Inertial effects in the fractional translational diffusion of a Brownian particle in a double-well potential

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The anomalous translational diffusion including inertial effects of nonlinear Brownian oscillators in a double well potential $V(x)=ax^2/2+bx^4/4$ is considered. An exact solution of the fractional Klein-Kramers (Fokker-Planck) equation is obtained allowing one to calculate via matrix continued fractions the positional autocorrelation function and dynamic susceptibility describing the position response to a small external field. The result is a generalization of the solution for the normal Brownian motion in a double well potential to fractional dynamics (giving rise to anomalous diffusion).

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I. INTRODUCTION

The Brownian motion in a field of force is of fundamental importance in problems involving relaxation and resonance phenomena in stochastic systems [1,2]. An example is the translational diffusion of noninteracting Brownian particles due to Einstein [3] with a host of applications in physics chemistry, biology, etc. Einstein's theory relies on the diffusion limit of a discrete time random walk. Here the random walker or particle makes a jump of a fixed mean square length in a fixed time and the inertia is ignored so that the velocity distribution instantaneously attains its equilibrium value. Thus the only random variable is the jump direction leading automatically via the central limit theorem (in the limit of a large sequence of jumps) to the Wiener process describing the normal Brownian motion. The Einstein theory of normal diffusion has been generalized to fractional diffusion (see Refs. [4–6] for a review) in order to describe anomalous relaxation and diffusion processes in disordered complex systems (such as amorphous polymers, glass forming liquids, etc.). These exhibit temporal nonlocal behavior arising from energetic disorder causing obstacles or traps simultaneously slowing down the motion of the walker and introducing memory effects. Thus in one dimension the dynamics of the particle are described by a fractional diffusion equation for the distribution function $f(x,t)$ in configuration space incorporating both a waiting time probability density function governing the random time intervals between single microscopic jumps of the particles and a jump length probability distribution. The fractional diffusion equation stems from the integral equation for a continuous time random walk (CTRW) introduced by Montroll and Weiss [7,8]. In the most general case of the CTRW, the random walker may jump an arbitrary length in arbitrary time. However, the jump length and jump time random variables are not statistically independent [7–9]. In other words a given jump length is penalized by a time cost, and vice versa.

A simple case of the CTRW arises by assuming that the jump length and jump time random variables are decoupled. Such walks possessing a discrete hierarchy of time scales, without the same probability of occurrence, are known as fractal time random walks [5]. They lead in the limit of a large sequence of jump times and the non inertial limit to the following fractional Fokker-Planck equation in configuration space (for a review see Refs. [5,7])

$$\frac{\partial f(x,t)}{\partial t} = {}_0D_t^{1-\sigma} K_\sigma \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} f(x,t) + \frac{f(x,t)}{kT}\frac{\partial}{\partial x} V(x,t)\right]. \quad (1)$$

Here x specifies the position of the walker at time t, $-\infty < x < \infty$, kT is the thermal energy, $K_\sigma = \zeta_\sigma / kT$ is a generalized diffusion coefficient, ζ_σ is a generalized viscous drag coefficient arising from the heat bath and $V(x,t)$ denotes the external potential. The operator ${}_0D_t^{1-\sigma} \equiv \frac{\partial}{\partial t}\,{}_0D_t^{-\sigma}$ in Eq. (1) is given by the convolution (the Riemann-Liouville fractional integral definition) [6]

$${}_0D_t^{-\sigma} f(x,t) = \frac{1}{\Gamma(\sigma)} \int_0^t \frac{f(x,t')dt'}{(t-t')^{1-\sigma}}, \quad (2)$$

where $\Gamma(z)$ is the gamma function. The physical meaning of the parameter σ is the order of the fractional derivative in the fractional differential equation describing the continuum limit of a random walk with a chaotic set of waiting times (fractal time random walk). Values of σ in the range $0<\sigma<1$ correspond to subdiffusion phenomena ($\sigma=1$ corresponds to normal diffusion).

Since inertial effects are ignored the fractional Fokker-Planck equation in configuration space Eq. (1) only describes the long time (low frequency) behavior of the ensemble of particles. In order to give a physically meaningful description of the short time (high frequency) behavior, inertial effects must be taken into account just as in normal diffusion

[1,10]. Inertial effects in the normal Brownian motion are included via the Fokker-Planck equation (which for a separable and additive Hamiltonian is known as the Klein-Kramers equation) for the distribution function of particles $W(x,p,t)$ in phase space (x,p) [1,10]. In order to incorporate these effects in anomalous translational diffusion, Metzler [12] and Metzler and Klafter [13] have proposed a fractional Klein-Kramers equation (FKKE) for the distribution function $W=W(x,\dot{x},t)$ in phase space

