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Anomalous diffusion in nonhomogeneous media: Power spectral density of signals generated by time-subordinated nonlinear Langevin equations

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HIGHLIGHTS

- We obtained time-subordinated nonlinear SDEs generating signals with power law distributions.
- The analytical expression of power spectral density has been derived.
- For some parameters our equations generate signals having $1/f$ spectrum.

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ABSTRACT

Subdiffusive behavior of one-dimensional stochastic systems can be described by time-subordinated Langevin equations. The corresponding probability density satisfies the time-fractional Fokker–Planck equations. In the homogeneous systems the power spectral density of the signals generated by such Langevin equations has power-law dependency on the frequency with the exponent smaller than 1. In this paper we consider nonhomogeneous systems and show that in such systems the power spectral density can have power-law behavior with the exponent equal to or larger than 1 in a wide range of intermediate frequencies.

1. Introduction

A number of experimental observations show that more complex diffusion processes in which the mean-square displacement is not proportional to the time t take place in various systems. A broad family of processes described by certain deviations from the classical Brownian linear time dependence of the centered second moment is called anomalous diffusion. Anomalous diffusion in one dimension is characterized by the occurrence of a mean square displacement of the form

$$\langle (\Delta x)^2 \rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha, \tag{1}$$

which deviates from the linear Brownian dependence on time [1]. Eq. (1) introduces the anomalous diffusion coefficient K_α. Such a deviation from classical diffusive behavior can be observed in many systems [2–4] and leads to many interesting physical properties [5]. Applications of anomalous diffusion have been found in physics, chemistry and biology [1,5,6]. In general, anomalous diffusion occurs in complex structures exhibiting the presence of long-range correlations or memory

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effects [1]. In the physics of complex systems, anomalous transport properties and their description have attracted considerable interest starting with the pioneering papers of Montroll and his collaborators [7].

An important subclass of anomalous diffusion processes constitute subdiffusion processes, characterized by the sublinear dependence with the power-law exponent in the range $0 < \alpha < 1$. In this situation no finite mean jump time Δt exists [2]. Subdiffusion processes have been reported in condensed matter systems [2], ecology [3], and biology [4]. Continuous time random walks (CTRWs) with on-site waiting-time distributions falling slowly as $t^{-\alpha-1}$ and lacking the first moment predict a subdiffusive behavior and are powerful tools to describe systems which display subdiffusion [2,8]. Starting from the generalized master equation or from the CTRW the fractional Fokker–Planck equation can be rigorously derived [9,10]. Fractional Fokker–Planck equation provides a useful approach for the description of transport dynamics in complex systems which are governed by anomalous diffusion [2] and nonexponential relaxation patterns [11]. It has been used to model dynamics of protein systems and for reactions occurring in disordered media [2,12–18]. Description equivalent to a fractional Fokker–Planck equation consists of a Markovian dynamics governed by an ordinary Langevin equation but proceeding in an auxiliary, operational time instead of the physical time [19]. This Markovian process is subordinated to the process defining the physical time; the subordinator introduces memory effects [20]. Other approaches for the theoretical description of the subdiffusion use the generalized Langevin equation [21–23], fractional Brownian motion [24], or the Langevin equation with multiplicative noise [25].

The traditional CTRW provides a homogeneous description of the medium. More complex situation is the diffusion in nonhomogeneous media, for example diffusion on fractals and multifractals [26]. Nonhomogeneous systems exhibit not only subdiffusion related to traps, but also enhanced diffusion can occur: for example, transport of interacting particles in a weakly disordered media is superdiffusive due to the disorder and subdiffusive without the disorder [27]. Anomalous diffusion in heterogeneous fractal medium has been considered in Ref. [28] where it was proposed that in one dimension the mean square displacement has the form $\langle(\Delta x)^2\rangle \sim x^{-\theta}t^{\alpha}$ instead of Eq. (1). Heterogeneous fractional Fokker–Planck equation on heterogeneous fractal structure media has been investigated in Refs. [29–32]. In nonhomogeneous media the properties of a trap can reflect the medium structure, therefore in the description of transport in such a medium the waiting time should explicitly depend on the position. This dependence can be introduced by using the position-dependent subdiffusion exponents [33–35]. Another way is to consider position-dependent time subordinator [36].

In the homogeneous systems the power spectral density (PSD) of the signals generated by time-subordinated Langevin equations has power-law dependency $S(f) \sim f^{\alpha-1}$ on the frequency as $f \to 0$ [37]. Since $0 < \alpha < 1$, the power-law exponent $1-\alpha$ is smaller than 1. The purpose of this paper is to consider the PSD in nonhomogeneous systems exhibiting anomalous diffusion. We demonstrate, that in such systems the PSD can have power-law behavior with the exponent equal to or larger than 1 in a wide range of intermediate frequencies.

The paper is organized as follows: in Section 2 we introduce the time-fractional Fokker–Planck equation describing subdiffusion in nonhomogeneous media. The expression for the power spectral density of the fluctuations of the diffusing particle in such a medium is obtained in Section 3. In Section 4 we consider a particular case of the time-fractional Fokker–Planck equation involving the coefficients with power-law dependence on the position. Numerical methods of solution are discussed in Section 5. Section 6 summarizes our findings.

2. Time-fractional Fokker–Planck equation for nonhomogeneous media

In this section we derive the time-fractional Fokker–Planck equation describing diffusion of a particle in nonhomogeneous media. Usually the description of the anomalous diffusion is given by the CTRW theory assuming heavy-tailed waiting-time distributions between successive jumps of the diffusing particle. Here we use the method of the derivation that is similar to that outlined in Refs. [19,38]. We start with the Markovian process described by the Itô stochastic differential equation (SDE)

$$\mathrm{d}x(\tau) = a(x(\tau))\mathrm{d}\tau + b(x(\tau))\mathrm{d}W(\tau). \tag{2}$$

Here $W(\tau)$ is the standard Brownian motion (Wiener process). The drift coefficient $a(x)$ and the diffusion coefficient $b(x)$ explicitly depend on the particle position x. This dependence on the position reflects the nonhomogeneity of a medium. Following Ref. [19] we interpret the time τ in Eq. (2) as an internal, operational time. Eq. (2) we consider together with an additional equation that relates the operational time τ to the physical time t. The difference between physical time t and the operational time τ occurs due to trapping of the diffusing particle. For the trapping processes that have distribution of the trapping times with power law tails, the physical time $t = T(\tau)$ is given by the strictly increasing α-stable Lévy motion defined by the Laplace transform

$$\langle \mathrm{e}^{-kT(\tau)}\rangle = \mathrm{e}^{-\tau k^{\alpha}}. \tag{3}$$

