Anomalous diffusion: Exact solution of the generalized Langevin equation for harmonically bounded particle

A. D. Viñales[1,*] and M. A. Despósito[1,2]
[1]Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina
[2]Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina
(Received 18 August 2005; published 12 January 2006)

We study the effect of a disordered or fractal environment in the irreversible dynamics of a harmonic oscillator. Starting from a generalized Langevin equation and using Laplace analysis, we derive exact expressions for the mean values, variances, and velocity autocorrelation function of the particle in terms of generalized Mittag-Leffler functions. The long-time behaviors of these quantities are obtained and the presence of a whip-back effect is analyzed.

DOI: 10.1103/PhysRevE.73.016111 PACS number(s): 02.50.−r, 05.40.−a, 02.50.Ey

The study of stochastic phenomena in disordered systems has been the subject of numerous investigations in the last years [1–4]. In simple systems, one assumes that the time correlation function for the system-environment interactions could be described by an exponential decay with a constant characteristic time. Nevertheless, complex out-of-equilibrium dynamics is characterized by a slow relaxation extended by several orders of magnitude and with the presence of power-law decay in the range of intermediate times. Some examples of these phenomena are the dynamics in polymers [5], charge transport in amorphous semiconductors [6], decorrelation processes in microemulsions [7], and diffusion in fractals [8].

It is now well established that power-law correlations are the physical origin of the so-called anomalous diffusion [2,4]. Dissipation in disordered media have mostly been discussed in a classical framework and for a free particle. In this case, the stochastic process is said to exhibit anomalous diffusion when the variance of its displacement after time t has the asymptotic form t^{λ}. The process is called subdiffusive when $\lambda<1$ and superdiffusive when $\lambda>1$; the case $\lambda=1$ corresponds to normal diffusion. Nevertheless, in several fields of physics, one encounters harmonic motion perturbed by some stochastic interaction with a macroscopic object. This situation typically corresponds to the residual coupling between one or various normal modes of a quantum fluid or many body system to the remaining, i.e., unresolved, microscopic degrees of freedom. In this paper, we analyze the effects associated with the disordered nature of an environment through the study of the dissipative dynamics of a harmonic oscillator immersed in a disordered environment.

For this purpose, we consider the dynamics of a particle under the influence of a random force modeled as Gaussian colored noise and an external field $f(X)=\omega^2 X$. In this situation, the generalized Langevin equation (GLE) for the diffusing particle is written as follows:

$$\ddot{X}(t) + \int_0^t dt'\,\gamma(t-t')\dot{X}(t') + \omega^2 X = F(t), \tag{1}$$

where $\gamma(t)$ is the dissipative memory kernel and $F(t)$ is a zero-centered and stationary Gaussian random force with correlation function

$$\langle F(t)F(t')\rangle = C(|t-t'|) = C(\tau). \tag{2}$$

In the case of internal noise, the memory kernel $\gamma(t)$ is related to the correlation function of the noise via the second fluctuation-dissipation theorem [9]

$$C(t) = k_B T \gamma(t), \tag{3}$$

where T is the absolute temperature, and k_B is the Boltzmann constant. In this case, the noise and dissipation stem from the same source and the system will finally reach the equilibrium state.

On the other hand, in the case of external noise, the fluctuation and dissipation come from different sources, and the memory kernel and the correlation function of the noise are independent. Thus, we cannot use the fluctuation-dissipation theorem. In this situation, the system will not reach the equilibrium state [10].

In what follows, we consider the Langevin equation (1) with the deterministic initial conditions

$$x_0 = X(0), \quad v_0 = \dot{X}(0). \tag{4}$$

By means of the Laplace transformation, one can easily obtain a formal expression for the displacement $X(t)$ and the velocity $\dot{X}(t)$. The displacement $X(t)$ satisfies that

$$X(t) = \langle X(t)\rangle + \int_0^t dt'\,G(t-t')F(t'), \tag{5}$$

where

$$\langle X(t)\rangle = v_0 G(t) + x_0[1-\omega^2 I(t)]. \tag{6}$$

The relaxation function $G(t)$ is the Laplace inversion of

*Corresponding author. Email address: dvinales@df.uba.ar

$$\hat{G}(s) = \frac{1}{s^2 + \hat{\gamma}(s)s + \omega^2}, \tag{7}$$

where $\hat{\gamma}(s)$ is the Laplace transform of the damping kernel and

$$I(t) = \int_0^t dt' G(t'). \tag{8}$$

On the other hand, the velocity $\dot{X}(t)$ satisfies that

$$\dot{X}(t) = \langle \dot{X}(t) \rangle + \int_0^t dt' g(t-t') F(t'), \tag{9}$$

where

$$\langle \dot{X}(t) \rangle = v_0 g(t) - \omega^2 x_0 G(t), \tag{10}$$

and the relaxation function $g(t)$ is the derivative of $G(t)$, i.e.,

$$g(t) = G'(t). \tag{11}$$

As in the free particle case [11], one can demonstrate that the relaxation function $g(t)$ is related with the long-time behavior of the normalized velocity autocorrelation function (VACF) $C_v(t)$ as [12]

$$C_v(\tau) = \lim_{t\to\infty} \frac{\langle \dot{X}(t)\dot{X}(t+\tau)\rangle}{\langle \dot{X}(t)\dot{X}(t)\rangle} = g(\tau). \tag{12}$$

