Different diffusive regimes, generalized Langevin and diffusion equations

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We investigate a generalized Langevin equation (GLE) in the presence of an additive noise characterized by the mixture of the usual white noise and an arbitrary one. This scenario lead us to a wide class of diffusive processes, in particular the ones whose noise correlation functions are governed by power laws, exponentials, and Mittag-Leffler functions. The results show the presence of different diffusive regimes related to the spreading of the system. In addition, we obtain a fractional diffusion-like equation from the GLE, confirming the results for long time.

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I. INTRODUCTION

Since Richardson’s work in 1926 [1], a large number of observations related to anomalous diffusion [2–6] have been reported in several fields of science, for instance, brain studies [7,8], social systems [9], biological cells [10,11], animal foraging behavior [12], nanoscience [13,14], and geophysical systems [15,16]. One of the main aspects of these situations is the anomalous spreading of the system or the unusual behavior of the correlation functions, which may be related to the non-Markovian nature of the stochastic process present in these systems. In this context, a typical behavior for the mean square displacement is \((\langle x(0) - x(t) \rangle^2) \propto t^\alpha\), where \(\alpha < 1\) and \(\alpha > 1\) correspond to the sub- and superdiffusive cases and \(\alpha = 1\) refers to the usual case. For processes governed by Lévy distributions, this quantity is not finite. Situations with different diffusive regimes are also possible and can be verified in biological systems [17–19], motion of colloidal particles [20], systems with long-range interactions [21,22], and adsorption-desorption process [23–25]. These situations have been investigated by using several approaches, such as nonlinear diffusion equations [26], fractional diffusion equations [27–30], random walks [31,32], and generalized Langevin equations (GLE) [33–36], which can be connected to a fractional diffusion equation [37]. From the previous discussion, we observe the relevance of these diffusion processes and, consequently, the formalisms employed to describe them. It is also important to point out that to know the physical mechanisms behind these processes lead us to the suitable approach to describe them. In this sense, recent and valuable discussions concerning this theme can be found in Refs. [38,39].

Here, we address this work to investigate a GLE by considering a large class of noise correlation functions, which may be used as a powerful tool to investigate several physical systems. For example, stochastic dynamics of non-Markovian processes present in several scenarios such as nuclear fusion reactions [40] where the nonlocality on time induces a memory effect in the particle velocity, anomalous polymer dynamics [41] connected to the mean relaxation of the polymer to local strains, viscoelastic media [42], nonexponential decay of the distribution of waiting times between successive turnovers of a single enzyme molecule [43], diffusion over a fluctuating barrier [44], quantum system with nonstationary coupling [45], and in the subdiffusion within a single protein molecule [46].

We start by considering two additive noises in the Langevin equation: a white noise and another one with the correlation function given by a power law. This choice is very interesting and leads us to a situation characterized by different diffusive regimes. One of them is the usual diffusion and the other, connected to anomalous diffusion, depends on the power law considered. A typical situation where this GLE with this additive noise can find application is in the investigation of the electrical response of the systems described in Ref. [47], which are characterized by different diffusive regimes. In the same context, the electrical response of the water [48] may be described in terms of the GLE used here, since the fractional diffusion equation used in Ref. [48] can be obtained from it by suitable considerations. After, we consider a noise with a general correlation function, instead of the power law. By using this development, the sum of white and Mittag-Leffler correlated noises is also investigated. In addition, based on the approach proposed in Ref. [37], we obtain a diffusion-like equation corresponding to the GLE and, by means of the mean square displacement, we show that these approaches are equivalent when long time scales are considered. These results may be connected to fractional diffusion equations [27–30], situations characterized by a finite collision time, and non-Markovian processes. We present these developments in Secs. II and III. The last section, i.e., Sec. IV, is devoted to the discussions and conclusions.

II. GENERALIZED LANGEVIN EQUATION

Let us start our analysis by considering a GLE in the absence of a deterministic field. For this case, it can be expressed in the following form:

\[ \ddot{x}(t) + \int_0^t dt' \zeta(t-t') \dot{x}(t') = \tilde{\xi}(t), \]

(1)

which is a nonlocal equation, where the mass is considered unitary (without loss of generality), \(\zeta(t - t')\) is the dissipative memory kernel related to a fractional force, and \(\tilde{\xi}(t)\) is a random force (noise source) with zero mean \(\langle \tilde{\xi}(t) \rangle = 0\). If the system described by Eq. (1) is in thermal equilibrium (the case
considered here), the relationship between these microscopic forces is given by the fluctuation-dissipation theorem [33]:

\[
\langle \xi(t)\xi(t') \rangle = C(|t - t'|) = k_B T \xi(|t - t'|),
\]

where \( k_B \) is the Boltzmann constant, \( T \) is the absolute temperature of the system, and \( C(|t - t'|) \) is the noise correlation function. For a white noise (uncorrelated noise), the correlation function is given by a Dirac delta function and for colored noises (correlated noise) it may be expressed, for example, in terms of exponential functions [49], power laws [50], and Mittag-Leffler functions [51,52].