Here the parameter α takes the values from the interval $0 < \alpha < 1$. Thus the physical time t obeys the SDE

$$\mathrm{d}t(\tau) = \mathrm{d}L^{\alpha}(\tau), \tag{4}$$

where $\mathrm{d}L^{\alpha}(\tau)$ stands for the increments of the strictly increasing α-stable Lévy motion $L^{\alpha}(\tau)$. For such physical time t the operational time τ is related to the physical time t via the inverse α-stable subordinator [39,40]

$$S(t) = \inf\{\tau : T(\tau) > t\}. \tag{5}$$

The processes $x(\tau)$ and $S(t)$ are assumed to be independent. Eqs. (2) and (4) define the subordinated process $y(t)$ obtained by a random change of time

$$y(t) = x(S(t)). \tag{6}$$

The process $y(t)$ describes the diffusion of a particle in a medium with traps.

We will derive the equation for the probability density function (PDF) of y. For the derivation we use the method of Laplace transform. The PDF $P_x(x, \tau)$ of the stochastic variable x as a function of the operational time τ obeys the Fokker–Planck equation corresponding to the Itô SDE (2)

$$\frac{\partial}{\partial \tau} P_x(x, \tau) = L_{\mathrm{FP}}(x) P_x(x, \tau), \tag{7}$$

where $L_{\mathrm{FP}}(x)$ is the time-independent Fokker–Planck operator [41]

$$L_{\mathrm{FP}}(x) = -\frac{\partial}{\partial x} a(x) + \frac{1}{2} \frac{\partial^2}{\partial x^2} b^2(x). \tag{8}$$

The Laplace transform of Eq. (7) is

$$k\tilde{P}_x(x, k) - P_x(x, 0) = L_{\mathrm{FP}}(x)\tilde{P}_x(x, k). \tag{9}$$

Since the processes $x(\tau)$ and $S(t)$ are independent, the PDF of the random process $x(S(t))$ is given by

$$P(x, t) = \int P_x(x, \tau) P_S(\tau, t)\, \mathrm{d}\tau. \tag{10}$$

Here $P_S(\tau, t)$ is the PDF of the inverse α-stable subordinator $S(t)$. From Eq. (10) it follows that the Laplace transform $\tilde{P}(x, k)$ of the PDF $P(x, t)$ is related to the Laplace transform $\tilde{P}_S(\tau, k)$ of the inverse subordinator $S(t)$:

$$\tilde{P}(x, k) = \int P_x(x, \tau)\tilde{P}_S(\tau, k)\, \mathrm{d}\tau. \tag{11}$$

The Laplace transform $\tilde{P}_S(\tau, k)$ of the inverse subordinator $S(t)$ we obtain as follows: from the definition of the inverse subordinator (5) we have $\Pr(S(t) < \tau) = \Pr(T(\tau) \geqslant t)$, therefore

$$P_S(\tau, t) = -\frac{\partial}{\partial \tau} \int_0^t P_T(t', \tau)\, \mathrm{d}t'. \tag{12}$$

Here $P_T(t, \tau)$ is the PDF of the strictly increasing α-stable Lévy motion $T(\tau)$. The PDF $P_T(t, \tau)$ fulfills the scaling relation

$$P_T(t, \tau) = \frac{1}{\tau^{\frac{1}{\alpha}}} P_T\left(\frac{t}{\tau^{\frac{1}{\alpha}}}, 1\right), \tag{13}$$

since the strictly increasing α-stable Lévy motion is $1/\alpha$ self-similar [42]. Combining Eqs. (12) and (13) we obtain

$$P_S(\tau, t) = \frac{t}{\alpha\tau} P_T(t, \tau). \tag{14}$$

Consequently, the Laplace transform of $P_S(\tau, t)$ is equal to

$$\tilde{P}_S(\tau, k) = k^{\alpha-1} \mathrm{e}^{-\tau k^{\alpha}}. \tag{15}$$

Here we used Eq. (3) for the Laplace transform of $P_T(t, \tau)$.

Using Eqs. (11) and (15) we get

$$\tilde{P}(x, k) = k^{\alpha-1}\tilde{P}_x(x, k^{\alpha}). \tag{16}$$

Acting with the operator $L_{\mathrm{FP}}(x)$ on Eq. (16) we have

$$\tilde{P}(x, k) = k^{-1} P_x(x, 0) + k^{-\alpha} L_{\mathrm{FP}}(x)\tilde{P}(x, k). \tag{17}$$

The inverse Laplace transform of this equation yields

$$P(x, t) = P_x(x, 0) + \frac{1}{\Gamma(\alpha)} \int_0^t \mathrm{d}t'\, (t - t')^{\alpha-1} L_{\mathrm{FP}}(x) P(x, t'). \tag{18}$$

Introducing the fractional Riemann–Liouville operator [43]

$${}_0D_t^{-\alpha} f(t) \equiv \frac{1}{\Gamma(\alpha)} \int_0^t \frac{f(t')}{(t - t')^{1-\alpha}} \mathrm{d}t', \quad 0 < \alpha < 1 \tag{19}$$

we can write Eq. (18) as

$$P(x,t) = P_x(x,0) + {}_0D_t^{-\alpha} L_{\mathrm{FP}}(x) P(x,t). \tag{20}$$

By differentiating this equation with respect to time we get the time-fractional Fokker–Planck equation

$$\frac{\partial}{\partial t} P(x,t) = {}_0D_t^{1-\alpha} \left(-\frac{\partial}{\partial x}[a(x)P] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b^2(x)P] \right), \tag{21}$$

where

$${}_0D_t^{1-\alpha} f(t) \equiv \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{f(t')}{(t-t')^{1-\alpha}} \mathrm{d}t', \quad 0 < \alpha < 1. \tag{22}$$

The operator ${}_0D_t^{1-\alpha}$ is expressed via the convolution with a slowly decaying kernel, which is typical for memory effects in complex systems [44]. Eq. (21) is the equation describing the subdiffusion of particles in an inhomogeneous medium. This equation generalizes the previously obtained time-fractional Fokker–Planck equation with the position-independent diffusion coefficient.

