

Generalized Langevin equation with fractional derivative and long-time correlation function

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(Received 6 April 2006; published 23 June 2006)

We investigate the motion of a particle governed by a generalized Langevin equation with fractional derivative, nonlocal dissipative force, and long-time correlation function. We derive general expressions for the variances with a linear external force. We also analyze their asymptotic behaviors for the power-law correlation function without external force.

DOI: [10.1103/PhysRevE.73.061104](https://doi.org/10.1103/PhysRevE.73.061104)

PACS number(s): 02.50.-r, 05.10.Gg, 05.40.-a

I. INTRODUCTION

One of the fundamental mechanisms for transport of materials in physical systems is related to diffusion. A well-known example of a diffusion process is Brownian motion. Diffusion processes are classified according to their mean-square displacements: in normal diffusion the mean-square displacement grows linearly with time and in other situations the processes are said to exhibit anomalous diffusion. Nowadays, there are several approaches to describe anomalous diffusion processes, and they can be applied to many situations of natural systems [1–3]. One of the most interesting features incorporated into these approaches is that related to the memory effect. In particular, the memory effect incorporated into the Langevin approach can be associated with the retardation of friction and fractal media [4–9]. Moreover, it has been suggested to substitute the ordinary derivative by the fractional derivative when separation of the microscopic and macroscopic time scales does not exist [4]. Let us consider the following generalized Langevin equation:

$${}_0D_t^\alpha v + \int_0^t dt_1 \gamma(t-t_1)v + U(x) = F(t) \quad \text{for } 0 < \alpha < 1, \quad (1)$$

where v is the velocity, $\gamma(t)$ is the dissipative memory kernel, $U(x)$ is an external force, $F(t)$ is a Gaussian random force with mean zero and correlation function given by

$$\langle F(t_1)F(t_2) \rangle = C(|t_1 - t_2|), \quad (2)$$

${}_0D_t^\alpha v$ is the Caputo fractional derivative [10] defined by

$${}_0D_t^\alpha v = \frac{1}{\Gamma[1-\alpha]} \int_0^t dt_1 \frac{dv/dt_1}{(t-t_1)^\alpha}, \quad (3)$$

and $\Gamma[z]$ is the Gamma function. We note that the fractional Langevin equation (1) with the use of the Riemann-Liouville fractional derivative and white noise has been investigated in [11]. Further, the ordinary Langevin equation with correlated noise has been investigated in [12] and it can also produce anomalous diffusion processes.

It is known that for ordinary derivatives ($\alpha=1$) the internal noise is related to the dissipative memory kernel. Two types of correlation function are usually employed to study the above system: power-law and exponential correlations. In particular, the anomalous diffusion processes can be generated by an internal power-law correlation function [5,6].

In this work we investigate the generalized Langevin equation given by (1) which includes the fractional derivative and nonlocal dissipative force. We obtain expressions for the variances with a linear external force. We show that these expressions for the variances can be very general due to the fact that they are independent of the fractional parameter α . We also analyze their asymptotic behaviors for the power-law correlation function.

II. GENERAL EXPRESSIONS FOR THE VARIANCES WITH $U(x) = \omega_\alpha^2 x$

Before analyzing the details of the above system for some specific correlation function and dissipative memory kernel, we can obtain formal expressions for the first moments and general expressions for the variances. Equation (1) can be solved by using the Laplace transform, with the initial conditions $x_0 = x(0)$ and $v_0 = v(0)$. The displacement $x(t)$ is given by

$$x(t) = \langle x \rangle + \int_0^t dt_1 G(t-t_1)F(t_1), \quad (4)$$

where

$$\langle x \rangle = x_0(1 - \omega_\alpha^2 I) + \frac{v_0}{\Gamma[1-\alpha]} \int_0^t dt_1 \frac{G(t-t_1)}{t_1^\alpha} \quad (5)$$

and $I = \int_0^t dt_1 G(t-t_1)$. The kernel $G(t)$ is the Laplace inversion of

$$\bar{G} = \frac{1}{s^{1+\alpha} + s\bar{\gamma} + \omega_\alpha^2}, \quad (6)$$

where $\bar{\gamma}$ is the Laplace transform of the damping kernel $\gamma(t)$.