On the other hand, from Eqs. (6) and (10) and taking into account the symmetry property of the correlation function and Eq. (3), one can obtain the explicit expressions of the variances

$$\beta\sigma_{xx}(t) = 2I(t) - G^2(t) - \omega^2 I^2(t), \tag{13}$$

$$\beta\sigma_{vv}(t) = 1 - g^2(t) - \omega^2 G^2(t), \tag{14}$$

$$\beta\sigma_{xv}(t) = G(t)\{1 - g(t) - \omega^2 I(t)\}, \tag{15}$$

where $\beta = 1/k_B T$.

It is well known that if the correlation function (2) is a Dirac delta function, the stochastic process is Markovian and its dynamics can be straightforwardly obtained [13]. However, if one considers a disordered or fractal environment, one must take into account that the process is non-Markovian due to the long-time correlation function behavior. The lack of characteristic length leads to a lack of characteristic time [7,14,15]. On the other hand, as a consequence of the physical limits of the fractal media, one must introduce characteristic lower and upper frequencies. Therefore, in this situation, one must consider a process with long-time tail noise characterized by a correlation function of the fluctuating force exhibiting a power-law time decay [2,16]

$$C(t) = C_0(\lambda) t^{-\lambda}. \tag{16}$$

The exponent λ can be taken as $0 < \lambda < 1$ or $1 < \lambda < 2$, which is determined by the dynamical mechanism of the physical process considered. The proportionality coefficient $C_0(\lambda)$ is independent of time, but dependent on the exponent λ.

Using the fluctuation-dissipation theorem (3), the memory kernel $\gamma(t)$ can be written as

$$\gamma(t) = \gamma_0(\lambda) t^{-\lambda}, \tag{17}$$

where $\gamma_0(\lambda) = \beta C_0(\lambda)$. Then, its Laplace transform reads

$$\hat{\gamma}(s) = \gamma_\lambda s^{\lambda-1}, \tag{18}$$

with $\gamma_\lambda = \gamma_0(\lambda)\Gamma(1-\lambda)$ being positive for $0 < \lambda < 1$ and negative for $1 < \lambda < 2$.

The kernel integral $I(t)$ is the Laplace inversion of

$$\hat{I}(s) = \frac{\hat{G}(s)}{s} = \frac{s^{-1}}{s^2 + \gamma_\lambda s^\lambda + \omega^2}, \tag{19}$$

which can be obtained using the recipes given in Ref. [17]. In this case, we get

$$I(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \omega^{2k} t^{2(k+1)} E^{(k)}_{2-\lambda,3+\lambda k}(-(\omega_\lambda t)^{2-\lambda}), \tag{20}$$

where $E_{\alpha,\beta}(y)$ is the generalized Mittag-Leffler function [18] defined by the series expansion

$$E_{\alpha,\beta}(y) = \sum_{j=0}^{\infty} \frac{y^j}{\Gamma(\alpha j + \beta)}, \quad \alpha > 0, \quad \beta > 0. \tag{21}$$

$E^{(k)}_{\alpha,\beta}(y)$ is the derivative of the Mittag-Leffler function

$$E^{(k)}_{\alpha,\beta}(y) = \frac{d^k}{dy^k} E_{\alpha,\beta}(y) = \sum_{j=0}^{\infty} \frac{(j+k)!\, y^j}{j!\,\Gamma(\alpha(j+k)+\beta)}, \tag{22}$$

and ${\omega_\lambda}^{2-\lambda} = |\gamma_\lambda|$.

The kernels $G(t)$ and $g(t)$ can be calculated using the relation [17]

$$\frac{d}{dt}(t^{\alpha k+\beta-1} E^{(k)}_{\alpha,\beta}(-\gamma t^\alpha)) = t^{\alpha k+\beta-2} E^{(k)}_{\alpha,\beta-1}(-\gamma t^\alpha) \tag{23}$$

to give

$$G(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \omega^{2k} t^{2k+1} E^{(k)}_{2-\lambda,2+\lambda k}(-(\omega_\lambda t)^{2-\lambda}) \tag{24}$$

and

$$g(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} (\omega t)^{2k} E^{(k)}_{2-\lambda,1+\lambda k}(-(\omega_\lambda t)^{2-\lambda}). \tag{25}$$

It is worth mentioning that expressions (20), (24), and (25) fully determine the temporal evolution of the mean values (6) and (10), variances (13)–(15), and velocity autocorrelation function (12).