2.1. Position-dependent trapping time

The properties of a trap in a nonhomogeneous medium can reflect the structure of the medium. In the description of the transport in such a medium the waiting time should explicitly depend on the position [36]. Instead of Eq. (4) we assume that the physical time t is related to the operational time τ via the SDE

$$\mathrm{d}t(\tau) = g(x(\tau))\mathrm{d}L^\alpha(\tau). \tag{23}$$

Here the positive function $g(x)$ is the intensity of random time and models the position of structures responsible for either trapping or accelerating the particle. Large values of $g(x)$ correspond to trapping of the particle, whereas small $g(x)$ leads to the acceleration of diffusion. A similar equation has been used in Ref. [36]. We interpret Eq. (23) according to the Itô stochastic calculus: the values of x and t at operational time τ are determined by events prior to the application of the stochastic force $\mathrm{d}L^\alpha$, which acts only from time τ to $\tau + \mathrm{d}\tau$. This assumption leads to the decoupling of the changes of x and the changes of t occurring during an infinitesimal increment of the operational time $\mathrm{d}\tau$. Note, that the increments of the strictly increasing α-stable Lévy motion $L^\alpha(\tau)$ are characterized by long tails and thus only moments of order smaller than α are finite.

For fixed particle position x the coefficient $g(x)$ in Eq. (23) is constant and Eq. (23) corresponds to the fractional Fokker–Planck equation

$$\frac{\partial}{\partial \tau} P(t;\tau|x) = -{}_0D_t^\alpha g(x)^\alpha P(t;\tau|x). \tag{24}$$

This equation can be obtained by noting that from the definition of the strictly increasing α-stable Lévy motion (3) the Laplace transform of the PDF $P(t;\tau|x)$ is $\tilde{P}(k;\tau|x) = \exp\{-\tau[g(x)k]^\alpha\}$. Differentiating this expression with respect to τ and taking the inverse Laplace transform one gets Eq. (24). Alternatively, one can obtain the fractional Fokker–Planck equation using the methods of Refs. [26,45,46]. The fractional derivative in the Fokker–Planck equation appears as a consequence of the increments of Lévy α-stable motion in Eq. (23).

Eqs. (2) and (23) together define the subordinated process. However, now the processes $x(\tau)$ and $t(\tau)$ are not independent and the derivation of the Fokker–Planck equation presented in previous subsection is not applicable. Nevertheless, we can show that also with position dependent trapping time the resulting equation has the form of Eq. (21). To do this let us consider the joint PDF $P_{x,t}(x,t;\tau)$ of the stochastic variables x and t.

SDEs (2) and (23) correspond to the following two-dimensional fractional Fokker–Planck equation:

$$\frac{\partial}{\partial \tau} P_{x,t}(x,t;\tau) = L_{\mathrm{FP}}(x) P_{x,t} - {}_0D_t^\alpha g(x)^\alpha P_{x,t}. \tag{25}$$

This equation is a combination of Eqs. (7) and (24). Two-dimensional fractional Fokker–Planck equation (25) for the PDF of two stochastic variables x and t can be rigorously derived from the SDEs (2) and (23) driven by Lévy stable noises as in Refs. [26,45,46] (the Gaussian noise in Eq. (2) is a particular case of a Lévy stable noise with index of stability $\alpha = 2$).

The zero of the physical time t coincides with the zero of the operational time τ, therefore, the initial condition for Eq. (25) is $P_{x,t}(x,t;0) = P_x(x,0)\delta(t)$. In addition, since t is strictly increasing, we have a boundary condition $P_{x,t}(x,0;\tau) = 0$ when $\tau > 0$. The fractional Riemann–Liouville operator ${}_0D_t^\alpha$ in Eq. (25) we can write as ${}_0D_t^\alpha = \frac{\partial}{\partial t} {}_0D_t^{\alpha-1}$.

Now let us consider x and τ as stochastic variables instead of x and t. Since the stochastic variable t is related to the operational time τ via Eq. (23), the joint PDF $P_{x,\tau}(x,\tau;t)$ of the stochastic variables x and τ is related to the PDF $P_{x,t}(x,t;\tau)$ according to the equation

$$P_{x,\tau}(x,\tau;t) = {}_0D_t^{\alpha-1} g(x)^\alpha P_{x,t}(x,t;\tau). \tag{26}$$

This equation can be obtained by noting that the last term in Eq. (25) contains derivative $\frac{\partial}{\partial t}$ and thus should be equal to $-\frac{\partial}{\partial t}P_{x,\tau}$. From Eq. (26) it follows that

$$P_{x,t} = {}_0D_t^{1-\alpha}\frac{1}{g(x)^{\alpha}}P_{x,\tau}. \tag{27}$$

Using Eqs. (25) and (27) we obtain

$$\frac{\partial}{\partial t}P_{x,\tau}(x,\tau;t) = {}_0D_t^{1-\alpha}L_{\mathrm{FP}}(x)\frac{1}{g(x)^{\alpha}}P_{x,\tau} - \frac{\partial}{\partial \tau}{}_0D_t^{1-\alpha}\frac{1}{g(x)^{\alpha}}P_{x,\tau}. \tag{28}$$

The PDF $P_{x,\tau}$ has the initial condition $P_{x,\tau}(x,\tau;0) = P_x(x,0)\delta(\tau)$ and the boundary condition $P_{x,\tau}(x,0;t) = 0$. The PDF of the subordinated random process $x(t)$ is $P(x,t) = \int P_{x,\tau}(x,\tau;t)\,\mathrm{d}\tau$. Integrating both sides of Eq. (28) we get

$$\frac{\partial}{\partial t}P(x,t) = {}_0D_t^{1-\alpha}L'_{\mathrm{FP}}(x)P, \tag{29}$$

where the new Fokker–Planck operator is

$$L'_{\mathrm{FP}}(x) = -\frac{\partial}{\partial x}a'(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}b'(x)^2. \tag{30}$$

Here the new drift and the diffusion coefficient are

$$a'(x) = \frac{a(x)}{g(x)^{\alpha}}, \qquad b'(x) = \frac{b(x)}{g(x)^{\frac{\alpha}{2}}}. \tag{31}$$

Thus position-dependent trapping leads to position-dependent coefficients in the time-fractional Fokker–Planck equation, even if the initial SDE (2) has constant coefficients. Eq. (29) is the same as Eq. (21) when $g(x)$ is constant and does not depend on position.

3. Power spectral density and time-fractional Fokker–Planck equation

In this section we derive a general expression for the PSD of the fluctuations of the diffusing particle in nonhomogeneous medium. The evolution of the PDF of particle position x is described by the time-fractional Fokker–Planck equation (21). For calculation of the spectrum we use the eigenfunction expansion of the Fokker–Planck operator L_{FP}. Method of eigenfunctions for solving of time-dependent fractional Fokker–Planck equation has been used in Ref. [47]. Spectrum of fluctuations when the diffusion coefficient is constant has been obtained in Ref. [37]. Similar derivation of the spectrum for nonlinear SDE has been performed in Ref. [48].