From Eq. (4) one can obtain the velocity $v(t)$ which is given by

$$v(t) = \langle v \rangle + \int_0^t dt_1 g(t-t_1)F(t_1) \quad (7)$$

with $G(0)=0$, where

$$\langle v \rangle = v_{00}D_t^\alpha G - x_0\omega_\alpha^2 G(t) \quad (8)$$

and $g(t) = dG/dt$. We note that for $\alpha=1$ (ordinary derivative) we recover the results obtained in [7].

From the solutions (4) and (7) and taking into account the symmetry of the correlation function, one can obtain the explicit expressions of the variances,

$$\sigma_{xx} = \langle x^2 \rangle - \langle x \rangle^2 = 2 \int_0^t dt_1 G(t_1) \int_0^{t_1} dt_2 G(t_2) C(t_1 - t_2), \quad (9)$$

$$\sigma_{xv} = \frac{1}{2} \frac{d\sigma_{xx}}{dt} = G(t) \int_0^t dt_1 G(t_1) C(t - t_1), \quad (10)$$

and

$$\sigma_{vv} = \langle v^2 \rangle - \langle v \rangle^2 = 2 \int_0^t dt_1 g(t_1) \int_0^{t_1} dt_2 g(t_2) C(t_1 - t_2). \quad (11)$$

We note that the solutions (4), (7), and (9)–(11) provide very general expressions due to the fact that they do not depend explicitly on the parameter α . In fact, they maintain the same expressions as the solutions of the ordinary derivative [7,9]. The order of the fractional derivative α appears in the kernel $G(t)$, $\langle x \rangle$, and $\langle v \rangle$.

In the case of $C(t)$ proportional to the dissipative memory kernel $C(t) = c\gamma(t)$ the expressions (9)–(11) can be simplified to

$$\begin{aligned} \sigma_{xx} &= 2 \int_0^t dt_1 G(t_1) \int_0^{t_1} dt_2 G(t_2) C(t_1 - t_2) \\ &= c \left(2I(t) - 2 \int_0^t dt_1 G(t_1) {}_0D_{t_1}^\alpha G(t_1) - \omega_\alpha^2 I^2(t) \right), \quad (12) \end{aligned}$$

$$\sigma_{xv} = \frac{1}{2} \frac{d\sigma_{xx}}{dt} = cG(t) [1 - {}_0D_t^\alpha G(t) - \omega_\alpha^2 I(t)], \quad (13)$$

and

$$\begin{aligned} \sigma_{vv} &= 2 \int_0^t dt_1 g(t_1) \int_0^{t_1} dt_2 g(t_2) C(t_1 - t_2) \\ &= 2c \int_0^t dt_1 g(t_1) [-{}_0D_{(*)t_1}^\alpha g(t_1) - \omega_\alpha^2 G(t_1)] \\ &= c \left(-2 \int_0^t dt_1 g(t_1) {}_0D_{(*)t_1}^\alpha g(t_1) - \omega_\alpha^2 G^2(t) \right), \quad (14) \end{aligned}$$

where ${}_0D_{(*)t}^\alpha g(t)$ is the Riemann-Liouville fractional derivative defined by

$${}_0D_{(*)t}^\alpha g(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t dt_1 \frac{g(t_1)}{(t-t_1)^\alpha}. \quad (15)$$

We note that for $\alpha=1$ we recover the results obtained in [7,9] which are given by

$$\sigma_{xx} = c[2I(t) - G^2(t) - \omega^2 I^2(t)], \quad (16)$$

$$\sigma_{xv} = cG(t)[1 - g(t) - \omega^2 I(t)], \quad (17)$$

and

$$\sigma_{vv} = c[1 - g^2(t) - \omega^2 G^2(t)]. \quad (18)$$

III. LONG-TIME CORRELATION FUNCTION AND ASYMPTOTIC BEHAVIORS WITH $U(x)=0$

In order to investigate some detail of the above system one considers two well-known correlation functions: the exponential and power-law correlations. Moreover, we set $U(x)=0$.