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\alpha}\tau^{1-\alpha}\left[-\dot{x}\frac{\partial W}{\partial x} + \frac{1}{m}\frac{\partial V}{\partial x}\frac{\partial W}{\partial \dot{x}} + \beta\left(\frac{\partial}{\partial \dot{x}}(\dot{x}W) + \frac{kT}{m}\frac{\partial^2 W}{\partial \dot{x}^2}\right)\right], \tag{3}$$

where $\tau=\langle x^2\rangle_0/K_1$ has the meaning of the intertrapping time (waiting time between jumps), $K_1=kT/(m\beta)$ is the diffusion coefficient for normal diffusion, $\beta=\zeta_1/m$ is a friction coefficient arising from the heat bath, and the angular brackets denote the equilibrium ensemble average. Equation (3) describes a multiple trapping picture, whereby the tagged particle executes translational Brownian motion. However, the particle gets successively immobilized in traps whose mean distance apart is $\Delta=(kT/m)\tau$, where τ is the mean time between successive trapping events. The time intervals spent in the traps are governed by the waiting time probability density function $w(t)\sim A_\alpha t^{-1-\alpha}$ $(0<\alpha<1)$. The entire Klein-Kramers operator in the square brackets of Eq. (3) acts nonlocally in time, i.e., drift friction and diffusion terms are under the time convolution and are thus affected by the memory. However, a model based on a FKKE of the form of Eq. (3) provides a physically unacceptable picture of the behavior of physical parameters such as the dynamic susceptibility in the high frequency limit $\omega\to\infty$ (in particular, it predicts infinite integral absorption [10]; see Sec. IV below). The root of this difficulty apparently being that in writing Eq. (3), the convective derivative or Liouville term, in the underlying Klein-Kramers equation, is operated upon by the fractional derivative. This problem does not arise in the FKKE proposed by Barkai and Silbey [15], where the fractional derivative term acts solely on the dissipative part of the normal Klein-Kramers operator [see Eq. (3)]

$$\frac{\partial W}{\partial t} = -\dot{x}\frac{\partial W}{\partial x} + \frac{1}{m}\frac{\partial V}{\partial x}\frac{\partial W}{\partial \dot{x}} + {}_0D_t^{1-\alpha}\tau^{1-\alpha}\beta\left[\frac{\partial}{\partial \dot{x}}(\dot{x}W) + \frac{kT}{m}\frac{\partial^2 W}{\partial \dot{x}^2}\right]. \tag{4}$$

In order to justify a diffusion equation of the form of Eq. (4), Barkai and Silbey [15] consider a "Brownian" test particle moving freely in one dimension and colliding elastically at random times with particles of the heat bath which are assumed to move much more rapidly than the test particle. The times between collision events are assumed to be independent, identically distributed, random variables, implying that the number of collisions in a time interval $(0,t)$ is a renewal process. This is reasonable, according to Barkai and Silbey, when the bath particles thermalize rapidly and when the motion of the test particle is slow. The FKKEs of Metzler and Klafter and Barkai and Silbey have recently been extended to the analogous fractional rotational diffusion models in a periodic potential by Coffey *et al.* [10,16].

As an example of application of the FKKE to a particular problem, we shall now present a solution for the Barkai and Silbey kinetic model of anomalous diffusion of a particle in a double-well potential, viz.,

$$V(x) = ax^2/2 + bx^4/4, \tag{5}$$

where a and b are constants (the Metzler and Klafter model can be treated in like manner). The model of normal diffusion in the potential given by Eq. (5) is almost invariably used to describe the noise driven motion in bistable physical and chemical systems. Examples are such diverse subjects as simple isometrization processes [17–21], chemical reaction rate theory [22–30], bistable nonlinear oscillators [31–33], second order phase transitions [34], nuclear fission and fusion [35,36], stochastic resonance [37,38], etc. If the inertial effects are taken into account, a large number of specialized solutions exist mostly for particular parameters in the above problem. For example, the normalized position correlation function and its spectra for small dumping were treated in Refs. [32,39–41]. Voigtlaender and Risken [42] calculated eigenvalues and eigenfunctions of the Kramers (Fokker-Planck) equation for a Brownian particle in the double-well potential (5) and evaluated the Fourier transforms of the position and velocity correlation functions. The method is as follows. First the distribution function is expanded in Hermite functions in the velocity and then in Hermite functions in the position. Next by inserting this distribution function into the Fokker-Planck equation they obtain a recursion relation for the expansion coefficients. By introducing a suitable vector and matrix notation this recurrence relation becomes a tridiagonal vector recurrence relation. Finally, this vector recurrence relation is solved by matrix continued fractions. The matrix continued fraction solution of the problem in question has been further developed in Ref. [43].

Fractional Klein-Kramers equations can in principle be solved by the same methods as the normal Klein-Kramers equation, e.g., by the method of separation of the variables. The separation procedure yields an equation of Sturm-Liouville type. Anomalous subdiffusion in the harmonic potential and double-well potential (5) has been treated by this method in Refs. [44–46] when inertial effects are ignored using an eigenfunction expansion with Mittag-Leffler temporal behavior. This method has recently been extended to the analogous fractional rotational diffusion models in a periodic potential by Coffey *et al.* [10,47]. There, the authors have developed effective methods of solution of fractional diffusion equations based on ordinary and matrix continued fractions (as is well known continued fractions are an extremely powerful tool in the solution of normal diffusion equations [1]). Here we apply the methods of Coffey *et al.* [10,43,47] to account for inertial effects in fractional translational diffusion. The main objective of the present paper is to ascertain how these effects in anomalous diffusion in a bistable potential modify the behavior of the normalized position correlation function $\langle x(0)x(t)\rangle_0/\langle x^2(0)\rangle_0$ and its spectra (characterizing the anomalous relaxation).