The eigenfunctions of the Fokker–Planck operator $L_{\mathrm{FP}}(x)$ are the solutions of the equation

$$L_{\mathrm{FP}}(x)P_{\lambda}(x) = -\lambda P_{\lambda}(x). \tag{32}$$

Here $P_{\lambda}(x)$ are the eigenfunctions and $\lambda \geqslant 0$ are the corresponding eigenvalues. The eigenfunctions obey the orthonormality relation [49]

$$\int \mathrm{e}^{\Phi(x)}P_{\lambda}(x)P_{\lambda'}(x)\mathrm{d}x = \delta_{\lambda,\lambda'}, \tag{33}$$

where

$$\Phi(x) = -\ln P_0(x) \tag{34}$$

is the potential associated with the operator $L_{\mathrm{FP}}(x)$. Here $P_0(x)$ is the steady-state solution of Eq. (21).

We can write the time-dependent solution of the fractional Fokker–Planck equation (21) corresponding to a single eigenfunction as

$$P(x,t) = P_{\lambda}(x)f_{\lambda}(t). \tag{35}$$

Inserting into Eq. (21) we get that the function $f(t)$ obeys the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}f_{\lambda}(t) = -\lambda {}_0D_t^{1-\alpha}f_{\lambda}(t) \tag{36}$$

with the initial condition $f(0) = 1$. The Laplace transform of this equation yields

$$k\tilde{f}_{\lambda}(k) = 1 - \lambda k^{1-\alpha}\tilde{f}_{\lambda}(k). \tag{37}$$

The solution of Eq. (37) is

$$\tilde{f}_{\lambda}(k) = \frac{1}{k + \lambda k^{1-\alpha}}. \tag{38}$$

The inverse Laplace transform is given in terms of the monotonically decreasing Mittag-Leffler function [47]

$$f_\lambda(t) = E_\alpha(-\lambda t^\alpha). \tag{39}$$

The Mittag-Leffler function has a series expansion

$$E_\alpha(z) \equiv E_{\alpha,1}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}. \tag{40}$$

The autocorrelation function can be calculated from the transition probability $P(x, t|x_0, 0)$ (the conditional probability that at time t the stochastic variable has value x with the condition that at time $t = 0$ it had the value x_0):

$$C(t) = \int \mathrm{d}x \int \mathrm{d}x_0\, x_0 x P_0(x_0) P(x, t|x_0, 0) - \left[\int \mathrm{d}x\, x P_0(x)\right]^2. \tag{41}$$

The transition probability is the solution of the Fokker–Planck equation (21) with the initial condition $P(x, 0|x_0, 0) = \delta(x - x_0)$. Expansion of the transition probability density in a series of the eigenfunctions has the form

$$P(x, t|x_0, 0) = \sum_\lambda P_\lambda(x) \mathrm{e}^{\Phi(x_0)} P_\lambda(x_0) E_\alpha(-\lambda t^\alpha), \tag{42}$$

where we used Eqs. (35) and (39). Inserting Eq. (42) into Eq. (41) we get the expression for the autocorrelation function

$$C(t) = \sum_{\lambda>0} X_\lambda^2 E_\alpha(-\lambda t^\alpha). \tag{43}$$

Here

$$X_\lambda = \int x P_\lambda(x)\, \mathrm{d}x \tag{44}$$

is the first moment of the stochastic variable x evaluated with the λ-th eigenfunction $P_\lambda(x)$. Such an expression for the autocorrelation function has been obtained in Ref. [37].

According to Wiener–Khintchine relations, the power spectral density is related to the autocorrelation function:

$$S(f) = 4 \int_0^\infty C(t) \cos(\omega t)\, \mathrm{d}t, \tag{45}$$

where $\omega = 2\pi f$. Using Eq. (43) we obtain

$$S(f) = 4 \sum_{\lambda>0} X_\lambda^2 \int_0^\infty E_\alpha(-\lambda t^\alpha) \cos(\omega t)\, \mathrm{d}t. \tag{46}$$

The integral can be calculated by noting that the Laplace transform of $E_\alpha(-\lambda t^\alpha)$ is given by Eq. (38). We obtain the desired expression for the PSD

$$S(f) = 4 \frac{\sin\left(\frac{\pi}{2}\alpha\right)}{\omega^{1-\alpha}} \sum_\lambda \frac{\lambda}{\lambda^2 + \omega^{2\alpha} + 2\lambda\omega^\alpha \cos\left(\frac{\pi}{2}\alpha\right)} X_\lambda^2. \tag{47}$$

Eq. (47) becomes the usual expression for the PSD when $\alpha \to 1$. Similar expression for the spectrum has been obtained in Ref. [37].

For small frequencies $\omega \ll \lambda_1^{1/\alpha}$ we can neglect the frequency when it appears together with the eigenvalues λ. Here λ_1 is the smallest eigenvalue larger than zero. Thus for small frequencies Eq. (47) approximately is

$$S(f) \approx 4 \frac{\sin\left(\frac{\pi}{2}\alpha\right)}{\omega^{1-\alpha}} \sum_\lambda \frac{X_\lambda^2}{\lambda}. \tag{48}$$

We obtain that for small frequencies the PSD has a power-law dependency on the frequency $S(f) \sim f^{-(1-\alpha)}$. However, the power-law exponent is always smaller than 1, since $0 < \alpha < 1$. It is not possible to get pure $1/f$ spectrum this way. In the next section we show that it is possible to get larger power-law exponents in the PSD in a wide range of intermediate frequencies when the diffusion coefficient is not constant and depends on x.

4. Time-fractional Fokker–Planck equation with power-law coefficients

In this section we consider a particular case of the time-fractional Fokker–Planck equation (21). We assume that the diffusion coefficient has a power-law dependence on the particle position x and Eq. (21) takes the form

$$\frac{\partial}{\partial t}P(x,t)=\sigma^2{}_0D_t^{1-\alpha}\left\{\left(\frac{\nu}{2}-\eta\right)\frac{\partial}{\partial x}\left[x^{2\eta-1}P(x,t)\right]+\frac{1}{2}\frac{\partial^2}{\partial x^2}\left[x^{2\eta}P(x,t)\right]\right\}. \tag{49}$$

Here η is the power-law exponent of the multiplicative noise in Eq. (2) and ν defines the behavior of the steady-state PDF $P_0(x)$. Eq. (49) should be considered together with the boundary conditions that restrict the stochastic variable x to the positive values.