We first consider the case of frictional memory kernel given by $\gamma(t) = \gamma_0 e^{-\lambda t}$ and ordinary derivative ($\alpha=1$). The Laplace transform of $\gamma(t)$ is $\bar{\gamma}(s) = \gamma_0/(s+\lambda)$. By using (6), we obtain

$$G(t) = \frac{\lambda}{\gamma_0} [1 - A_1 e^{-\lambda t/2} \sin(\lambda_1 t + \phi)], \quad \gamma_0 > \frac{\lambda^2}{4}, \quad (19)$$

$$G(t) = \frac{4}{\lambda} \left[1 - e^{-\lambda t/2} \left(1 + \frac{\lambda}{4} t \right) \right], \quad \gamma_0 = \frac{\lambda^2}{4}, \quad (20)$$

$$\begin{aligned} G(t) &= \frac{\lambda}{\gamma_0} \left(1 - \frac{A_2 + 1}{2} e^{-(\lambda/2 - \lambda_2)t} + \frac{A_2 - 1}{2} e^{-(\lambda/2 + \lambda_2)t} \right), \\ \gamma_0 &< \frac{\lambda^2}{4}, \quad (21) \end{aligned}$$

where

$$\begin{aligned} A_1 &= \frac{\gamma_0}{\lambda \lambda_1}, \quad A_2 = \frac{\lambda^2 - 2\gamma_0}{2\lambda \lambda_2}, \quad \lambda_1 = \sqrt{\gamma_0 - \frac{\lambda^2}{4}}, \\ \lambda_2 &= \sqrt{\frac{\lambda^2}{4} - \gamma_0}, \quad (22) \end{aligned}$$

and

$$\phi = \arctan\left(\frac{\lambda \lambda_1}{\lambda^2/2 - \gamma_0}\right). \quad (23)$$

The solution (19) has been obtained in [6], but the authors have not considered the other two cases. We see that the behavior of $G(t)$ changes with the damping parameter. In the case of internal noise, the correlation function is related to the dissipative memory kernel given by $C(t) = (D/2\tau_c) e^{-t/\tau_c}$ and $\gamma(t) = C(t)/k_B T$ [6], where τ_c is the correlation time, k_B is the Boltzmann constant, and T is the absolute temperature of the environment. Then, $\lambda = 1/\tau_c$ and $\gamma_0 = D/(2\tau_c k_B T)$. For this case, the change of behavior of the kernel $G(t)$ can be associated with the noise intensity D . For $D > k_B T/2\tau_c$, $G(t)$ oscillates. For $D = k_B T/2\tau_c$, $G(t)$ does not oscillate; however, it contains a term of type e^{-z} . For $D < k_B T/2\tau_c$, $G(t)$ contains a combination of exponential terms. These behaviors are also obtained for the variances as shown below.

From the solutions (19)–(21) one can obtain the variances σ_{xx} and σ_{vv} which are given by

$$\begin{aligned} \sigma_{xx} = & -\frac{4(k_B T)^3 A_1}{D^2} \{ \sin \phi + 2\lambda_1 \tau_c \cos \phi \\ & - e^{-t/2\tau_c} [3 \sin(\lambda_1 t + \phi) + 2\lambda_1 \tau_c \cos(\lambda_1 t + \phi)] \} \\ & + \frac{(2k_B T)^2}{D} t - \frac{4(k_B T)^3}{D^2} [1 + A_1^2 e^{-t/\tau_c} \sin^2(\lambda_1 t + \phi)], \\ & D > k_B T / 2\tau_c, \end{aligned} \quad (24)$$

$$\begin{aligned} \sigma_{xx} = & \frac{(2k_B T)^2}{D} \left(t - 4\tau_c + \frac{2D\tau_c^2}{k_B T} - \frac{k_B T}{D} \right) \\ & + \frac{8(k_B T)^2 \tau_c e^{-t/2\tau_c}}{D} \left[1 + \left(1 + \frac{t}{2\tau_c} \right) \left(1 - \frac{D\tau_c}{k_B T} \right) \right] \\ & + \frac{8(k_B T)^3 e^{-t/2\tau_c}}{D^2} \left[1 + \left(1 - \frac{D\tau_c}{k_B T} \right) \frac{t}{2\tau_c} \right] \left(1 - \frac{e^{-t/2\tau_c}}{2} \right), \\ & D = k_B T / 2\tau_c, \end{aligned} \quad (25)$$