II. BASIC EQUATIONS

By introducing the normalized variables as in [43]

$$y = \frac{x}{\langle x^2\rangle_0^{1/2}}, \quad A = \frac{a\langle x^2\rangle_0}{2kT}, \quad B = \frac{b\langle x^2\rangle_0^2}{4kT},$$

$$\eta = \sqrt{\frac{m\langle x^2\rangle_0}{2kT}}, \quad \beta' = \eta\beta, \tag{6}$$

the fractional kinetic Eq. (4) becomes

$$\eta\frac{\partial W}{\partial t} + \eta\dot{y}\frac{\partial W}{\partial y} - \frac{1}{2\eta}\frac{dV}{dy}\frac{\partial W}{\partial \dot{y}} = \tau^{1-\alpha}\beta'\,{}_0D_t^{1-\alpha}\left[\frac{\partial}{\partial \dot{y}}(\dot{y}W) + \frac{1}{2\eta^2}\frac{\partial^2 W}{\partial \dot{y}^2}\right], \tag{7}$$

where $\tau=2\beta'\eta$ and $V(y)=Ay^2+By^4$. For $A>0$ and $B>0$, the potential $V(y)$ has only one minimum. For $A<0$ and $B>0$ (which is the case of interest), the potential $V(y)$ has two minima separated by a maximum at $y=0$ with the potential barrier $\Delta V=Q=A^2/4B$. The new normalization condition $\langle y^2\rangle_0=1$ implies that the constants A and B are not independent and are related via [48]

$$B = B(Q) = \frac{1}{8}\left[\frac{D_{-3/2}[\mathrm{sgn}(A)\sqrt{2Q}]}{D_{-1/2}[\mathrm{sgn}(A)\sqrt{2Q}]}\right]^2, \tag{8}$$

where $D_v(z)$ is Whitaker's parabolic cylinder function of order v [14]. According to Barkai and Silbey [15], Eq. (7) has hitherto been regarded as been valid for subdiffusion in velocity space, $0<\alpha<1$. However, the subdiffusion in velocity space gives rise to *enhanced* diffusion in configuration space [10,47]. Furthermore, if $1<\alpha<2$, Eq. (7) is also regarded as describing *enhanced* diffusion in velocity space, then the enhanced diffusion in velocity space gives rise to subdiffusion in configuration space [10,47].

Just as normal diffusion [42,43], one may seek a general solution of Eq. (7) in the form

$$W(y,\dot{y},t) = \frac{\eta\kappa}{\pi}e^{-\eta^2\dot{y}^2-[\kappa^2y^2+V(y)]/2}\sum_{n=0}^{\infty}\sum_{q=0}^{\infty}\frac{1}{\sqrt{2^{n+q}n!q!}}c_{n,q}(t) \times H_q(\kappa y)H_n(\eta\dot{y}), \tag{9}$$

where $H_n(z)$ are the orthogonal Hermite polynomials [14], $\kappa=\Lambda B^{1/4}$ and Λ is a scaling factor with value chosen so as to ensure optimum convergence of the continued fractions involved as suggested by Voigtlaender and Risken [42] (all results for the observables are independent of Λ). By substituting Eq. (9) into Eq. (7) and noting that [14]

$$\frac{d}{dz}H_n(z) = 2nH_{n-1}(z), \quad H_{n+1}(z) = 2zH_n(z) - 2nH_{n-1}(z),$$

we have the fractional differential recurrence relations for the functions $c_{n,q}(t)$

$$\eta\frac{d}{dt}c_{n,q}(t) = -n\beta'\tau^{1-\alpha}\,{}_0D_t^{1-\alpha}c_{n,q}(t) + \sqrt{n+1}[e_qc_{n+1,q+3}(t) + d_q^-c_{n+1,q+1}(t) + d_{q-1}^+c_{n+1,q-1}(t) + e_{q-3}c_{n+1,q-3}(t)] - \sqrt{n}[e_qc_{n-1,q+3}(t) + d_q^+c_{n-1,q+1}(t) + d_{q-1}^-c_{n-1,q-1}(t) + e_{q-3}c_{n-1,q-3}(t)], \tag{10}$$

where

$$d_q^{\pm} = \frac{B^{1/4}\sqrt{q+1}}{2\Lambda^3}[3(q+1) - 2\Lambda^2\sqrt{Q} \pm \alpha^4], \tag{11}$$

$$e_q = \frac{B^{1/4}\sqrt{q+1}}{2\Lambda^3}\sqrt{(q+3)(q+2)(q+1)}. \tag{12}$$

For $\alpha=1$, Eq. (10) coincides with that for normal diffusion [42,43].