The steady-state PDF $P_0(x)$ obtained from Eq. (49) has a power-law form

$$P_0(x)\sim x^{-\nu}. \tag{50}$$

For $\nu \geq 1$ the PDF $P_0(x)$ diverges as $x \to 0$, thus the diffusion should be restricted at least from the side of small values. This can be done by introducing an additional potential that becomes large only when x acquires values outside of the interval $[x_{\min}, x_{\max}]$ into the drift term of Eq. (49). The simplest choice is the reflective boundaries at $x = x_{\min}$ and $x = x_{\max}$.

The power-law form of the diffusion coefficient is natural for systems exhibiting self-similarity, for example disordered materials, and has been used to describe diffusion on fractals [50,51], turbulent two-particle diffusion, transport of fast electrons in a hot plasma [52,53]. Eq. (49) is a generalization of the Fokker–Planck equation resulting from nonlinear SDEs proposed in Refs. [54,55]. Such nonlinear SDEs generate signals having $1/f$ spectrum in a wide range of frequencies and have been used to describe signals in socio-economical systems [56,57] and Brownian motion in inhomogeneous media [58].

In Ref. [48] an approximate expression for the first moment X_λ has been obtained for the Fokker–Planck operator appearing in Eq. (49) assuming reflective boundaries at $x_{\min} = 1$ and $x_{\max} = \xi$, $\xi \gg 1$. According to the results of Ref. [48]

$$X_\lambda\sim\frac{c_\lambda}{|1-\eta|}\frac{1}{\rho^{\beta_1}}, \tag{51}$$

where

$$c_\lambda=\sqrt{\frac{|1-\eta|}{z_{\max}}\frac{\nu-1}{1-\xi^{1-\nu}}\pi\rho},\qquad \rho=\frac{\sqrt{2\lambda}}{|\eta-1|},\qquad \beta_1=1+\frac{\nu-3}{2(\eta-1)}. \tag{52}$$

The parameters $z_{\min}$ and $z_{\max}$ depend on the boundaries $x_{\min}$ and $x_{\max}$. When $\rho z_{\max} \gg 1$, replacing summation by integration in Eq. (47) we obtain the expression for the PSD

$$S(f)\approx 4\frac{\sin\left(\frac{\pi}{2}\alpha\right)}{\omega^{1-\alpha}}\int\frac{\lambda}{\lambda^2+\omega^{2\alpha}+2\lambda\omega^\alpha\cos\left(\frac{\pi}{2}\alpha\right)}X_\lambda^2 D(\lambda)\,\mathrm{d}\lambda. \tag{53}$$

The density of eigenvalues $D(\lambda)$ has been estimated as [48]

$$D(\lambda)\sim\frac{1}{\sqrt{\lambda}}. \tag{54}$$

Using Eqs. (51) and (54) we get

$$S(f)\sim 4\frac{\sin\left(\frac{\pi}{2}\alpha\right)}{\omega^{1+\alpha(\beta_1-1)}}\int_{\frac{z_{\max}^{-2}}{\omega^\alpha}}^{\frac{z_{\min}^{-2}}{\omega^\alpha}}\frac{1}{u^{\beta_1-1}}\frac{1}{\left(u^2+1+2u\cos\left(\frac{\pi}{2}\alpha\right)\right)}\mathrm{d}u. \tag{55}$$

Here the upper range of integration is limited because X_λ becomes small when $\rho z_{\min} \gg 1$ [48]. When $z_{\max}^{-2} \ll \omega^\alpha \ll z_{\min}^{-2}$ and $0 < \beta_1 < 2$ then we can approximate the lower limit of integration by 0 and the upper limit by ∞. In this case the PSD depends on the frequency as $S(f) \sim f^{-1-\alpha(\beta_1-1)}$. When $\beta_1 > 2$ then the largest contribution is from the lower limit of the integration. Thus, when $z_{\max}^{-2} \ll \omega^\alpha \ll z_{\min}^{-2}$ then the leading term in the expansion of the approximate expression for the PSD in the power series of ω is

$$S(f)\sim\begin{cases}\dfrac{1}{\omega^{1+\alpha(\beta_1-1)}}, & 0<\beta_1<2,\\[2mm] \dfrac{1}{\omega^{1+\alpha}}, & \beta_1>2.\end{cases} \tag{56}$$

This expression for PSD can also be written as

$$S(f)\sim\begin{cases}\dfrac{1}{\omega^{\beta}}, & 1-\alpha<\beta<1+\alpha,\\[2mm] \dfrac{1}{\omega^{1+\alpha}}, & \beta>1+\alpha.\end{cases} \tag{57}$$

Here

$$\beta = 1 + \alpha(\beta_1 - 1) = 1 + \frac{\alpha(\nu - 3)}{2(\eta - 1)} \tag{58}$$

is the power-law exponent of the PSD. Eq. (58) generalizes the expression for the power-law exponent obtained for nonlinear SDEs [55]. When $\nu = 3$ then from Eq. (58) follows that we obtain $1/f$ spectrum.

4.1. Power spectral density from scaling properties

Power-law exponent (58) in the PSD can be obtained from the scaling properties of Eq. (49), similarly as it has been done for the nonlinear SDEs [59]. Changing the variable x to the scaled variable $x_s = ax$ in Eq. (49) yields

$$\frac{\partial}{\partial t}P(x_s, t) = \frac{\sigma^2}{a^{2(\eta-1)}}\,{}_0D_t^{1-\alpha}\left\{\left(\frac{\lambda}{2} - \eta\right)\frac{\partial}{\partial x_s}\left[x_s^{2\eta-1}P(x_s, t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x_s^2}\left[x_s^{2\eta}P(x_s, t)\right]\right\}. \tag{59}$$

The Riemann–Liouville fractional derivative has the following scaling property: ${}_0D_t^{1-\alpha}f(ct) = c^{1-\alpha}\,{}_0D_{ct}^{1-\alpha}f(ct)$. Thus, changing the time t to the scaled time $t_s = a^{\mu}t$ we get

$$a^{\mu}\frac{\partial}{\partial t_s}P(x, t_s) = \sigma^2\,{}_0a^{\mu(1-\alpha)}D_{t_s}^{1-\alpha}\left\{\left(\frac{\lambda}{2} - \eta\right)\frac{\partial}{\partial x}\left[x^{2\eta-1}P(x, t_s)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[x^{2\eta}P(x, t_s)\right]\right\}. \tag{60}$$

The change of the variable x to the scaled variable ax or the change of the time t to the scaled time $a^{\mu}t$ produces the same fractional Fokker–Planck equation if

$$\mu = \frac{2(\eta - 1)}{\alpha}. \tag{61}$$

It follows, that the transition probability $P(x, t|x_0, 0)$ has the following scaling property:

$$aP(ax, t|ax_0, 0) = P(x, a^{\mu}t|x_0, 0). \tag{62}$$

As has been shown in Ref. [59], the power-law steady state PDF $P_0(x) \sim x^{-\nu}$ and the scaling property of the transition probability (62) lead to the power-law form PSD $S(f) \sim f^{-\beta}$ in a wide range of frequencies. The power-law exponent β is given by

$$\beta = 1 + (\nu - 3)/\mu. \tag{63}$$

Using Eq. (61) we obtain the same expression for β as in Eq. (58).

