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Spectral density of fluctuations in fractional bistable Klein-Kramers systems

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We investigate the stationary spectral density of fractional bistable Klein-Kramers systems. First, we deduce a dissipation-fluctuation relation between the stationary spectral density at thermal equilibrium and the linear response of the system to an applied perturbation. Second, we describe how to obtain the linear dynamic susceptibility from the method of moments, and thus we derive the fluctuating spectral density from the dissipation-fluctuation relation. Finally, we exhibit the structure of this fluctuating spectral distribution and explore the effect of the subdiffusion on it. Compared with the standard bistable Klein-Kramers systems, our observation on the spectral distribution in fractional systems reveals that the subdiffusion weakens the oscillatory components of the intrawell oscillation and the above-barrier motion. This phenomenon should reflect a fact that the particles tend to stand still in separate wells in subdiffusive processes.

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I. INTRODUCTION

Diffusive processes in nature can be classed as either normal or anomalous [1]. In normal diffusion the second-order central moment is linear in time, namely, $\langle[x(t)-\langle x(t)\rangle]^2\rangle\propto t$, while in anomalous diffusion this physical quantity is generally characterized by a power-law relation, i.e., $\langle[x(t)-\langle x(t)\rangle]^2\rangle\propto t^\sigma$ with $\sigma\neq 1$. Here σ is called the diffusive exponent, and provides additional classification with phenomena categorized as superdiffusive ($\sigma>1$) or as subdiffusive ($0<\sigma<1$). Recently, there has been a continuously growing interest in exploring the complex stochastic dynamics connected with anomalous diffusion that has been increasingly observed in fluid transport within porous media, surface growth, diffusion of plasma, diffusion at liquid surfaces, two-dimensional rotating flow to name a few [1–4].

To describe such anomalous diffusion processes, several fractional Fokker-Planck equations (FFPE) have been introduced by replacing some integer-order derivatives in the standard equations with fractional analogs [5–11]. Due to slowly decaying characteristic kernels showing strong memory effect and nonexponential relaxation, as well as the straightforward inclusion of time-independent external fields, the FFPE approach has proved to be powerful in describing relaxation behavior. Several numerical schemes including direct simulation [12], the prediction-correction technique [13], the matrix continued fraction method [14], and the subordination method [15], have been proposed to numerically solve or directly simulate fractional dynamics. However, most of this body of work mainly concentrates on calculating the probability distribution. In contrast, the focus of this paper concerns the calculation of the spectral density of the bistable fractional Klein-Kramers (FKK) equation and the effect of subdiffusion on its dynamics.

For many problems of spectroscopy and for radiophysics, the spectral distribution is of key interest [16–18]. Generally speaking, when nonlinear stochastic systems are involved, their spectral density is frequently obtained from the autocorrelation function through the Wiener-Khintchine theorem, and as a result one must use certain transient methods to derive the transition probability density function and the correlation function. Nevertheless, we adopt here a different means. Applying the general frame [19] to subdiffusive processes described by the bistable FKK equation, we derive a dissipation-fluctuation relation between the linear dynamical susceptibility and the spectral density of fluctuations, which is similar to that found in the normal diffusion [20], and therefore with the relation, we obtain the fluctuating spectral distribution by calculating the linear dynamic susceptibility using an asymptotical numerical method. To do this, we will demonstrate how to calculate the linear dynamic susceptibility by extending the method of moments to a formal time-periodically modulated bistable FKK equation. Although the genuine physical meaning of such time-dependent FKK equations has not been verified from the viewpoint of the continuous limit of a continuous-time random walk with a Mittag-Leffler residence time density [21,22], it is useful in calculating the stationary spectral density of the original time-independent bistable FKK equation. After that, we will analyze the subdiffusive effect on fluctuating spectral densities by observing their evolution as noise intensity increases.