Aiming to investigate some aspects of Eq. (1), i.e., the behavior of its solutions, and how it is possible to get different diffusive behaviors from Eq. (1), subjected to the initial conditions \( x(0) = x_0 \) and \( \dot{x}(0) = v_0 \), we first consider the sum of two distinct random forces: \( \tilde{\xi}(t) = \alpha \xi(t) + \beta \eta(t) \), where \( \xi(t) \) and \( \eta(t) \) are stochastic variables with zero mean and correlation functions given by [34]

\[
\langle \xi(t)\xi(t') \rangle = A\delta(t - t'),
\]

\[
\langle \eta(t)\eta(t') \rangle = B|t - t'|^\gamma,
\]

with \( \langle \xi(t)\eta(t') \rangle = 0 \), where \( A \) and \( B \) are non-negative parameters and \( 0 < \gamma < 1 \). In order to satisfy the fluctuation-dissipation theorem, we have that

\[
a^2\langle \xi(t)\xi(t') \rangle + \beta^2\langle \eta(t)\eta(t') \rangle = k_B T \xi(|t - t'|)\xi(|t - t'|).
\]

Note that Eq. (1) is linear for \( x(t) \). However, the solution of Eq. (1) with \( \tilde{\xi}(t) = \alpha \xi(t) + \beta \eta(t) \) is not equal to the sum of the solutions for \( \xi(t) = \alpha \tilde{\xi}(t) \) and \( \tilde{\xi}(t) = \beta \eta(t) \) considered separately. In addition, Eqs. (3) and (4) incorporated in Eq. (5) lead us to a mixture of the usual and the anomalous cases. A direct consequence of this mixture is the presence of different diffusive regimes depending on the time scale considered.

Similar choices, characterized by different diffusive regimes, have been applied to describe the single-file diffusion [53–55] (one-dimensional motion of interacting particles in pores that are so narrow that the mutual passage of particles is excluded [56]) and can be used to investigate the electrical response of the systems such as those worked out in Refs. [47,48]. In particular, for single-file diffusion, the presence of the non-Gaussian noise source is related to the mechanism of subdiffusion, i.e., the collisional interaction between the file components which leads to long-range correlations or memory effects.

In our analysis about diffusive processes and Langevin equations, we have to solve Eq. (1) and investigate the mean square displacement related to the variable \( x \). In this direction, we apply the Laplace transform in Eqs. (1) and (5) to simplify our calculations. Therefore, we obtain that

\[
x(s) = \langle x(s) \rangle x_0 + v_0 \hat{G}(s) + \tilde{\xi}(s)\hat{G}(s),
\]

with

\[
\hat{G}(s) = \frac{1}{s^2 + \zeta^2(s)}
\]

and \( \zeta(s) = \tilde{\Lambda} + \tilde{B}s^{\gamma-1} \), where \( \tilde{\Lambda} = \alpha^2 \tilde{A}/k_B T \) and \( \tilde{B} = \beta^2 \tilde{B}/k_B T \). The inverse Laplace transform lead us to

\[
x(t) = \langle x(t) \rangle + \alpha \int_0^t dt'\xi(t'G(t-t')) + \beta \int_0^t dt'\eta(t')G(t-t'),
\]

with \( \langle x(t) \rangle = v_0\hat{G}(t) + x_0 \) and the inverse Laplace transform of \( \hat{G}(s) \) given by

\[
\hat{G}(t) = \sum_{n=0}^{\infty} \frac{t}{(1+n)!} (-\tilde{B}t^{-\gamma})^n E_{\gamma,\beta}^{(n)}(-\tilde{\Lambda}t),
\]

where \( \tilde{\alpha} = 1 \) and \( \tilde{\beta} = 2 + (2 - \gamma)n \). The function \( E_{\gamma,\beta}(x) \) represents the generalized Mittag-Leffler function, whose definition is given by

\[
E_{\gamma,\beta}(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(\beta + \alpha n)},
\]

with \( \tilde{\beta} > 0 \) and \( \tilde{\alpha} > 0 \). The asymptotic limit of \( E_{\gamma,\beta}(x) \) for \( x \rightarrow \infty \) is given by \( E_{\gamma,\beta}(x) \sim -1/[\Gamma(\tilde{\beta} - \tilde{\alpha}x)] \). The presence of its derivative of the order \( n \), i.e., \( E_{\gamma,\beta}(x) \equiv d^n E_{\gamma,\beta}(x)/dx^n \) [57], in \( G(t) \) indicates that the relaxation is not unique. This feature can be verified by analyzing the asymptotic limit of \( \hat{G}(s) \), which lead us to a power-law behavior instead of an exponential one.