The presence of restrictions at $x = x_{\min}$ and $x = x_{\max}$ makes the scaling (62) not exact. This limits the power-law part of the PSD to a finite range of frequencies $f_{\min} \ll f \ll f_{\max}$. Similarly as in Ref. [59], we estimate the limiting frequencies as

$$\begin{aligned} &\sigma^{\frac{2}{\alpha}}x_{\min}^{\frac{2}{\alpha}(\eta-1)} \ll 2\pi f \ll \sigma^{\frac{2}{\alpha}}x_{\max}^{\frac{2}{\alpha}(\eta-1)}, \quad \eta > 1,\\ &\sigma^{\frac{2}{\alpha}}x_{\max}^{-\frac{2}{\alpha}(1-\eta)} \ll 2\pi f \ll \sigma^{\frac{2}{\alpha}}x_{\min}^{-\frac{2}{\alpha}(1-\eta)}, \quad \eta < 1. \end{aligned} \tag{64}$$

This equation shows that the frequency range grows with decrease of α. By increasing the ratio $x_{\max}/x_{\min}$ one can get an arbitrarily wide range of the frequencies where the PSD has $1/f^{\beta}$ behavior.

5. Numerical approach

5.1. Numerical approximation of sample paths

Since analytical solution of time-fractional Fokker–Planck equation can be obtained only in separate cases, there is a need of numerical solution. Numerical solution of time-fractional Fokker–Planck equation is complicated [60]. It is easier to numerically solve Langevin equations (2), (4) instead. The desired properties of the solution of the Fokker–Planck equation then can be calculated by averaging over many sample paths obtained by solving the Langevin equations. The numerical method of solution of the Langevin equations with constant drift coefficient is outlined in Refs. [38,61]. We can use the same method also when the drift coefficient is position-dependent.

Choosing the time step $\Delta\tau$ of the operational time τ the inverse subordinator $S(t)$ is approximated as [62]

$$S_{\Delta\tau}(t) = [\min\{n \in \mathbb{N} : T(n\Delta\tau) > t\} - 1]\Delta\tau. \tag{65}$$

Such approximation satisfies [63]

$$\sup_{0\leqslant t\leqslant T}[S_{\Delta\tau}(t) - S(t)] \leqslant \Delta\tau. \tag{66}$$

The values $T(n\Delta\tau)$ are generated by summing up the independent and stationary increments of the Lévy process:

$$T(n\Delta\tau) = T([n-1]\Delta\tau) + \Delta\tau^{1/\alpha}\xi_n. \tag{67}$$

Here ξ_n are independent totally skewed positive α-stable random variables with the distribution specified by the Laplace transform $\langle e^{-k\xi}\rangle = e^{-k^\alpha}$. Such variables can be generated using the formula [64]

$$\xi = \frac{\sin\left[\alpha\left(U+\frac{\pi}{2}\right)\right]}{\cos(U)^{\frac{1}{\alpha}}}\left(\frac{\cos\left[U-\alpha\left(U+\frac{\pi}{2}\right)\right]}{W}\right)^{\frac{1-\alpha}{\alpha}}. \tag{68}$$

Here U is uniformly distributed on $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ and W has an exponential distribution with mean 1. Note, that in Ref. [38] an incorrect formula for generating totally skewed positive α-stable random variables has been used. The definition of the Lévy α-stable distribution using the Laplace transform (3) differs from the more common definition using the Fourier transform. This has been corrected in Ref. [61].

The SDE (2) in the operational time τ can be numerically solved using the Euler–Maruyama scheme with the time step $\Delta\tau$. For each value of the stochastic variable x_k we assign the physical time t_k generated by the process $T(\tau)$ using Eq. (67). Thus the numerical method of solution of Langevin equations (2), (4) is given by the following equations:

$$x_{k+1} = x_k + a(x_k)\Delta\tau + b(x_k)\sqrt{\Delta\tau}\varepsilon_k, \tag{69}$$

$$t_{k+1} = t_k + \Delta\tau^{\frac{1}{\alpha}}\xi_k. \tag{70}$$

Here ε_k are i.i.d. random variables having standard normal distribution.

For numerical solution of nonlinear equations, such as those resulting in Eq. (49), the fixed time step $\Delta\tau$ can be inefficient. For example, in Eq. (49) with $\eta > 1$ large values of stochastic variable x lead to large coefficients and thus require a very small time step. A more efficient way of solution is to use a variable time step that adapts to the coefficients in the equation. Similar method has been used in Refs. [54,55] for solving nonlinear SDEs. Such a variable time step is equivalent to changing of the operational time τ to the position-dependent operational time τ'. If we choose the intensity of random time in Eq. (23) as $g(x) = b(x)^{-\frac{2}{\alpha}}$, then according to Eq. (31) instead of initial Langevin equations (2), (4) we get the new Langevin equations

$$dx(\tau') = \frac{a(x(\tau'))}{b(x(\tau'))^2} + dW(\tau'), \tag{71}$$

$$dt(\tau') = b(x(\tau'))^{-\frac{2}{\alpha}} dL^\alpha(\tau'). \tag{72}$$

Discretizing the operational time τ' with the time step $\Delta\tau'$ and using the Euler–Maruyama approximation for Eq. (71) instead of Eqs. (69), (70) we have

$$x_{k+1} = x_k + \frac{a(x_k)}{b(x_k)^2}\Delta\tau' + \sqrt{\Delta\tau'}\varepsilon_k, \tag{73}$$

$$t_{k+1} = t_k + \left(\frac{\Delta\tau'}{b(x_k)^2}\right)^{\frac{1}{\alpha}}\xi_k. \tag{74}$$