On the other hand, taking the limit $\omega \to 0$ in Eqs. (20), (24), and (25), we reobtain the solutions for the free particle, previously obtained in Refs. [19–21]. In this case, we get

$$I(t) = t^2 E_{2-\lambda,3}(-(\omega_\lambda t)^{2-\lambda}), \tag{26}$$

$$G(t) = t E_{2-\lambda,2}(-(\omega_\lambda t)^{2-\lambda}), \tag{27}$$

$$g(t) = E_{2-\lambda}(-(\omega_\lambda t)^{2-\lambda}), \quad (28)$$

where $E_\alpha(y)$ denotes the Mittag-Leffler function [18] defined through the series

$$E_\alpha(y) = E_{\alpha,1}(y) = \sum_{j=0}^{\infty} \frac{y^j}{\Gamma(\alpha j + 1)}, \quad \alpha > 0. \quad (29)$$

Let us analyze the asymptotic behavior of the kernels $I(t)$, $G(t)$, and $g(t)$. Introducing the long-time limit of the generalized Mittag-Leffler function [17]

$$E_{\alpha,\beta}(y) \sim [y\Gamma(\beta-\alpha)]^{-1} \quad (30)$$

in (20), using (22) and after some computations, one gets that for $\omega_\lambda t \gg 1$ the asymptotic behavior for $I(t)$ reads

$$I(t) \approx -\frac{1}{\omega^2}\left\{E_\lambda\left(-\left(\frac{\omega}{\omega_\lambda}\right)^2(\omega_\lambda t)^\lambda\right) - 1\right\}. \quad (31)$$

Then, from (8) and (11) we get

$$G(t) \approx -\frac{1}{\omega^2}\frac{d}{dt}E_\lambda\left(-\left(\frac{\omega}{\omega_\lambda}\right)^2(\omega_\lambda t)^\lambda\right), \quad (32)$$

and

$$g(t) \approx -\frac{1}{\omega^2}\frac{d^2}{d^2 t}E_\lambda\left(-\left(\frac{\omega}{\omega_\lambda}\right)^2(\omega_\lambda t)^\lambda\right). \quad (33)$$

Moreover, using the asymptotic behavior at large y of the Mittag-Leffler function [22]

$$E_\alpha(y) \sim [y\Gamma(1-\alpha)]^{-1} \quad (34)$$

in Eqs. (31)–(33), the asymptotic behavior of the kernels $I(t)$, $G(t)$, and $g(t)$ (i.e., $\omega \gtrsim \omega_\lambda$) can be written as

$$I(t) \approx \frac{1}{\omega^2} - \frac{\omega_\lambda^{2-\lambda}}{\omega^4}\frac{\sin(\lambda\pi)}{\pi}\frac{\Gamma(\lambda)}{t^\lambda}, \quad (35)$$

$$G(t) \approx \frac{\omega_\lambda^{2-\lambda}}{\omega^4}\frac{\sin(\lambda\pi)}{\pi}\frac{\Gamma(\lambda+1)}{t^{\lambda+1}}, \quad (36)$$

$$g(t) \approx -\frac{\omega_\lambda^{2-\lambda}}{\omega^4}\frac{\sin(\lambda\pi)}{\pi}\frac{\Gamma(\lambda+2)}{t^{\lambda+2}}, \quad (37)$$

where we use the fact that [17]

$$\Gamma(\lambda)\Gamma(1-\lambda) = \frac{\pi}{\sin(\lambda\pi)}, \quad \lambda \neq 0,1,2. \quad (38)$$

Substitution of the asymptotic expansions (35)–(37) into Eqs. (6) and (10) allows us to obtain the long-time behavior of the mean displacement $\langle X(t)\rangle$ and the mean velocity $\langle \dot{X}(t)\rangle$, which can be written as

$$\langle X(t)\rangle \approx \frac{\omega_\lambda^{2-\lambda}}{\omega^2}\frac{\sin(\lambda\pi)}{\pi}\left\{x_0\frac{\Gamma(\lambda)}{t^\lambda} + \frac{v_0}{\omega^2}\frac{\Gamma(\lambda+1)}{t^{\lambda+1}}\right\}, \quad (39)$$

$$\langle \dot{X}(t)\rangle \approx -\frac{\omega_\lambda^{2-\lambda}}{\omega^2}\frac{\sin(\lambda\pi)}{\pi}\left\{x_0\frac{\Gamma(\lambda+1)}{t^{\lambda+1}} + \frac{v_0}{\omega^2}\frac{\Gamma(\lambda+2)}{t^{\lambda+2}}\right\}. \quad (40)$$