By using these equations, it is possible to find the behavior of the mean square displacement for the \( x \) variable. In fact, performing some calculations, it is possible to show that [52]

\[
\sigma^2_x(t) = 2\tilde{\tau}(t) - \tilde{G}^2(t),
\]

with \( \tilde{\tau}(t) = \int_0^t dt' G(t') \) and \( k_B T = 1 \) (without loss of generality). The time-dependent behavior manifested by Eq. (11) provides information about the spreading of the system governed by Eq. (1). The presence of different diffusive regimes may be verified by analyzing the time-dependent behavior of Eq. (11). In fact, the behavior of Eq. (11) can be approximated to

\[
\sigma^2_x \approx \frac{2\tilde{\tau}}{3} t^3 + (3 - \gamma) \frac{2\tilde{B}t^4 - \gamma}{\Gamma(5 - \gamma)}
\]

for small times \( (t < (3/2\tilde{A}))^{1/3} \),

\[
\sigma^2_x \approx \frac{2\tilde{\tau}}{\tilde{A}}
\]

for intermediate times \( (3/2\tilde{A})^{1/3} < t < (\tilde{A}/[\Gamma(1 + \gamma)\tilde{B}])^{1/(1-\gamma)} \), and

\[
\sigma^2_x \approx \frac{2\tilde{\tau}^{1-\gamma}}{\Gamma(1 + \gamma)\tilde{B}}
\]

for long times \( (\tilde{A}/[\Gamma(1 + \gamma)\tilde{B}])^{1/(1-\gamma)} \ll t < \infty \). These approximations were obtained by considering \( \tilde{B} < \tilde{\Lambda} \). For the cases where this condition is not verified, the intermediated regime is not evidenced as in the previous case. This feature can be verified when comparing Fig. 1 with Fig. 2. In this situation, the more convenient approximation to cover intermediate and long times is given by the following equation:

\[
\sigma^2_x \approx \frac{2\tilde{\tau}}{\tilde{A}} E_{2,1-\gamma}(-\frac{\tilde{B}}{\tilde{A}} t^{1-\gamma}).
\]

These asymptotic behaviors show us that the spreading of the solution has different diffusive behaviors. In Fig. 1, we illustrate the behavior of \( \sigma^2_x(t) \) obtained from Eq. (11), as well as the asymptotic expansions. Notice also that the first term in Eq. (12) is not governed by the values of \( \gamma \) if \( 0 < \gamma < 1 \), in
contrast with Eq. (13), which has a strong dependence on $\gamma$. In particular, it is interesting to note that the behavior obtained for Eq. (12) is the same founded in the usual scenario, i.e., in absence of nonwhite noise ($B = 0$) and for short time. In Fig. 2, we consider $\bar{A} > \bar{B}$ to illustrate the presence of an intermediate regime governed by the usual white noise. This figure also shows that the system may present different diffusive regimes depending on the noises incorporated in the Langevin equation. The crossover time, $t_c$, between the different regimes can be estimated from the mean square displacement by considering the asymptotic results. In this sense, the first crossover time occurs at $t_c^{(1)} \sim \sqrt{3}/\bar{A}$ and the second one at $t_c^{(2)} \sim [\bar{A}/(\Gamma(1+\gamma)\bar{B})]^{1/(1-\gamma)}$.