The paper is organized into five sections. Following this introduction, a dissipation-fluctuation relation is presented in Sec. II for subdiffusive processes characterized by the time-independent FKK equation. To calculate the linear dynamics, we generalize in Sec. III the method of moments from the standard time-periodically modulated bistable FKK equation to treat the fractional case. The calculated spectral density of fluctuations is displayed and the effect of subdiffusion on it is discussed in Sec. IV. Finally, conclusions are drawn in Sec.V.

II. DISSIPATION-FLUCTUATION RELATION IN FRACTIONAL KLEIN-KRAMERS SYSTEMS

Consider a subdiffusive particle of velocity v and displacement x moving within a time-independent bistable potential $U(x)=x^4/4-x^2/2$. Then according to Refs. [7,8], we have for the probability density function $p(x,v,t)$ in phase

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space the following dimensionless FKK equation

$$\frac{\partial p(x,v,t)}{\partial t} = {}_0D_t^{1-\sigma}\left[-v\frac{\partial}{\partial x} + \frac{\partial}{\partial v}(\gamma v + x^3 - x) + \gamma D\frac{\partial^2}{\partial v^2}\right]p(x,v,t), \quad 0 < \sigma < 1, \tag{1}$$

where γ denotes the friction constant and D is the Boltzmann temperature. The fractional Riemann-Liouville operator ${}_0D_t^{1-\sigma}$ is defined via an integral operator of a slowly decaying power-law kernel [23] as

$${}_0D_t^{1-\sigma}p(x,v,t) = \frac{1}{\Gamma(\sigma)}\frac{\partial}{\partial t}\int_0^t dt' \frac{p(x,v,t')}{(t-t')^{1-\sigma}} \tag{2}$$

for $0<\sigma<1$. When $\sigma\to 1$, the standard Klein-Kramers equation is recovered. Since the Riemann-Liouville operator acts exclusively on variable t, it is easy to verify that the steady solution of Eq. (1) still is the Gibbs-Boltzmann equilibrium distribution

$$p_0(x,v) = Z\exp[-(v^2/2 + x^4/4 - x^2/2)/D] \tag{3}$$

with Z being the normalized constant.

In an effort to develop the relation connecting the stationary spectral density with the linear dynamical susceptibility of the fractional system Eq. (1), let us start with a time-periodically modulated fractional system, which is formally derived from Eq. (1) by replacing the time-independent bistable potential $U(x)$ with a time-periodically modulated potential $\tilde{U}(x)=x^4/4-x^2/2-x\varepsilon(t)$ with $\varepsilon(t)=\varepsilon e^{i\Omega t}$ being an external force. The time-periodically modulated fractional system is governed by

$$\frac{\partial}{\partial t}p(x,v,t) = {}_0D_t^{1-\sigma}[L_{FP}(x,v) + L_{ext}(x,v,t)]p(x,v,t), \quad 0 < \sigma < 1, \tag{4}$$

where the Fokker-Planck-type Klein-Kramers operator

$$L_{FP}(x,v) = -v\frac{\partial}{\partial x} + \frac{\partial}{\partial v}(\gamma v + x^3 - x - \varepsilon e^{i\Omega t}) + D\gamma\frac{\partial^2}{\partial v^2}$$

is time-independent and the perturbation part $L_{ext}(x,v,t) = -\frac{\partial}{\partial v}\varepsilon(t)$ is time dependent. Here we emphasize that throughout natural boundary conditions are always assumed.

Suppose the external force is very weak, namely, $\varepsilon \ll 1$, then within the linear response range [19,20,24–26] the long-time solution of Eq. (4) can be sought in the form

$$p_{as}(x,v,t) = p_0(x,v) + P_1(x,v,t) \tag{5}$$

with $P_1(x,v,t)$ as a perturbation to be determined. Substitution of Eq. (5) into Eq. (4) yields

$$\frac{\partial P_1(x,v,t)}{\partial t} = {}_0D_t^{1-\sigma}L_{FP}(x,v)P_1(x,v,t) + {}_0D_t^{1-\sigma}L_{ext}(x,v,t)p_0(x,v). \tag{6}$$