Equation (10) can be solved exactly using matrix continued fractions as described in Appendix A. Having determined $c_{0,2q-1}(t)$, one can then calculate the position correlation function $C_\alpha(t)=\langle y(0)y(t)\rangle_0$ (see Appendix B)

$$C_\alpha(t) = \frac{\Lambda Z B^{1/4}}{\sqrt{\pi}}\sum_{q=1}^{\infty}c_{0,2q-1}(0)c_{0,2q-1}(t), \tag{13}$$

its spectrum $\tilde{C}_\alpha(\omega)=\int_0^\infty C_\alpha(t)e^{-i\omega t}dt$, and the dynamic susceptibility $\hat{\chi}(\omega)=\chi'(\omega)-i\chi''(\omega)$ defined as

$$\hat{\chi}(\omega) = -\int_0^\infty e^{-i\omega t}\frac{d}{dt}C_\alpha(t)dt = 1 - i\omega\tilde{C}_\alpha(\omega). \tag{14}$$

Here Z is the partition function in configuration space given by [47]

$$Z = \int_{-\infty}^{\infty}e^{-Ay^2-By^4}dy = \sqrt{\pi}(2B)^{-1/4}D_{-1/2}(-\sqrt{2Q})e^{Q/2}. \tag{15}$$

We remark that the dynamic susceptibility $\chi(\omega)$ characterizes the ac response of the system to a small perturbation [42].

III. NONINERTIAL SUBDIFFUSION IN CONFIGURATION SPACE

In the high damping (or noninertial) limit, $\beta'\gg1$, and $1<\alpha<2$, i.e., noninertial subdiffusion in configuration space, the low-frequency behavior ($\omega\to0$) of the susceptibility may be evaluated as [47]

$$\chi(\omega) \approx 1 - (i\omega\tau)^{2-\alpha}\tau_{\mathrm{int}}/\tau + \cdots, \tag{16}$$

where the relaxation time τ_{int} is given by

$$\tau_{\mathrm{int}} = \int_0^\infty C_1(t)dt. \tag{17}$$

For normal diffusion, τ_{int} corresponds to the correlation (or integral relaxation) time [the area under the correlation function $C_1(t)$]. Now τ_{int} for normal diffusion in a double well

potential (5) may be expressed in exact closed form, viz. ([10], Chap. 6),

$$\tau_{\rm int} = \tau \frac{\sqrt{\pi} e^{Q/2} D_{-1/2}(-\sqrt{2Q})}{2^{3/4} D^2_{-3/2}(-\sqrt{2Q})} \int_0^\infty e^{(s-\sqrt{Q})^2} [1 - {\rm erf}(s-\sqrt{Q})]^2 \frac{ds}{\sqrt{s}}, \tag{18}$$

where ${\rm erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-z^2} dz$ is the error function [14]. The low frequency part of the susceptibility spectrum $\chi(\omega)$ may also be approximated by a Cole-Cole-like equation [16,46]

$$\chi(\omega) \approx \frac{1-\delta}{1 + (i\omega/\omega_R)^{2-\alpha}} + \delta, \tag{19}$$

where

$$\omega_R \approx \tau^{-1} (\tau \lambda_1)^{1/(2-\alpha)} \tag{20}$$

is the characteristic frequency, λ_1 is the smallest nonvanishing eigenvalue of the Fokker-Planck equation for normal diffusion, and δ is a parameter accounting for the contribution of the high-frequency modes. In the time domain, such a representation is equivalent to assuming that the correlation function $C_\alpha(t)$ may be approximated as

$$C_\alpha(t) \approx (1-\delta) E_{2-\alpha}[-\tau \lambda_1 (t/\tau)^{2-\alpha}] + \delta, \tag{21}$$

where $E_\sigma(z)$ is the Mittag-Leffler function defined as [4,5]

$$E_\sigma(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n\sigma)}.$$

The behavior of λ_1 for normal diffusion can be evaluated with very high accuracy from the approximate equation [10,46]

$$\lambda_1 = \frac{D_{-3/2}(-\sqrt{2Q})}{\tau D_{-1/2}(-\sqrt{2Q})} \left[\frac{e^Q}{1 + {\rm erf}(\sqrt{Q})} \int_0^\infty \int_0^\infty e^{-(s-\sqrt{Q})^2 - (t-\sqrt{Q})^2} \times \frac{{\rm erf}(\sqrt{2st})}{\sqrt{st}} ds dt \right]^{-1}. \tag{22}$$

In the low temperature limit ($Q \gg 1$) λ_1^{-1} and $\tau_{\rm int}$ have the simple asymptotic behavior [10,46]

$$1/\lambda_1 \sim \frac{\tau \pi e^Q}{4\sqrt{2}Q} \left(1 + \frac{5}{8Q} + \cdots \right),$$

$$\tau_{\rm int} \sim \frac{\tau \pi e^Q}{4\sqrt{2}Q} \left(1 + \frac{1}{2Q} + \cdots \right). \tag{23}$$

Equations (19)–(23) allow one to readily estimate the qualitative behavior of the susceptibility $\chi(\omega)$ and its characteristic frequency ω_R. In particular, $\omega_R \sim (4\sqrt{2}Q/\pi)^{1/(2-\alpha)} e^{-Q/(2-\alpha)}/\tau$ in the low temperature limit ($Q \gg 1$). Noninertial subdiffusion in a double well potential has been treated in detail in Ref. [46].