It is possible to consider other forms for Eq. (16), leading us to different diffusive processes which may be related to different diffusive regimes. In this direction, we extend one of these equations by considering an arbitrary correlation, i.e.,

$$\langle \eta(t)\eta(t') \rangle = B^\gamma \Upsilon(|t-t'|),$$

where $\Upsilon(|t|)$ is a time-dependent function that has Laplace transform defined. In general, $\Upsilon(|t|)$ enables us to connect Eq. (16) with correlation functions governed by exponentials, power-law, Mittag-Leffler, and other functions depending on the process considered. The main change produced in the previous results, by considering Eq. (16) instead of Eq. (4), is in Eq. (7). After some calculations using Eq. (16), we have that

$$\mathcal{G}(s) = \frac{1}{s^2 + s(\bar{A} + \bar{B}\Upsilon(s))},$$

which has as inverse Laplace transform,

$$\mathcal{G}(t) = \frac{1}{\bar{A}}(1 - e^{-\bar{A}t}) + \sum_{n=1}^{\infty} \frac{(-\bar{B})^n}{\Gamma(1+n)} \int_0^t dt' t'^{n+1} E_{1,2}(-\bar{A}t') \Upsilon_n(t-t'),$$

where

$$\Upsilon_n(t) = \int_0^t dt_n \Upsilon(t-t_n) \int_0^{t_n} dt_{n-1} \Upsilon(t_{n-1}) \cdots \int_0^{t_1} dt_1 \Upsilon(t_2-t_1) \Upsilon(t_1).$$

Note that, for $\bar{B}$ sufficiently small, the sum in Eq. (18) could be truncated at a given order in $\bar{B}$ to obtain an approximated solution. This procedure resembles a perturbation development in the sense that the solution of the GLE can be grouped in powers of $\bar{B}$.

Another interesting choice for Eq. (16) is to consider $\Upsilon(|t|) = E_\gamma(-|t|/\tau) / \tau^\gamma$ ($\tau$ is a characteristic time) (see also Refs. [51,52]) because it has two asymptotic behaviors: a stretched exponential one for short times and a power-law one for long times. These two different behaviors imply in different diffusive regimes, which can be related to anomalous...
diffusion. After substituting this colored noise into Eq. (18) and performing some calculations, we obtain that
\[ \mathcal{G}(t) = \frac{1}{A} (1-e^{-\tilde{A}t}) + \sum_{n=1}^{\infty} \left( \frac{-\tilde{B} t^n}{\Gamma(1+n)} \right) \int_0^t \int_0^{t'} e^{-\tilde{A}t'} \Delta_n(t-t'), \]
with
\[ \Delta_n(t) = \frac{t^n}{\tau^n} \left[ E_{\gamma,n}(t') - t' \right] + \frac{t^n}{\tau^n} E_{\gamma+1,n}(t') - \frac{t^n}{\tau^n} \right] \]
and \( v = 1 + (1 - \gamma)n \). The regimes and the influence of the noise on the solution obtained can be evidenced by analyzing the asymptotic behaviors for short and long times of Eq. (20).

In this direction, it is possible to show that
\[ \mathcal{G}(t) \approx t - \frac{1}{2} \tilde{A} t^2 + \frac{1}{6 \gamma} \tilde{A}^2 \frac{t^3}{\tau^3} - \tilde{B} t^3 \]
for short times and
\[ \mathcal{G}(t) \approx t + \sum_{n=0}^{\infty} \frac{1}{\Gamma(1+n)} \left( \frac{-\tilde{B} t^{2-\gamma} n}{\tau^{2-\gamma}} E_{\gamma,n}(t) - \tilde{A} t^3 \right) \]
for long times, with \( \tau = 2 + (1 - \gamma)n \). Notice again that, for short times, the relaxation process is not dominated by the \( \gamma \) values. On the other hand, the \( \gamma \) value plays an important role for long times.

### III. DERIVATION OF A DIFFUSIONLIKE EQUATION

Now, we dedicate this section to derive a generalized diffusionlike equation associated with the GLE based on the approach proposed by Khan and Reynolds [37]. In this sense, we start by considering the following generalized Kramers diffusionlike equation associated with the GLE based on the diffusion. After substituting this colored noise into Eq. (18) with \( \mathcal{G}(t) \), this equation is
\[ \frac{\partial^2 W}{\partial t^2} + \tilde{A} \frac{\partial W}{\partial t} + \tilde{B} \int_0^t d t' \gamma(t-t') \frac{\partial W}{\partial t'} = \frac{\partial^2}{\partial x^2} (W^2). \] (27)

Depending on the choice of \( \gamma(t) \) and the time scale considered, this equation may be connected to several cases, such as the fractional diffusion equations [28,30] and fractional diffusion equation of distributed order [60]. In particular, Eq. (27) can be considered as an extension of the Cattaneo equation; other extensions can be found in Ref. [61]. In this sense, it can be related to situations with finite collision time, which is not present in the usual diffusion equation. Indeed, the usual diffusion equation is an approximation valid only for time scales that are large enough when compared to the time scale related to the microscopic collisions. As pointed out in Ref. [62], one of the most striking nonphysical properties of the standard diffusion equation is an infinite velocity of information propagation. However, the inclusion of the finite collision frequency in the system may create additional difficulties to treat the problem; an approximation that makes the problem more tractable is discussed by Bourret [63] and may lead to an integral equation similar to Eq. (27) with a correlation function in the kernel [64]. In addition, it is interesting to note that Eq. (27) may also be connected to the situations discussed in Refs. [65–67], which are essentially non-Markovian.