Due to the smallness of both ${}_0D_t^{1-\sigma}L_{ext}(x,v,t)$ and $P_1(x,v,t)$, ${}_0D_t^{1-\sigma}L_{ext}(x,v,t)P_1(x,v,t)$ is neglected in the derivation of Eq. (6). Using Fourier transform techniques [19], a formal solution to Eq. (6) can be acquired as

$$P_1(x,v,t) = \frac{1}{D}\int_{-\infty}^{t} E_\sigma(L_{FP}(x,v)(t-t')^\sigma) \times {}_0D_{t'}^{1-\sigma}vp_0(x,v)dt', \tag{7}$$

where $E_\sigma(\cdot)$ is the Mittag-Leffler function defined by the series $E_\sigma(z)=\sum_{n=0}^{\infty}\frac{z^n}{\Gamma(1+\sigma n)}$.

To obtain an expression for the linear dynamical susceptibility, let us consider the deviation of the long-time displacement coordinate average from thermal equilibrium [20]. Using Eqs. (5) and (7) and changing the integration order, we find the deviation

$$\Delta x(t) = \int\int xP_1(x,v,t)dxdv = \int_{-\infty}^{t} R_{A,L}(t-t')\,{}_0D_{t'}^{1-\sigma}F(t')dt' \tag{8}$$

with linear response function

$$R_{x,L}(t) = \begin{cases} \frac{1}{D}\int\int xE_\sigma(L_{FP}(x,v)t^\sigma)vp_0(x,v)dxdv, & t \geq 0; \\ 0, & t < 0. \end{cases} \tag{9}$$

Noting the formal solution of Eq. (1)

$$P(x,v,t|x_0,v_0,0) = E_\sigma(L_{FP}(x,v)t^\sigma)\,\delta(x-x_0)\,\delta(v-v_0), \tag{10}$$

and letting t_1 and t_2 be two times after the fractional system attains thermal equilibrium, then between $x(t_1)$ and $x(t_2)$ with $t=t_1-t_2\geq 0$ we have stationary correlation function

$$K_{xv}(t) = \int\int xE_\sigma(L_{FP}(x,v)t^\sigma)vp_0(x,v)dxdv. \tag{11}$$

By virtue of $K_{xv}(t)=-\frac{d}{dt}K_{xx}(t)$, a comparison Eq. (9) with Eq. (11) yields

$$R_{x,L}(t) = \begin{cases} -\frac{1}{D}\frac{d}{dt}K_{xx}(t), & t \geq 0; \\ 0, & t < 0. \end{cases} \tag{12}$$

This is the dissipation-fluctuation relation for the fractional system Eq. (1).

Taking into account the spectral density of fluctuations $Q_0(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}K_{xx}(t)e^{-i\omega t}dt=\frac{1}{\pi}\int_0^{+\infty}K_{xx}(t)\cos(\omega t)dt$, a Fourier transform of Eq. (12) yields

$$\chi_x(\omega)=\frac{1}{D}\left\{K_{xx}(0)-i\omega\int_0^{+\infty}K_{xx}(t)[\cos(\omega t)-i\sin(\omega t)]dt\right\}. \quad (13)$$

Further equating imaginary parts gives the Kramers-Kronig relation

$$\text{Im}[\chi_x(\omega)]=\frac{\omega\pi}{D}Q_0(\omega), \quad (14)$$

where we have used the linear dynamical susceptibility $\chi_x(\omega)=\int_0^{+\infty}R_{x,L}(t)e^{-i\omega t}dt=\text{Re}\,\chi_x(\omega)-i\,\text{Im}\,\chi_x(\omega)$. Evidently, Eq. (14) establishes a connection between the spectral density of fluctuations and the dynamical susceptibility, and in this paper it provides a foundation for calculating the fluctuating spectral density by an asymptotic method.