IV. RESULTS AND DISCUSSION

The imaginary $\chi''(\omega)$ part of the dynamic susceptibility for various values of the barrier height Q, friction coefficient β', and fractional exponent α are shown in Figs. 1 and 2. The low-frequency asymptotes [Eq. (16)] are also shown here for comparison. Apparently for high damping, $\beta' \gg 1$, the low frequency part of the spectrum may by approximated by Eq. (19). This low frequency relaxation band is due to the slow overbarrier relaxation of the particles in the double-well potential. A very high-frequency band is also visible in Figs. 1 and 2 due to the fast inertial oscillations of the particles in the potential wells. As far as the behavior of the high-frequency band as a function of β' is concerned, its amplitude decreases progressively with increasing β', as one would intuitively expect. For large friction $\beta' \gg 1$ (small inertial effects), the characteristic frequency of this band can

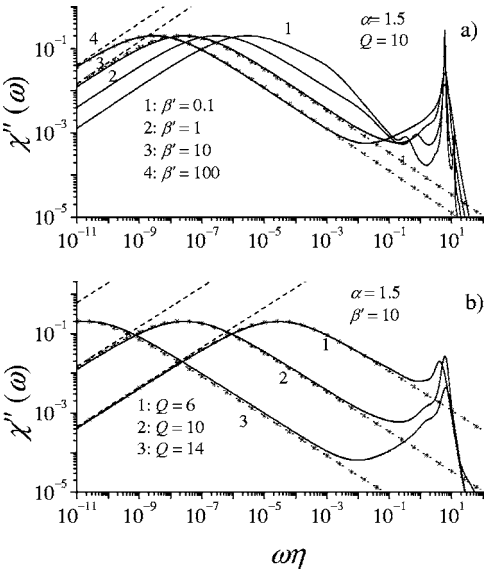

FIG. 1. The imaginary part of $\chi(\omega)$ vs $\omega\eta$ (solid lines) for the fractional exponent $\alpha = 1.5$ and various values of the damping coefficient β' and barrier height Q. The Cole-Cole-like spectra [Eq. (19)] and low frequency asymptotes [Eq. (16)] are shown by symbols and dashed lines, respectively.

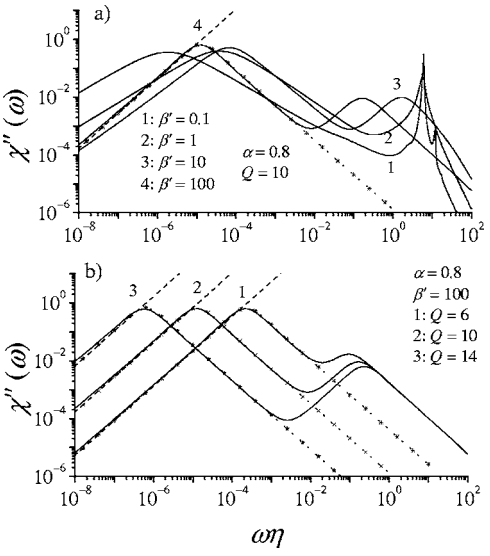

FIG. 2. The same as in Fig. 1 for $\alpha = 0.5$.

be estimated as $\omega_W \sim (8Q)^{1/(2-\alpha)}/\tau$ [46] (for $1<\alpha<2$). On the other hand, for very small friction $\beta' \ll 1$ (large inertial effects), two sharp peaks appear in the high-frequency part of the spectra. These peaks appear at the fundamental and second harmonic frequencies of the almost free periodic motion of the particle in the (anharmonic) potential $V(x) = ax^2/2 + bx^4/4$. For $Q \gg 1$, $\beta' \ll 1$, and $\alpha = 1$, the characteristic frequency of the high-frequency oscillations ω_L can be estimated from the analytic solution for the position correlation function $\langle x(0)x(t)\rangle_0$ at vanishing damping, $\beta' \to 0$, as $\omega_L \sim 2Q^{3/4}\eta^{-1}$ [32,42,43] (detailed discussion of the undamped case is given in Refs. [32,39,43]). Moreover, just as in normal Brownian dynamics, inertial effects cause a rapid falloff of $\chi''(\omega)$ at high frequencies. The "integral" absorption defined as $\int_0^\infty \omega\chi''(\omega)d\omega$ satisfies the sum rule [11]

$$\int_0^\infty \omega\chi''(\omega)d\omega = \int_0^\infty \omega^2 \mathrm{Re}[\tilde{C}(\omega)]d\omega$$