Comparison with Eqs. (69), (70) shows that Eqs. (73), (74) can be obtained by replacing the time step $\Delta\tau$ in Eqs. (69), (70) by

$$\Delta\tau \to \frac{\Delta\tau'}{b(x_k)^2}. \tag{75}$$

As an example, we solve the Langevin equations

$$dx = \left(\eta - \frac{\nu}{2}\right)x^{2\eta-1}d\tau + x^\eta dW(\tau), \tag{76}$$

$$dt = dL^\alpha(\tau) \tag{77}$$

resulting in the time-fractional Fokker–Planck equation (49). For restriction of the diffusion region we use the reflective boundaries at $x = x_{\min}$ and $x_{\max}$. More effective numerical solution scheme is obtained changing the operational time τ to the time τ' defined by the equation

$$dt(\tau') = x(\tau')^{-\frac{2}{\alpha}(\eta-1)}dL^\alpha(\tau'). \tag{78}$$

This change is equivalent to the introduction of the variable time step $\Delta\tau_k = \Delta\tau' x_k^{-2(\eta-1)}$. Discretizing the operational time τ' with the step $\Delta\tau'$ from Eqs. (76)–(78) we get the following numerical approximation:

$$x_{k+1} = x_k + \left(\eta - \frac{\nu}{2}\right)x_k\Delta\tau' + x_k\sqrt{\Delta\tau'}\varepsilon_k, \tag{79}$$

$$t_{k+1} = t_k + \left(\frac{\Delta\tau'}{x_k^{2(\eta-1)}}\right)^{\frac{1}{\alpha}}\xi_k. \tag{80}$$

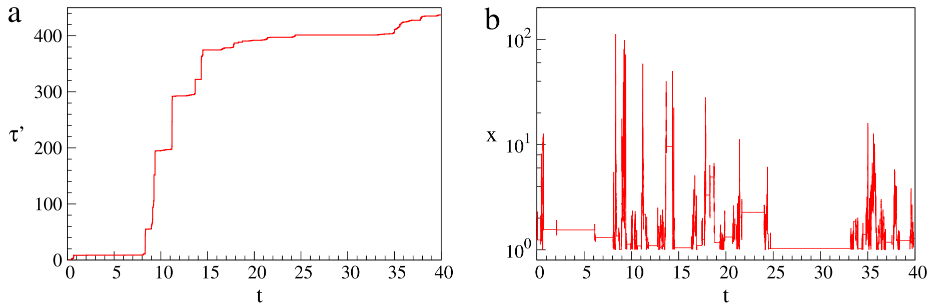

Fig. 1. Sample path obtained from Langevin equations (76), (77) using numerical solution scheme given by Eqs. (79), (80). (a) Dependence of the operational time τ', defined by Eq. (78), on the physical time t. (b). Dependence of the stochastic variable x on the physical time t. The parameters are $\alpha = 0.7$, $\eta = 2$, $\nu = 3$. Reflective boundaries are placed at $x_{\min} = 1$ and $x_{\max} = 1000$.

Sample path obtained using Eqs. (79), (80) with the parameters $\eta = 2$ and $\nu = 3$ is shown in Fig. 1. The change of the operational time τ' with the physical time t is shown in Fig. 1(a) and the dependence of the stochastic variable x on the physical time t is shown in Fig. 1(b). Due to nonlinear coefficients in Eq. (76) the sample path in Fig. 1(b) exhibits peaks or bursts, corresponding to the large deviations of the variable x. The intervals with x being constant indicate the heavy-tailed trapping times. Comparing Fig. 1(a) with Fig. 1(b) we see that the operational time τ' increases faster when x acquires larger values, in accordance to Eq. (78).

5.2. Power spectral density

Since the equations exhibit a slow (power-law instead of a usual exponential) relaxation [47], calculation of the PSD using sample paths is very slow. A more efficient way is to find the eigenvalues and eigenfunctions of the Fokker–Planck operator (8) and calculate the PSD using the rapidly converging series in Eq. (47). This is the approach for calculating the PSD used in Ref. [37] for the case of constant diffusion coefficient.

As an example let us calculate the PSD of the diffusion described by the time-fractional Fokker–Planck equation (49) with $\eta \neq 1$ and the reflective boundaries at $x_{\min} = 1$ and $x_{\max} = \xi$. Eq. (32) for the eigenfunctions of the Fokker–Planck operator that enters Eq. (49) is

$$-\left(\eta - \frac{\nu}{2}\right)\frac{\partial}{\partial x}x^{2\eta-1}P_\lambda(x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}x^{2\eta}P_\lambda(x) = -\lambda P_\lambda(x). \tag{81}$$

The reflective boundaries lead to the conditions $S_\lambda(1) = 0$ and $S_\lambda(\xi) = 0$, where

$$S_\lambda(x) = \left(\eta - \frac{\nu}{2}\right)x^{2\eta-1}P_\lambda(x) - \frac{1}{2}\frac{\partial}{\partial x}x^{2\eta}P_\lambda(x) \tag{82}$$

is the probability current related to the eigenfunction $P_\lambda(x)$. The steady state solution of Eq. (49) is

$$P_0(x) = \frac{\nu - 1}{1 - \xi^{1-\nu}}x^{-\nu}. \tag{83}$$

It is more convenient to transform Eq. (81) into the Schrödinger equation [49]. To do this we first make the diffusion coefficient constant by changing the variable x to

$$z = \frac{x^{1-\eta}}{|\eta - 1|}. \tag{84}$$

Eq. (81) then becomes

$$\frac{\nu'}{2}\frac{\partial}{\partial z}\frac{1}{z}P'_\lambda(z) + \frac{1}{2}\frac{\partial^2}{\partial z^2}P'_\lambda(z) = -\lambda P'_\lambda(z) \tag{85}$$

with the reflective boundaries at $z_{\min}$ and $z_{\max}$, where

$$z_{\min} = \begin{cases} \dfrac{1}{\eta - 1}\dfrac{1}{\xi^{\eta-1}}, & \eta > 1, \\ \dfrac{1}{1-\eta}, & \eta < 1, \end{cases} \qquad z_{\max} = \begin{cases} \dfrac{1}{\eta - 1}, & \eta > 1, \\ \dfrac{1}{1-\eta}\xi^{1-\eta}, & \eta < 1. \end{cases} \tag{86}$$