Now we make Fourier transform on Eq. (8) to obtain the deviation in the frequency domain

$$\Delta\tilde{x}(\omega)=2\pi\varepsilon(i\omega)^{1-\sigma}\chi_x(\omega)\delta(\omega-\Omega). \quad (15)$$

An inverse Fourier transform of Eq. (14) yields

$$\langle\Delta x(t)\rangle_{as}=\varepsilon(i\Omega)^{1-\sigma}\chi_x(\Omega)e^{i\Omega t}. \quad (16)$$

Combining Eqs. (14) and (16) indicates that if we can calculate the deviation of the long-time linear dynamics of the time-dependent system Eq. (4), then the spectral density of the time-independent system Eq. (1) can be acquired.

III. METHOD OF MOMENTS FOR CALCULATING THE LONG-TIME LINEAR DYNAMICS

In this section for calculating the long-time linear dynamics, we extend the method of moments [24] to the time-periodically modulated fractional system (4). Let $f(x,v)$ be some function of x and v, and suppose the expectation $\langle f(x,v)\rangle(t)=\int_{-\infty}^{\infty}f(x,v)p(x,v,t)dxdv$ exist, then from Eq. (4) we acquire the following evolutionary equation

$$\frac{\partial\langle f(x,v)\rangle(t)}{\partial t}={}_0D_t^{1-\sigma}\left\{\left\langle v\frac{\partial f}{\partial x}\right\rangle-\left\langle[U'(x)-\varepsilon(t)]\frac{\partial f}{\partial v}\right\rangle+\gamma\left[D\left\langle\frac{\partial^2 f(x,v)}{\partial v^2}\right\rangle-\left\langle v\frac{\partial f(x,v)}{\partial v}\right\rangle\right]\right\}. \quad (17)$$

We decompose $P_1(x,v,t)$ in Eq. (5) into a product of first-order harmonic and time-independent part [24–26], and then the long-time solution to Eq. (4) turns into

$$p(x,v,t)=p_0(x,v)+p_1(x,v)\varepsilon(t). \quad (18)$$

Substituting Eq. (18) into Eq. (17) and omitting the higher-order term $o(\varepsilon)$ yield

$$i\Omega\langle f(x,v)\rangle_1\varepsilon(t)=\left\{\left\langle v\frac{\partial f}{\partial x}\right\rangle_1-\left\langle U'(x)\frac{\partial f}{\partial v}\right\rangle_1+\left\langle\frac{\partial f}{\partial v}\right\rangle_0+\gamma\left[D\left\langle\frac{\partial^2 f(x,v)}{\partial v^2}\right\rangle_1-\left\langle v\frac{\partial f(x,v)}{\partial v}\right\rangle_1\right]\right\}{}_0D_t^{1-\sigma}\varepsilon(t). \quad (19)$$

Here $\langle f(x,v)\rangle_i=\int\int p_i(x,v)f(x,v)dxdv$, $i=0$, 1. A Fourier transform of Eq. (19) gives

$$(i\Omega)^\sigma\langle f(x,v)\rangle_1=\left\langle v\frac{\partial f}{\partial x}\right\rangle_1-\left\langle U'(x)\frac{\partial f}{\partial v}\right\rangle_1+\left\langle\frac{\partial f}{\partial v}\right\rangle_0+\gamma\left[D\left\langle\frac{\partial^2 f(x,v)}{\partial v^2}\right\rangle_1-\left\langle v\frac{\partial f(x,v)}{\partial v}\right\rangle_1\right]. \quad (20)$$

To determine $p_1(x,v)$, let us expand it into power series form

$$p_1(x,v)=p_0(x,v)\sum_{k=0}^{N}\sum_{j=0}^{k}C_{k,j}x^jv^{k-j}, \quad (21)$$

where N is the truncation order to be determined by numerical convergence. Choice of $f(x,v)=x^mv^l(m,\ l\geq 0,\ m+l>0)$ and insertion of the expansion (21) into Eq. (20) lead to

$$\sum_{k=0}^{N}\sum_{j=0}^{k}C_{k,j}\{[(i\Omega)^\sigma\langle x^{m+j}v^{k-j+l}\rangle_0-m\langle x^{j+m-1}v^{k-j+l+1}\rangle_0+l\langle U'(x)x^{j+m}v^{k-j+l-1}\rangle_0]-\gamma[Dl(l-1)\langle x^{m+j}v^{k-j+l-2}\rangle_0-l\langle x^{j+m}v^{k-j+l}\rangle_0]\}=l\langle x^mv^{l-1}\rangle_0. \quad (22)$$