$$= -\frac{\pi}{2}\ddot{C}(0)$$

$$= \frac{\pi}{2}\frac{\langle \dot{x}^2(0)\rangle_0}{\langle x^2(0)\rangle_0}$$

$$= \frac{\pi}{4\eta^2}, \tag{24}$$

which relates the second spectral moments of position autocorrelation functions to their second time derivative at $t=0$. The sum rule Eq. (24) dictates that the integral absorption remains finite. We remark, on the other hand, that for a model based on a FKKE of the form of Eq. (3), this sum rule is not fulfilled as here $\int_0^\infty \omega\chi''(\omega)d\omega = \infty$. The behavior of $\chi(\omega)$ and the low-frequency asymptotes [Eq. (16)] for high damping is shown in Figs. 3 and 4 for various values of the fractional exponent α. Apparently, the agreement between the exact continued fraction calculations and the approximate Eq. (16) at low frequencies is very good when $1<\alpha<2$, i.e., noninertial subdiffusion in configuration space. As far as the dependence of the characteristic frequency $\omega_R \approx \tau^{-1}(\tau\lambda_1)^{1/(2-\alpha)}$ [Eq. (20)] of the low-frequency band on the barrier height Q and fractional exponent α is concerned the frequency ω_R decreases exponentially $\sim e^{-Q/(2-\alpha)}$ as Q is raised and $\alpha \to 2$. This behavior occurs because for normal diffusion the probability of escape of a particle from one well to another over the potential barrier exponentially decreases with increasing Q.

The model we have outlined incorporates both relaxation and resonance behavior of a nonlinear Brownian oscillator and so may simultaneously explain both the anomalous (low-frequency) relaxation and high frequency resonance spectra. The present calculation also constitutes an example of the solution of the fractional Klein-Kramers equation for anomalous inertial translational diffusion in a double well potential and is to our knowledge the first example of such a solution. We remark that all the above results are obtained from the Barkai-Silbey fractional form of the Klein-Kramers Eq. (7) for the evolution of the probability distribution function in phase space. In that equation, the fractional derivative acts only on the diffusion term. Hence the form of the Liouville operator, or convective derivative is preserved so that Eq. (7) has the conventional form of a Boltzmann equation for the single particle distribution function. Thus the high frequency behavior is entirely controlled by the inertia of the system, and does not depend on the anomalous exponent. Although such a diffusion equation fully incorporates inertial effects and produces physically meaning results much work remains to be done in order to provide a rigorous justification for such inertial kinetic equations.

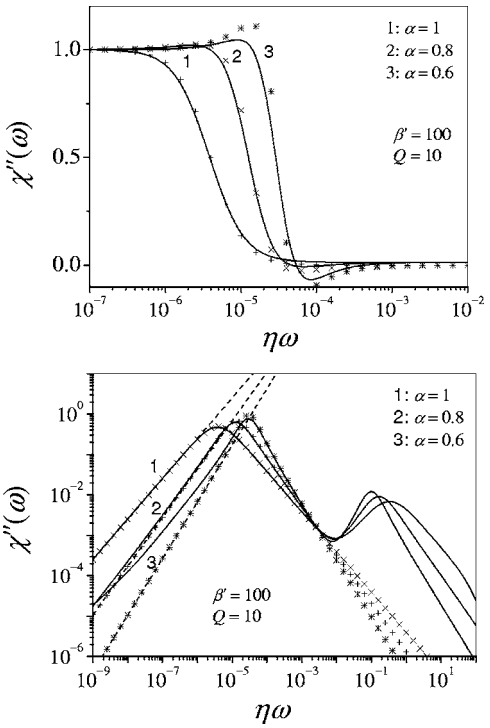

FIG. 3. The real χ' and imaginary χ'' parts of the dynamic susceptibility $\chi(\omega)$ vs $\omega\eta$ (solid lines) for various values of the fractional exponent $\alpha = 1$ (normal diffusion), 0.8, and 0.6; the barrier height $Q = 10$ and damping coefficient $\beta' = 100$. The Cole-Cole-like spectra [Eq. (19)] and low frequency asymptotes [Eq. (16)] are shown by symbols and dashed lines, respectively.

APPENDIX A: MATRIX CONTINUED FRACTION SOLUTION

The solution of Eq. (10) can be found by modifying the solution for normal diffusion [43]. We introduce the column vectors

$$\mathbf{C}_{2n-1}(t) = \begin{pmatrix} c_{2n-2,1}(t) \\ c_{2n-2,3}(t) \\ \vdots \end{pmatrix}, \quad \mathbf{C}_{2n}(t) = \begin{pmatrix} c_{2n-1,0}(t) \\ c_{2n-1,2}(t) \\ \vdots \end{pmatrix} \quad (n \geqslant 1).$$

Now, Eq. (10) can be rearranged as the set of matrix three-term recurrence equations for the one-sided Fourier transforms $\tilde{\mathbf{C}}_n(\omega) = \int_0^\infty \mathbf{C}_n(t)e^{-i\omega t}dt$, viz.,