Here

$$\nu' = \frac{\eta - \nu}{\eta - 1}. \tag{87}$$

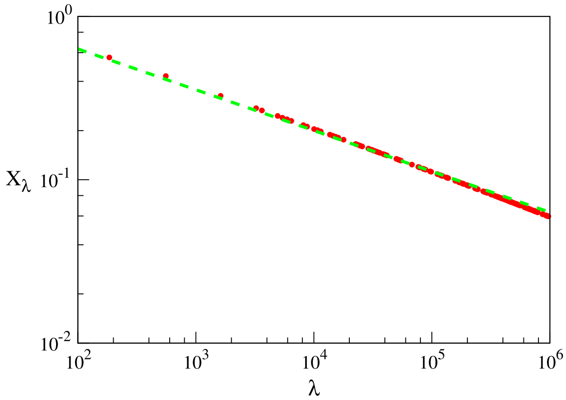

Fig. 2. (Color online) Dependence of numerically obtained first moments of the variable x on the eigenvalues λ for the lowest eigenvalues (red dots). Eigenvalues and eigenfunctions are obtained numerically solving Eq. (88). The dashed green line shows the slope $\lambda^{-0.25}$, predicted by Eq. (51). The parameters used are $\eta = \frac{5}{2}$, $\nu = 3$, $x_{\min} = 1$ and $x_{\max} = 1000$.

Eq. (85) can be transformed into the Schrödinger equation [49]

$$-\frac{1}{2}\frac{d^2}{dz^2}\psi_\lambda(z) + V(z)\psi_\lambda(z) = \lambda\psi_\lambda(z) \tag{88}$$

with the potential

$$V(z) = \frac{1}{8z^2}\nu'(2+\nu'). \tag{89}$$

Here $\psi_\lambda(z) = P'_\lambda(z)/\sqrt{P'_0(z)}$. The condition of zero probability current at the reflective boundaries $z = z_{\min}$ and $z = z_{\max}$ becomes

$$\left(\frac{d}{dz} + \frac{\nu'}{2}\frac{1}{z}\right)\psi_\lambda(z)\bigg|_{z=z_{\min},z_{\max}} = 0. \tag{90}$$

The solution of Eq. (88) corresponding to the eigenvalue $\lambda = 0$ is

$$\psi_0(z) = \sqrt{\frac{\nu'-1}{z_{\min}^{1-\nu'} - z_{\max}^{1-\nu'}}}\, z^{-\frac{\nu'}{2}}. \tag{91}$$

Eq. (88) can be solved using standard finite-difference or finite-element methods. Having the eigenfunction $\psi_\lambda(z)$ the first moment of the stochastic variable x can be calculated using the equation

$$X_\lambda = \int_{z_{\min}}^{z_{\max}} \psi_0(z)|\eta-1|^{\frac{1}{1-\eta}} z^{\frac{1}{1-\eta}}\psi_\lambda(z)\,dz. \tag{92}$$

Let us take the following values of the parameters in Eq. (49): $\eta = \frac{5}{2}$, $\nu = 3$. The dependence of the numerically calculated first moment X_λ on the eigenvalue λ for lowest eigenvalues is shown in Fig. 2. We see good agreement with the analytical prediction (51) of power-law dependence on λ. For larger eigenvalues λ than those shown in Fig. 2 the power-law dependence does not hold and X_λ decreases faster.

The PSD calculated using Eq. (47) is presented in Fig. 3. Eigenvalues λ and the first moments X_λ shown in Fig. 2 have been used. We see good agreement with the predicted power-law dependency of the PSD on the frequency for frequencies $f > f_{\min} \approx 1$. The power-law exponent coincides with Eq. (58). For smaller frequencies $f < 1$ the PSD exhibits the power-law behavior (48) with the exponent $1-\alpha$.

6. Conclusions

In summary, we proposed Eq. (21) describing the subdiffusion of particles in an inhomogeneous medium that generalizes the previously obtained time-fractional Fokker–Planck equation with the position-independent diffusion coefficient. Fokker–Planck equation with the position-independent diffusion coefficient has been used to model various phenomena such as ion channel gating [65] and the translocation dynamics of a polymer chain threaded through a nanopore [66]. Properties of such equations have been studied extensively. In this paper we analyzed a more general case when both drift and diffusion coefficients are position-dependent. We hope that the present model can serve as a basis to study trapping induced subdiffusion in complex inhomogeneous media.

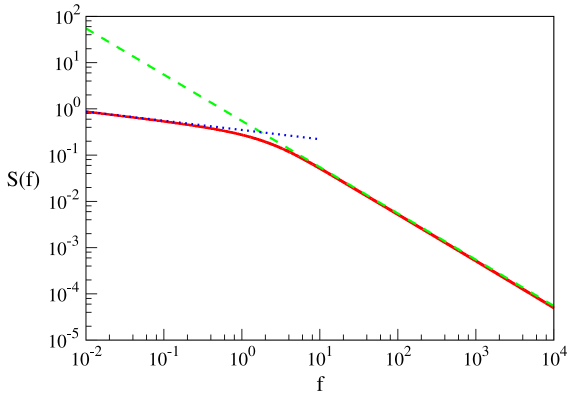

Fig. 3. (Color online) Power spectral density for the diffusion process defined by Eq. (49) with the parameter $\alpha = 0.8$. The solid red line shows the result of numerical calculation using Eq. (47). The dashed green line shows the slope $1/f$, whereas the dotted blue line shows the slope $f^{-0.2}$. Other parameters are the same as in Fig. 2.

We derived the analytical expression of power spectral density of signals described by the one-dimensional time fractional Fokker–Planck equation in a more general case when diffusion coefficient depends on the position. The general expression for the PSD (47) we applied to a particular case (49) when the drift and diffusion coefficients have power-law dependence on the position. The resulting PSD has a power-law form $S(f) \sim f^{-\beta}$ in a wide range of frequencies, with the power-law exponent β given by Eq. (58). This approximate result is confirmed by the numerical simulation (see Fig. 3). Thus, according to Eq. (58), time-fractional Fokker–Planck equation with power-law coefficients yields the PSD with the power-law exponent equal to or larger than 1 in a wide range of intermediate frequencies. In contrast, the PSD for small frequencies has a power-law dependency on the frequency in the form of $f^{-(1-\alpha)}$ even when the diffusion coefficient depends on the position.

Since an analytical solution of time-fractional Fokker–Planck equation can be obtained only in separate cases, there is a need of numerical solution. For the numerical solution of the nonlinear equations, such as those resulting in Eq. (49), we propose to use a variable time step that adapts to the coefficients in the equation. Such a variable time step is equivalent to changing of the operational time τ to the position-dependent operational time τ'.

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