Using $\partial p_0/\partial v=-vp_0/D$ and $\partial p_0/\partial x=-U'(x)p_0/D$ and along with the probability normalization requirement, Eq. (22) reduces to

$$\sum_{k=1}^{N}\sum_{j=0}^{k}C_{k,j}\{(i\Omega)^\sigma[\langle x^{m+j}v^{k-j+l}\rangle_0-\langle x^mv^l\rangle_0\langle x^jv^{k-j}\rangle_0]+D[m(j-k)+lj]\langle x^{j+m-1}v^{k-j+l-1}\rangle_0+\gamma Dl(k-j)\langle x^{m+j}v^{k-j+l-2}\rangle_0\}=l\langle x^mv^{l-1}\rangle_0. \quad (23)$$

It is clear that Eq. (23) is consistent with Eq. (13) in Ref. [24] when $\sigma\to 1$. For all m and l satisfying $1\leq m+l\leq N$, Eq. (23) is a linear algebraic system of $N(N+3)/2$ unknowns, and its solution can be sought with subroutine DLSARG in Microsoft's FORTRAN power station.

Once Eq. (23) is solved, a scaled Fourier coefficient

$$\hat{\chi}(\Omega)=\int\int xp_1(x,v)dxdv=\sum_{k=1}^{N}\sum_{j=0}^{k}C_{k,j}(\langle x^{j+1}v^{k-j}\rangle_0-\langle x\rangle_0\langle x^jv^{k-j}\rangle_0) \quad (24)$$

is obtained. We can then obtain the long-time deviation due to the external periodic modulation

$$\langle \Delta x(t) \rangle_{as} = \varepsilon \hat{\chi}(\Omega) e^{i\Omega t}. \tag{25}$$

Comparison of Eqs. (16) and (25) leads to

$$\hat{\chi}(\Omega) = (i\Omega)^{1-\sigma} \chi_x(\Omega). \tag{26}$$

Combining Eqs. (14) and (26) suggests that the spectral density of fluctuations $Q_0(\Omega)$ can be acquired by the method of moments.

IV. FLUCTUATING SPECTRAL DENSITY OF FRACTIONAL BISTABLE KLEIN-KRAMERS SYSTEMS

Before exploring the effect of the subdiffusion, we need to discuss the convergence of the method of moments. In normal diffusion it is well known that the method of moments has quick convergence when the friction constant is large, while in the limit of zero friction the convergence becomes quite slow [24]. However, in subdiffusion, we observe that a small diffusive exponent actually counteracts the effects of small friction constant. That is to say, when the diffusive exponent is small enough, a convergence precision can be accepted at a lower truncation order, such as at $N=12$, even if the friction constant is much less than 0.1. In the following numerical experiments, to guarantee the convergence both in the normal diffusive and subdiffusive cases, we fix $N=24$ to demonstrate the calculated spectral distribution of Eq. (1) for the parameters under concern.

For the standard bistable Klein-Kramers system, when the weak friction constant is small enough, three different types of stochastic motion are encountered, namely, the interwell jump, the intrawell oscillation and the above-barrier oscillation, and as a result of competition among these motions, there are three distinct spectral peaks coexisting within a certain noise range [27], which are referred to as the zero-frequency peak, the intrawell frequency peak, and the above-barrier frequency peak, respectively [24,28]. Here our interest is to explore how subdiffusion affects the complex fluctuating spectral distribution. To clarify this point, we plot in Fig. 1 the fluctuating spectral diagram for $\gamma=0.05$ and at three noise levels.