$$\begin{aligned} \sigma_{xx} = & \frac{2(k_B T)^2}{D} \left(2t + \frac{1+A_2}{\lambda/2 - \lambda_2} (e^{-(\lambda/2 - \lambda_2)t} - 1) \right. \\ & + \left. \frac{1-A_2}{\lambda/2 + \lambda_2} (e^{-(\lambda/2 + \lambda_2)t} - 1) \right) - \frac{4(k_B T)^3}{D^2} \left(1 - \frac{1+A_2}{2} \right. \\ & \times \left. e^{-(\lambda/2 - \lambda_2)t} - \frac{1-A_2}{2} e^{-(\lambda/2 + \lambda_2)t} \right)^2, \quad D < k_B T / 2\tau_c, \end{aligned} \quad (26)$$

$$\begin{aligned} \sigma_{vv} = & k_B T \left[1 - \frac{(2k_B T)^2 A_1^2}{D^2} e^{-t/\tau_c} \left(\frac{1}{2\tau_c} \sin(\lambda_1 t + \phi) \right. \right. \\ & \left. \left. - \lambda_1 \cos(\lambda_1 t + \phi) \right)^2 \right], \quad D > k_B T / 2\tau_c, \end{aligned} \quad (27)$$

$$\sigma_{vv} = k_B T \left[1 - \left(1 + \frac{t}{2\tau_c} \right)^2 e^{-t/\tau_c} \right], \quad D = k_B T / 2\tau_c, \quad (28)$$

and

$$\begin{aligned} \sigma_{vv} = & k_B T - \frac{(2k_B T)^3}{2D^2} \left[\frac{1+A_2}{2} \left(\frac{\lambda}{2} - \lambda_2 \right) e^{-(\lambda/2 - \lambda_2)t} \right. \\ & \left. + \frac{1-A_2}{2} \left(\frac{\lambda}{2} + \lambda_2 \right) e^{-(\lambda/2 + \lambda_2)t} \right]^2, \quad D < k_B T / 2\tau_c. \end{aligned} \quad (29)$$

It is easy to see that the asymptotic behaviors of these mean-square displacements are similar and they present normal diffusion, given by $\sigma_{xx} \sim \frac{(2k_B T)^2}{D} t$, whereas $\sigma_{vv} \sim k_B T$. The former result shows that the internal exponential correlation function does not generate anomalous diffusion processes, in contrast to the power-law correlation function [5–7].

Next, we consider a long-time correlation function given by $C(t) = C_\theta t^{-\theta}$ ($0 < \theta < 1$) and the frictional memory kernel as $\gamma(t) = \gamma_\lambda t^{-\lambda}$ ($0 < \lambda < 1$), for $0 < \alpha < 1$. Then, the Laplace transform of $\gamma(t)$ is $\bar{\gamma} = \gamma_\lambda \Gamma(1-\lambda) s^{\lambda-1}$. From Eq. (6) we obtain

$$G(t) = t^\alpha E_{1+\alpha-\lambda, 1+\alpha}[-\gamma_\lambda \Gamma(1-\lambda) t^{1+\alpha-\lambda}] \quad (30)$$

and

$$g(t) = t^{\alpha-1} E_{1+\alpha-\lambda, \alpha}[-\gamma_\lambda \Gamma(1-\lambda) t^{1+\alpha-\lambda}], \quad (31)$$

where $E_{\alpha, \beta}(z) = \sum_{n=0}^{\infty} z^n / \Gamma(\beta + \alpha n)$ is the generalized Mittag-Leffler function. Moreover, one can obtain explicit solutions for

$$\begin{aligned} \int_0^{t_1} dt_2 G(t_2) C(t_1 - t_2) \\ = C_\theta \Gamma(1-\theta) t_1^{1+\alpha-\theta} E_{1+\alpha-\lambda, 2+\alpha-\theta}[-\gamma_\lambda \Gamma(1-\lambda) t_1^{1+\alpha-\lambda}] \end{aligned} \quad (32)$$

and

$$\begin{aligned} \int_0^{t_1} dt_2 g(t_2) C(t_1 - t_2) \\ = C_\theta \Gamma(1-\theta) t_1^{\alpha-\theta} E_{1+\alpha-\lambda, 1+\alpha-\theta}[-\gamma_\lambda \Gamma(1-\lambda) t_1^{1+\alpha-\lambda}]. \end{aligned} \quad (33)$$

