Klein-Kramers dynamics for arbitrary potentials $\Phi(x)$ and with no restrictions on the parameters of the model, especially for any $0<\alpha<1$.

IV. CONCLUSIONS

We have introduced an algorithm for approximating sample paths of the anomalous diffusion process described by the FKKE (1). The algorithm is based on the derived stochastic representation of the FKKE. The structure of the stochastic process corresponding to Eq. (1) agrees with the two-stage scenario underlying the anomalous diffusion

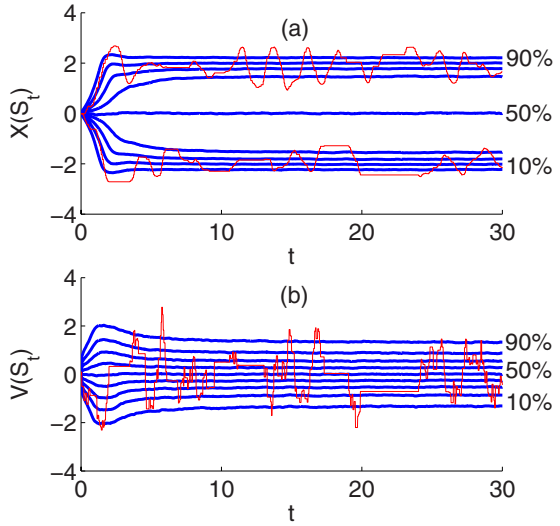

FIG. 4. (Color online) Exemplary sample paths (red lines) and estimated quantile lines (blue lines) $(10\%,20\%,\ldots,90\%)$ corresponding to the processes $X(S_t)$ and $V(S_t)$ in the presence of the double-well potential $\Phi(x)=x^4/4-2x^2$. In both cases the quantile lines are asymptotically parallel, which confirms that the stationary solution is reached. The quantile lines of the position process $X(S_t)$ are typical for the double-well potential with two stable states at $x=\pm 2$. The results were obtained with the help of Monte Carlo techniques on the basis of 10^4 simulated realizations. The parameters are $\alpha=0.9$ and $m=k_BT=\eta=1$.

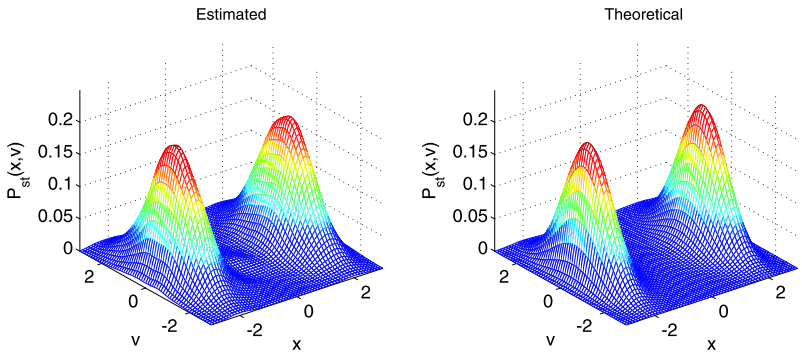

FIG. 5. (Color online) Comparison of the estimated and theoretical stationary solution of the FKKE (1) in the case of a double-well potential with two stable states at $x=\pm 2$. The similarity between the two PDFs confirms the correctness of the algorithm used. The estimated PDF was constructed on the basis of 10^4 simulated realizations of $(X(S_t), V(S_t))$ with $t=30$. Parameters as in Fig. 4.

mechanism, in which trapping events are superimposed onto the Langevin dynamics. The constant intervals of the subordinator S_t are related to the trapping periods of the test particle, whereas the motion of the particle between consecutive trapping events is governed by the Langevin dynamics described by the Brownian diffusion $(X(\tau), V(\tau))$. We have visualized these facts in the included figures (Figs. 1 and 2).

The statistical Monte Carlo techniques presented here allow us to approximate solutions of the FKKE with no restrictions on the set of parameters of the model (Fig. 3). Additionally, we are able to examine the properties of the anomalous diffusion in various external potentials. As an example, we have numerically investigated the model with a double-well potential and its asymptotic behavior (Figs. 4 and 5).

We hope that the results and statistical methods presented here will contribute to further investigations and to a better understanding of the fractional Klein-Kramers dynamics.

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