At the zero limit noise level of $D=0.001$ when $\sigma=1$, Fig. 1(a) exhibits an obvious intrawell frequency peak near $\omega_0 = \sqrt{2}$ that corresponds to the minimal unperturbed eigenfrequency at the well bottom, but the peak turns more and more obscure as σ continually decreases. For instance, when $\sigma=0.7$ the intrawell frequency peak has entirely vanished. At medium noise levels around $D=0.1$ when $\sigma=1$, Fig. 1(b) displays a double-frequency peak in the spectral distribution, the left being the above-barrier frequency peak and the right being the intrawell frequency peak, but both are weakened or vanish when $\sigma<1$. As for higher noise levels around $D=2.0$, when $\sigma=1$, there exists an exclusive above-barrier frequency peak and it has a similar weakening tendency as σ reduces. Evidently, the observation on Fig. 1 tends to imply that the components of both the intrawell oscillation and the above-barrier motion are inhibited by subdiffusive processes.

To further confirm this implication, we also exhibit the evolution of nonzero peak frequencies versus noise intensity for $\gamma=0.05$ in Figs. 2 and 3. Here the nonzero peak frequency refers to a nonzero frequency at which the spectral peak is observed. For $\sigma=0.95$ as shown in Fig. 2, there are two branches of peak frequency curves, and the left represents the intrawell peak frequency, while the right corresponds to the above-barrier peak frequency. As for $\sigma=0.8$, we note that no matter how the noise intensity changes, there