On the other hand, substitution of these asymptotic expansions into Eqs. (13)–(15) give the long-time behavior of the variances of the process. Hence,

$$\beta\sigma_{xx}(t) \approx \frac{1}{\omega^2} - \frac{\omega_\lambda^{2(2-\lambda)}}{\omega^6}\frac{\sin^2(\lambda\pi)}{\pi^2}\frac{\Gamma(\lambda)^2}{t^{2\lambda}}, \quad (41)$$

$$\beta\sigma_{vv}(t) \approx 1 - \frac{\omega_\lambda^{2(2-\lambda)}}{\omega^6}\frac{\sin^2(\lambda\pi)}{\pi^2}\frac{\Gamma(\lambda+1)^2}{t^{2(\lambda+1)}}, \quad (42)$$

$$\beta\sigma_{xv}(t) \approx \frac{\omega_\lambda^{2(2-\lambda)}}{\omega^6}\frac{\sin^2(\lambda\pi)}{\pi^2}\frac{\Gamma(\lambda)\Gamma(\lambda+1)}{t^{2\lambda+1}}. \quad (43)$$

The variances decay as a power law in contrast with the exponential equilibrium rate in normal diffusive regime. Moreover, as opposed to the free particle diffusion, the variance of the displacement approaches its equilibrium value due to the confining potential.

Finally, taking into account (12) and (37), the long-time behavior of the velocity autocorrelation function behaves as

$$C_v(t) \approx -\frac{\omega_\lambda^{2-\lambda}}{\omega^4}\frac{\sin(\lambda\pi)}{\pi}\frac{\Gamma(\lambda+2)}{t^{\lambda+2}}. \quad (44)$$

From Eq. (44), one realizes that the velocity autocorrelation function decays with a positive power-law tail for $1<\lambda<2$. This fact implies that the particle is more likely to move always in the same direction. However, when $0<\lambda<1$, the $C_v(t)$ function decays with a long negative tail. This negative correlation was called the whip-back effect [2,23,24] in the frame of the free particle situation. This behavior implies that if the particle moves in the positive direction at this instant, it is more likely to move in the negative direction in the next instant. This effect is responsible for the slower diffusion of the particle (subdiffusion).

This work was performed under PICT Grant No. 8450 from the Agencia Nacional de Promoción Científíca y Tecnológica, FONCYT, Argentina.

[1] J. P. Bouchaud and A. Georges, Phys. Rep. **195**, 127 (1990).
[2] K. G. Wang, Phys. Rev. A **45**, 833 (1992).
[3] A. Bunde, S. Havlin, J. Klafter, G. Graff, and A. Shehter, Phys. Rev. Lett. **78**, 3338 (1997).
[4] R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).
[5] F. Amblard, A. C. Maggs, B. Yurke, A. N. Pargellis, and S. Leibler, Phys. Rev. Lett. **77**, 4470 (1996).
[6] Q. Gu, E. A. Schiff, S. Grebner, F. Wang, and R. Schwarz, Phys. Rev. Lett. **76**, 3196 (1996).
[7] F. Sciortino and P. Tartaglia, Physica A **236**, 140 (1997).

[8] J. Stephenson, Physica A **222**, 234 (1995).
[9] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II. Non-Equilibrium Statistical Mechanics* (Springer, Berlin, 1985).
[10] K. G. Wang and M. Tokuyama, Physica A **265**, 341 (1999).
[11] J. M. Porra, K. G. Wang, and J. Masoliver, Phys. Rev. E **53**, 5872 (1996).
[12] A. D. Viñales and M. A. Despósito (unpublished).
[13] H. Risken, *The Fokker-Plank Equation* (Springer-Verlag, Berlin, 1989).
[14] J. A. White and S. Velasco, Phys. Rev. A **46**, 1880 (1992).
[15] S. Velasco and J. A. White, Phys. Rev. A **46**, 8015 (1992).
[16] A. D. Viñales and M. A. Despósito (unpublished).
[17] I. Podlubny, *Fractional Differential Equations* (Academic Press, London, 1999).
[18] A. Erdelyi *et al.*, *Higher Transcendental Functions* (Krieger, Malabar, 1981), Vol. 3.
[19] E. Lutz, Phys. Rev. E **64**, 051106 (2001).
[20] R. Kupferman, J. Stat. Phys. **114**, 291 (2004).
[21] N. Pottier, Physica A **317**, 371 (2003).
[22] F. Mainardi and R. Gorenflo, J. Comput. Appl. Math. **118**, 283 (2000).
[23] R. Muralidhar *et al.*, Physica A **167**, 539 (1990).
[24] E. Lutz, Europhys. Lett. **54**, 293 (2001).