The explicit solutions for $\langle x \rangle$ and $\langle v \rangle$ can be obtained from the solution (30), and they are given by

$$\langle x \rangle = x_0 + v_0 t E_{1+\alpha-\lambda, 2}[-\gamma_\lambda \Gamma(1-\lambda) t^{1+\alpha-\lambda}] \quad (34)$$

and

$$\langle v \rangle = v_0 E_{1+\alpha-\lambda}[-\gamma_\lambda \Gamma(1-\lambda) t^{1+\alpha-\lambda}]. \quad (35)$$

We note that these first moments can give the same results obtained from the fractional Fokker-Planck equation by identifying the parameter of the fractional order of the fractional Fokker-Planck equation with $1+\alpha-\lambda$ (for $\lambda \neq \alpha$) [13]. In the case of $\lambda = \alpha$, we obtain the same results of the normal Brownian motion.

The asymptotic behaviors of the above quantities can be obtained by using the long-time limit of the generalized Mittag-Leffler function [14]

$$E_{\alpha, \beta}(z) \sim -\frac{1}{z \Gamma(\beta - \alpha)}, \quad (36)$$

and we obtain

$$\langle x \rangle \sim \frac{v_0 t^{\lambda-\alpha}}{\gamma_\lambda \Gamma(1-\lambda) \Gamma(1+\lambda-\alpha)} \quad (37)$$

and

$$\langle v \rangle \sim \frac{v_0 t^{\lambda-\alpha-1}}{\gamma_\lambda \Gamma(1-\lambda) \Gamma(\lambda-\alpha)}, \quad (38)$$

where we have considered $x_0 = 0$. Equation (37) shows a net drift in a direction determined by the initial velocity v_0 . For $\lambda < \alpha$, Eq. (37) exhibits a slow power-law decay. We see that

there is a competition between the dissipative term and inertial term. In the normal Brownian motion $\langle v \rangle$ exhibits an exponential decay faster than the power-law decay exhibited by Eq. (38) for $\lambda \neq \alpha$ ($0 < \lambda < 1$ and $0 < \alpha < 1$). But, for $\lambda = \alpha$, $\langle v \rangle$ exhibits an exponential decay which has the same result of the normal Brownian motion.

Instead of determining the complete solutions of the variances by using (30)–(33), we are interested in determining the long-time behaviors of the mean-square displacement which can be obtained from Eq. (36). In this case, σ_{xx} is given by

$$\sigma_{xx} \sim \text{const}, \quad 2\lambda < \theta, \quad (39)$$

$$\sigma_{xx} \sim \ln(t), \quad 2\lambda = \theta, \quad (40)$$

and

$$\sigma_{xx} \sim t^{2\lambda-\theta}, \quad 2\lambda > \theta. \quad (41)$$

From Eq. (41) we have normal diffusion for $2\lambda - \theta = 1$, subdiffusion for $2\lambda - \theta < 1$, and superdiffusion for $2\lambda - \theta > 1$. It is interesting to note that the long-time behavior of the mean-square displacement does not depend on the parameter α of the inertial term. This means that the inertial term has no significant contribution to the long-time limit of the mean-square displacement as in the usual case [2].

IV. CONCLUSION

In this work we have investigated the motion of a particle governed by the generalized Langevin equation with fractional derivative (1) under the influence of a long-time correlation function and a linear external force $U(x) = \omega_\alpha^2 x$. In particular, the generalized Langevin equation with ordinary derivative and dissipative memory kernel has been studied and applied to several physical systems [3,5–9], whereas the generalized Langevin equation with fractional derivative has been studied and applied to financial systems [4]. Equation (1) generalizes the usual Langevin equation by using both the nonlocal dissipative force and fractional derivative which modifies the classical Newtonian force. We have obtained unifying expressions for the displacement, velocity, and variances due to the fact that they are independent of the fractional parameter α . The processes have been investigated by using the exponential and power-law correlation functions. The exponential correlation function has been applied to $\alpha = 1$ and it does not generate anomalous diffusion processes. However, the anomalous diffusion processes can be generated by the power-law correlation function, and they are confirmed in [7] and by the asymptotic solutions (40) and (41) of fractional derivative approach.

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