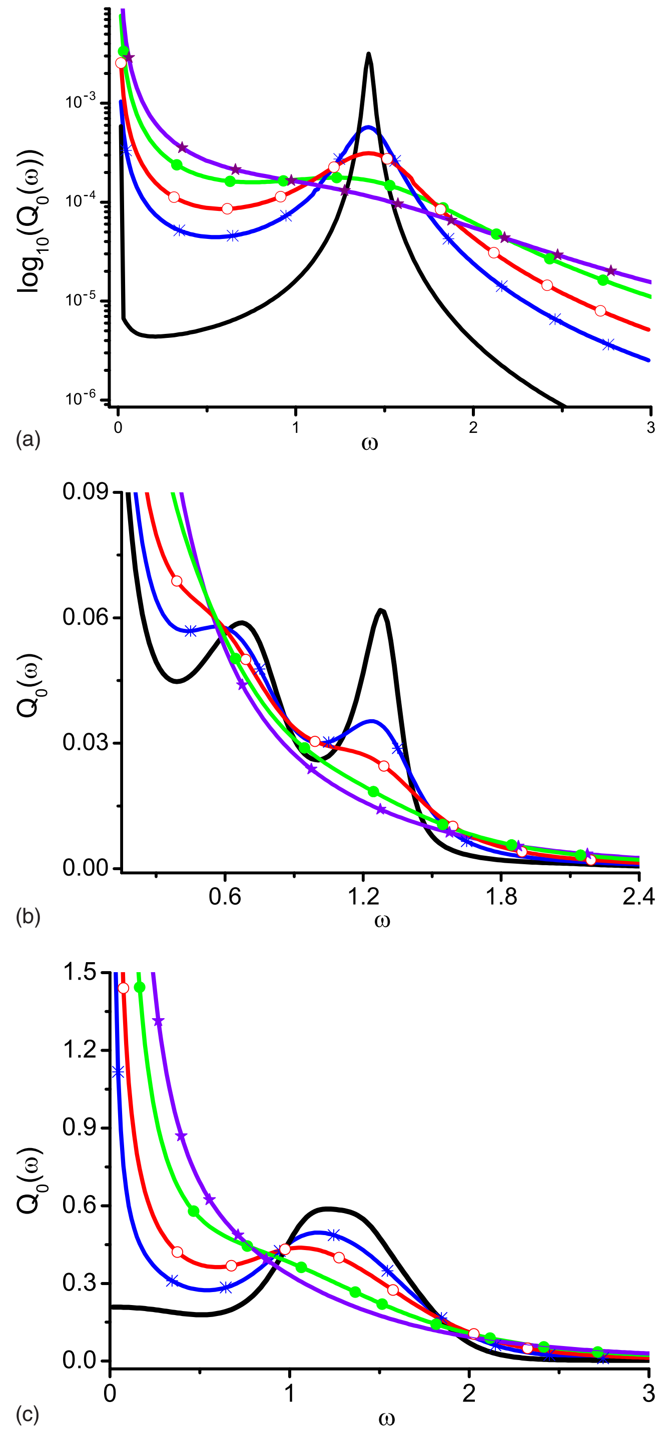

FIG. 1. (Color online) Fluctuating spectral distribution under different noise level with $\gamma=0.05$ and σ values of 1.0 (black line); 0.95 (blue line with asterisks); 0.9 (red line with empty circles); 0.8 (green line with solid circles) and 0.7 (purple line with pentacles). The noise intensity is (a) $D=0.001$; (b) $D=0.1$; (c) $D=2.0$.

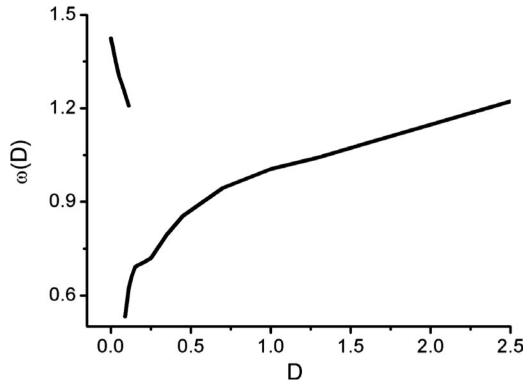

FIG. 2. Evolution of nonzero peak frequency via the noise intensity with $\gamma=0.05$ and $\sigma=0.95$.

is only one nonzero frequency spectral peak left in the spectral distribution, so there is only an intrawell frequency branch plotted in Fig. 3. On further scrutiny into cases with smaller subdiffusive exponents, say $\sigma=0.5$, it is obvious that we can no longer observe any nonzero peak frequencies. Clearly, these observations for Figs. 2 and 3 lead to the same conclusion as that for Fig. 1.

In addition, we also observe that although subdiffusion has a tendency to inhibit the intrawell oscillation and the above-barrier motion, the zero frequency spectral peak is always enhanced by reducing the subdiffusive exponent. Since the zero-frequency spectral peak correlates with the probability of the interwell jump events [24], the rise in height should infer that subdiffusion enhances the stochastic interwell jump in subdiffusive processes.

Why does such an interesting phenomenon occur? Let us seek a clue from the intuitive characteristics of such a subdiffusive process. In subdiffusive processes, the second-order central moment satisfies power law $\langle[x(t)-\langle x(t)\rangle]^2\rangle \propto t^{\sigma}$ for $0<\sigma<1$, signifying that the diffusion in the particle's displacement is much slower than the change in time. Therefore we can imagine that the subdiffusive particle spends more time standing still in each well rather than oscillating near the well bottom or above the barrier. This inference is to some extent coincident with the sample path derived in Ref. [15]. Besides, as further support, we demonstrate the phenomenon in Figs. 4 and 5 by exhibiting some numerical results for a larger friction constant $\gamma=0.3$. As shown in the figures, a double-frequency spectral peak does not appear. Especially when $\sigma=0.8$, the exclusive intrawell spectral peak in Fig. 3 also disappears, so for larger friction constants we do not give a similar plot to Fig. 3.

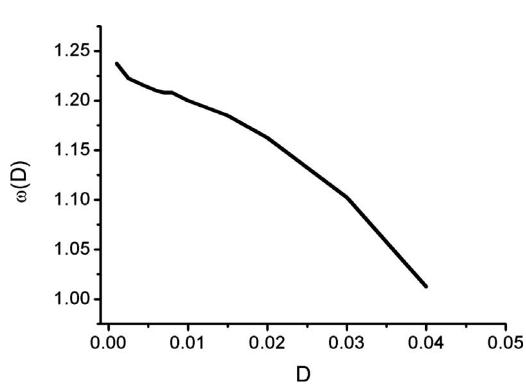

FIG. 3. Evolution of nonzero peak frequency via the noise intensity with $\gamma=0.05$ and $\sigma=0.8$.