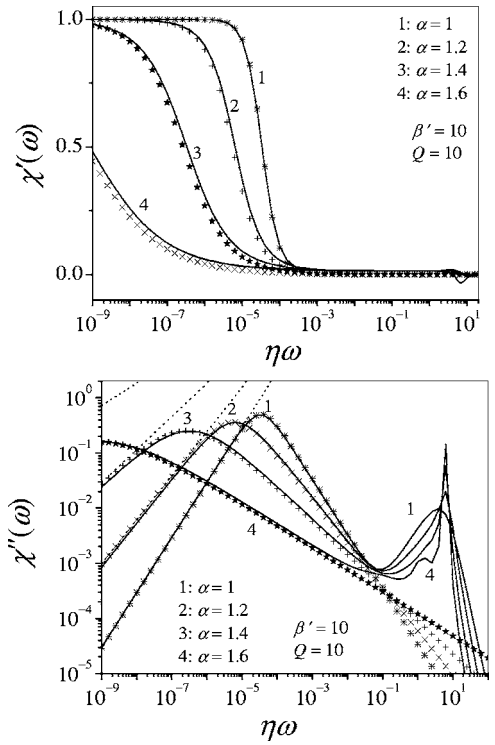

FIG. 4. The same as in Fig. 3 for $\alpha=1$ (normal diffusion), 1.2, and 1.4; $\beta'=10$ and $Q=10$.

$$[i\eta\omega+\beta'(i\omega\tau)^{1-\alpha}(n-1)]\tilde{\mathbf{C}}_n(\omega)-\mathbf{Q}_n^-\tilde{\mathbf{C}}_{n-1}(\omega)-\mathbf{Q}_n^+\tilde{\mathbf{C}}_{n+1}(\omega)=\eta\delta_{n,1}\mathbf{C}_1(0), \tag{A1}$$

where $\mathbf{Q}_n^+$ and $\mathbf{Q}_n^-$ are the four-diagonal matrices. Their matrix elements are given by

$$(\mathbf{Q}_{2n}^-)_{p,q}=-\sqrt{2n-1}(\delta_{p,q+2}e_{2p-5}+\delta_{p,q+1}d_{2p-3}^-+\delta_{p,q}d_{2(p-1)}^+ +\delta_{p,q-1}e_{2(p-1)}),$$

$$(\mathbf{Q}_{2n}^+)_{p,q}=\sqrt{2n}(\delta_{p,q+2}e_{2p-5}+\delta_{p,q+1}d_{2p-3}^+ +\delta_{p,q}d_{2(p-1)}^- +\delta_{p,q-1}e_{2(p-1)}),$$

$$(\mathbf{Q}_{2n-1}^-)_{p,q}=-\sqrt{2n-2}(\delta_{p,q+1}e_{2(p-2)}+\delta_{p,q}d_{2(p-1)}^- +\delta_{p,q-1}d_{2p-1}^+ +\delta_{p,q-2}e_{2p-1}),$$

$$(\mathbf{Q}_{2n-1}^+)_{p,q}=\sqrt{2n-1}(\delta_{p,q+1}e_{2(p-2)}+\delta_{p,q}d_{2(p-1)}^+ +\delta_{p,q-1}d_{2p-1}^- +\delta_{p,q-2}e_{2p-1}),$$

where $d_q^\pm$ and e_q are defined by Eqs. (11) and (12).

By invoking the general method [10] for solving the matrix recursion Eq. (A1), we have the exact solution for the spectrum $\tilde{\mathbf{C}}_1(\omega)$ in terms of a matrix continued fraction, viz.

$$\tilde{\mathbf{C}}_1(\omega)=\eta\mathbf{\Delta}_1(\omega)\mathbf{C}_1(0), \tag{A2}$$

where the matrix continued fraction $\Delta_1(\omega)$ is defined by the recurrence equation

$$\mathbf{\Delta}_n(\omega)=\{[i\eta\omega+\beta'(i\tau\omega)^{1-\alpha}(n-1)]\mathbf{I}-\mathbf{Q}_n^+\mathbf{\Delta}_{n+1}(\omega)\mathbf{Q}_{n+1}^-\}^{-1}.$$

and $\mathbf{I}$ is the unit matrix. Having determined $\tilde{\mathbf{C}}_1(\omega)$ [whose elements are $\tilde{c}_{0,2q-1}(\omega)$, $q\geqslant 1$], we can evaluate the spectrum of the position correlation function $C_\alpha(t)=\langle y(0)y(t)\rangle$ defined by Eq. (13) [here the initial values $c_{0,2q-1}(0)$ are calculated from Eq. (B2) of the Appendix B].