By using Eq. (27), a generalized diffusionlike equation related to the GLE with two additive noises can be obtained when Eqs. (3), (5), and (16) are considered. It is given by
\[ \frac{d^2 W}{dt^2} + \tilde{A} \frac{d W}{dt} + \tilde{B} \int_0^t d t' \gamma(t-t') \frac{d W}{d t'} = \frac{d^2}{d x^2} (W^2) \] (28)
(\( \tilde{A} = \alpha^2 A/k_B T \) and \( \tilde{B} = \beta^2 B/k_B T \)). This equation presents different diffusive regimes depending on the time scale considered; a similar situation is found in Ref. [61]. These different behaviors can be verified by analyzing the mean square displacement (or the second moment depending on the initial condition), which is a measure of the spreading of the system. With this purpose, by multiplying Eq. (28) by \( x^2 \) and integrating it with respect to \( x \) variable, we have that
\[ \frac{d^2}{dx^2} \langle x^2(t) \rangle + \tilde{A} \frac{d}{dt} \langle x^2(t) \rangle + \tilde{B} \int_0^t d t' \gamma(t-t') \frac{d}{dt'} \langle x^2(t') \rangle \]
\[ = 2 \langle v^2 \rangle(t), \] (29)
where \( \langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 W dx \) and \( \langle v^2 \rangle(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v^2 \rho(x,v,t) dv dx \). Note that, to obtain \( \langle x^2 \rangle \), we need to know the time dependence of \( \langle v^2 \rangle \). However, we are interested in the behavior of Eq. (28) for long times, i.e., when it can be connected to a fractional diffusion equation of distributed order for a suitable choice of \( \gamma(t) \). In order to cover this scenario, we approximate \( \langle v^2 \rangle \) to a constant, i.e., \( \langle v^2 \rangle \approx D \). Applying the Laplace transform with \( \langle x(0) \rangle = 0 \), it is possible to obtain the second
D = Eqs. (11) and (32) have a different behavior due to the approximations the straight red line is the GLE approach. Note that, for small times, square displacement $\langle x^2 \rangle \sim t$. After some calculations, we obtain

$$\sigma^2_t = 2D \sum_{n=0}^{\infty} \frac{t^n}{\Gamma(1+n)} (-\bar{B}t^{2-\gamma})^n E_{\alpha,\beta}^{(n)}(-\bar{A}t),$$  

(32)

where $\bar{a} = 1$ and $\bar{B} = n(1-\gamma) + 3$. In Fig. 3, we compare this result with the one found in the GLE approach by plotting Eqs. (11) and (32). As we can see, this figure shows a good agreement between Eqs. (11) and (32) when long times are considered, as expected from the previous discussion. In particular, the asymptotic limits for Eq. (32) are $\sigma^2_t \sim 2(1-\bar{A}t/3)$ for short times, $\sigma^2_t \sim 2(1-\bar{A}t/\bar{A})$ for intermediate times, and $\sigma^2_t \sim 2(1-\bar{A}t/\gamma \bar{B})$ for long times. Notice that Eqs. (11) and (32) are proportional to $t$ for intermediate times and to $t^\gamma$ for long times when $\bar{B} < \bar{A}$. This fact is a consequence of the presence of the usual and power-law relaxations in the system; the last one is evidenced by the presence of the generalized Mittag-Leffler functions.

**IV. SUMMARY AND CONCLUSIONS**

We have investigated a Langevin equation by taking additive noises into account. In particular, different diffusive regimes may be manifested depending on the time scale considered. This feature is evidenced when the Langevin equation is analyzed by incorporating the sum of two noises, one of them being white. Furthermore, since any noise can be decoupled as a sum of two others, this approach may be viewed as a kind of perturbative approach, where the nonwhite noise is considered as a perturbation. After this, we have analyzed the diffusionlike equations that are related to these Langevin equations by using the procedure present in [37]. The diffusion equation also manifests, similar to the Langevin equation, different diffusive regimes. In addition, we verify that the spreading, for an initial condition obtained for this diffusion equation, is equivalent to the Langevin equation when long times are considered. Finally, we hope that the results presented here can be useful to investigate situations related to anomalous diffusion.

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