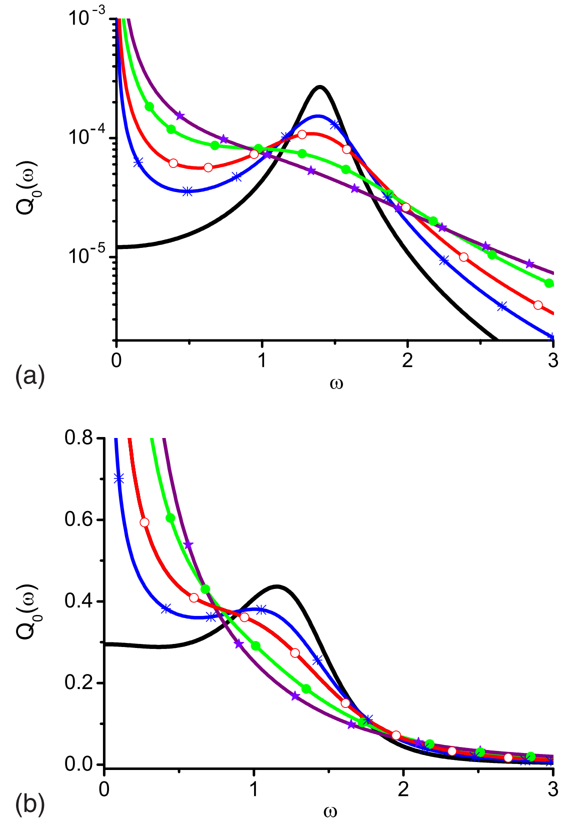

FIG. 4. (Color online) Fluctuating spectral distribution under different noise level with $\gamma=0.3$ and σ being 1.0 (black line); 0.95 (blue line with asterisks); 0.9 (red line with empty circles); 0.8 (green line with solid circles) and 0.7 (purple line with pentacles). The noise intensity is (a) $D=0.0005$; (b) $D=1.5$.

V. CONCLUSIONS

Using the dissipation-fluctuation relation between the linear dynamical susceptibility and the spectral density of fluc-

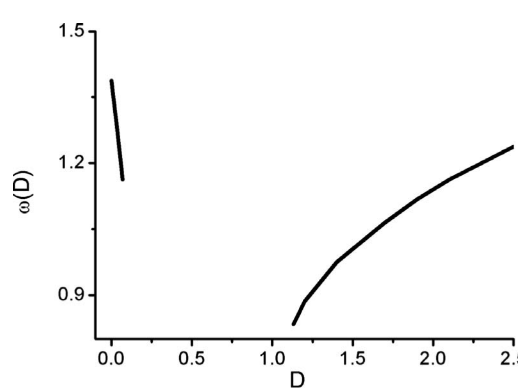

FIG. 5. Evolution of nonzero peak frequency via the noise intensity with $\gamma=0.3$ and $\sigma=0.95$.

tuations, the stationary spectral distribution of the time-independent bistable FKK systems has been investigated by the method of moments. Compared with normal diffusive processes described by the standard bistable Klein-Kramers equation, subdiffusive processes described by the fractional equation have a simple spectral structure. When the diffusive exponent is near unity, the spectral distribution of the subdiffusive process resembles that of the normal diffusive process. However, as the diffusive exponent further decreases, the change in the spectral distribution shows that both the intrawell oscillation and the above-barrier motion will become weak or vanish. We infer that the effect of subdiffusion on the fluctuating spectral density should be due to the characteristics of the subdiffusive process, which make the subdiffusive particle spend more time in residing quietly in each well. At the same time, the continuous rise in the height of the zero-frequency spectral peak seems to imply an enhanced occurrence of the interwell jump that is worthy of further theoretical consideration particularly from the viewpoint of fractional survival probability.

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