The exact matrix continued fraction solution [Eq. (A2)] we have obtained is easily computed. As far as practical calculations of the infinite matrix continued fraction are concerned, we approximate it by a matrix continued fraction of finite order (by putting $\Delta_{n+1}=\mathbf{0}$ at some $n=N$); simultaneously, we confine the dimensions of the infinite matrices $\mathbf{Q}_n^-$, $\mathbf{Q}_n^+$, and $\mathbf{I}$ to a finite value $M\times M$. N and M are determined so that further increase of N and M does not alter the results. Both N and M depend mainly on the dimensionless barrier (Q) and damping (β') parameters and must be chosen taking into account the desired degree of accuracy of the calculation. The final results are independent of the scaling factor Λ. The advantage of choosing an optimal value of Λ is, however, that the dimensions N and M can be minimized. Both N and M increase with decreasing β' and increasing Q.

APPENDIX B: DERIVATION OF EQ. (13)

Equation (13) follows from the definition of the correlation function $C_\alpha(t)$, viz.,

$$C_\alpha(t)=\langle y(0)y(t)\rangle_0=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}yy_0W(y,\dot{y},t|y_0,\dot{y}_0,0)\times W_0(y_0,\dot{y}_0)dydy_0d\dot{y}d\dot{y}_0,$$

where $y_0=y(0)$, $W_0(y_0,\dot{y}_0)=(\eta/\sqrt{\pi}Z)e^{-\eta^2\dot{y}_0^2-V(y_0)}$ is the equilibrium (Boltzmann) distribution function, and $W(y,\dot{y},t|y_0,\dot{y}_0,0)$ is the transition probability, which satisfies Eq. (7) with the initial condition $W(y,\dot{y},0|y_0,\dot{y}_0,0)=\delta(y-y_0)\delta(\dot{y}-\dot{y}_0)$ and is defined as

$$W(y,\dot{y},t|y_0,\dot{y}_0,0)=\frac{\kappa\eta}{\pi}e^{-\eta^2\dot{y}^2-[\kappa^2(y^2+y_0^2)+V(y)-V(y_0)]/2}\sum_{n=0}^{\infty}\sum_{q=0}^{\infty}\sum_{m=0}^{\infty}\sum_{p=0}^{\infty}\times\frac{[\mathbf{G}(t)]_{q,p}^{n,m}H_p(\kappa y_0)H_m(\eta\dot{y}_0)H_q(\kappa y)H_n(\eta\dot{y})}{\sqrt{2^{n+m+p+q}m!p!n!q!}}, \tag{B1}$$

where $[\mathbf{G}(t)]_{q,p}^{n,m}$ are the matrix elements of the system matrix $\mathbf{G}(t)$ defined as

$$[\mathbf{G}(t)]_{q,p}^{n,m}=\frac{\kappa\eta}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dydy_0d\dot{y}d\dot{y}_0W(y,\dot{y},t|y_0,\dot{y}_0,0)\times H_p(\kappa y_0)H_m(\eta\dot{y}_0)H_q(\kappa y)H_n(\eta\dot{y})\times e^{-\eta^2\dot{y}_0^2-[\kappa^2(y^2+y_0^2)-V(y)-V(y_0)]/2}.$$

The coefficients $c_{n,q}(t)$ can be presented in terms of $[\mathbf{G}(t)]_{q,p}^{n,m}$ as [42]

$$c_{n,q}(t) = \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} [\mathbf{G}(t)]_{q,p}^{n,m} c_{m,p}(0).$$

Whence

$$c_{0,q}(t) = \sum_{p=0}^{\infty} [\mathbf{G}(t)]_{q,p}^{0,0} c_{0,p}(0)$$

with the initial conditions

$$c_{0,p}(0) = \frac{1}{Z\sqrt{2^p p! B}} \int_{-\infty}^{\infty} x H_p(\Lambda x) e^{-(\Lambda^2 x^2 - 2Qx^2 + x^4)/2} dx. \tag{B2}$$

Noting that $[G(0)]_{q,p}^{m,n} = \delta_{q,p}\delta_{m,n}$, we have from Eq. (B1)

$$W(y,\dot{y},0|y_0,\dot{y}_0,0) = \frac{\kappa\eta}{\pi} e^{-\eta^2\dot{y}^2 - [\kappa^2(y^2+y_0^2)+V(y)-V(y_0)]/2} \times \sum_{p=0}^{\infty} \frac{H_p(\kappa y_0) H_p(\kappa y)}{2^p p!} \times \sum_{m=0}^{\infty} \frac{H_m(\eta\dot{y}_0) H_m(\eta\dot{y})}{2^m m!}.$$

Taking into account that [1]

$$f_\lambda(y,y_0) = \sum_{p=0}^{\infty} \frac{\lambda^p}{p!} H_p(\kappa y) H_p(\kappa y_0) = \frac{1}{\sqrt{1-4\lambda^2}} \exp\left[\frac{4\lambda\kappa^2}{1-4\lambda^2}(yy_0 - \lambda y^2 - \lambda y_0^2)\right]$$

and

$$\lim_{\lambda \to 1/2} f_\lambda(y,y_0) = \frac{\sqrt{\pi}}{\kappa} e^{\kappa^2 y_0^2} \delta(y - y_0),$$

we have Eq. (13).

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