Velocity autocorrelation of a free particle driven by a Mittag-Leffler noise: Fractional dynamics and temporal behaviors

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We investigate the dynamical phase diagram of the generalized Langevin equation of the free particle driven by a Mittag-Leffler noise and show critical curves and a critical value of the exponent parameter of the Mittag-Leffler function that mark different dynamical regimes. By considering that the modeling of a Mittag-Leffer memory kernel corresponds to a power-law second-order memory kernel, we show that the generalized Langevin equation of the velocity autocorrelation function (VACF) is transformed in a fractional Langevin equation. In the superdiffusive case our results exhibit oscillations and negative correlations of the VACF that are not provided by the usual power-law noise model.

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I. INTRODUCTION

The study of anomalous diffusion in a complex or disordered medium has achieved a substantial progress during the last years [1–9]. Anomalous diffusion in physical and biological systems can be formulated in the framework of the generalized Langevin equation (GLE) [1,2,8,10–19]. If one considers the dynamics of a particle under the influence of a random force modeled as Gaussian colored noise, the corresponding GLE is written as [12,13,20]

$$\dot{v}(t) + \int_0^t dt' \gamma(t - t') v(t') = \xi(t),$$
(1)

where v(t) represents the velocity of a particle of mass m = 1 at time t, and $\gamma(t)$ is the frictional memory kernel. The random force $\xi(t)$ is a zero centered and stationary Gaussian that obeys the fluctuation-dissipation theorem [21,22],

$$\langle \xi(t)\xi(t')\rangle = C(|t-t'|) = k_B T \gamma(|t-t'|),$$
 (2)

where k_B is the Boltzmann constant, and *T* is the absolute temperature of the environment.

It is now well established that the physical origin of anomalous diffusion is related to the long-time tail correlations [1-3]. Therefore, in order to model the anomalous diffusion process, pure power-law correlation functions are usually employed [1,2,11,13,20,23,24].

The GLE with a power-law-type memory kernel is very useful for modeling anomalous diffusion processes; however, the corresponding power-law correlated noises have some nonphysical properties like absence of a characteristic memory time and infinite variance.

In Ref. [25] a more general noise whose correlation is proportional to a Mittag-Leffler function was introduced. Remarkably, for certain values of the parameters that characterize this noise, one can reproduce a power-law correlation function, a standard Ornstein-Uhlenbeck noise with an exponential one, and a white noise. This correlation behaves as a power law for large times, but is nonsingular at the origin due to the inclusion of a characteristic time and as a consequence has finite variance. Some applications of a generalized Langevin equation with a Mittag-Leffler noise can be seen in [26–28]. In [28], the anomalous diffusive behavior of a harmonic oscillator driven by a Mittag-Leffler noise is studied, and the results for free particle given in [25] are recovered as the limit case.

The normalized velocity autocorrelation function (VACF) is defined as

$$C_{v}(t) = \frac{\langle v(t)v(0) \rangle}{\langle v(0)^{2} \rangle}.$$
(3)

This function is an important quantity that can be measured in the laboratory and from which it is possible to obtain experimentally the physical properties of the system, in particular, information about the diffusive behavior [29,30].

Although the VACF of a free particle driven by a Mittag-Leffler noise was obtained analytically in [25] [see relaxation function g(t) given by Eqs. (32) and (33)], its practical use from a numerical point of view is limited because it is expressed as an infinite double series with high-order derivatives of Mittag-Leffler functions. On the other hand, the detailed study of the temporal behavior of the VACF is still missing in the literature. This is quite surprising given the relevance of colored noise and viscoelasticity for biological systems. In this way, our main purpose in this paper is to investigate the dynamical effects of the Mittag-Leffler noise on a free particle governed by the GLE (1) making use of an effective approach based in a hierarchical relationship between memory kernels. Remarkably, this approach turns out to be a valuable method that allows us, among other dynamics characteristics, to investigate the dynamical phase diagram obtaining critical curves and a critical value of the exponent parameter of the Mittag-Leffler function that mark different dynamical regimes in the behavior of the system.

We first began with a generalized Langevin equation for the VACF with a memory kernel $\gamma(t)$. In turn, we assume that $\gamma(t)$ satisfies a generalized Langevin equation with a memory kernel $\eta(t)$ that plays the role of a second-order memory kernel. In particular, we show that if the memory kernel $\gamma(t)$

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is a Mittag-Leffler function, then the second-order memory kernel $\eta(t)$ is a power-law function. From this relationship, a fractional Langevin equation of the VACF for the superdiffusive case can be obtained, which is formally the same as that corresponding to the normalized position autocorrelation function of a particle harmonically bounded in the subdiffusive case. The solution in the last case is a known matter in the literature [31,32]. As a consequence of this approach we found that-for the superdiffusive case-the VACF may exhibit different types of relaxations and oscillations depending on the values of the noise parameters. We show the existence of critical curves that mark different dynamical regimes in the behavior of the VACF. In addition, we determine a critical value of the exponent parameter of Mittag-Leffler noise and the phase diagrams that define the different dynamical behavior. This paper is organized as follows. In Sec. II, we show that there exists a correspondence between the VACF of a free particle driven by a noise with the memory kernel $\gamma(t)$ and the autocorrelation position of a harmonic oscillator driven by a noise with the memory kernel $\eta(t)$. In Sec. III we discuss some characteristics of the Mittag-Leffler noise. In Sec. IV, we obtain the analytical expression of the VACF for a free particle driven by a Mittag-Leffler noise using the correspondence described in Sec. II. In Sec. V we obtain the temporal limits behavior of the VACF, and in Sec. VI we derive the temporal behavior of the VACF in the superdiffusive case obtaining a phase diagram with critical curves and critical value of the exponent parameter of the Mittag-Leffler function that points out different dynamical behaviors. The conclusions are presented in Sec. VII. Finally, the appendixes deal with the analytical expression of the VACF for particular cases.

II. LANGEVIN EQUATION FOR THE VACF

We multiply Eq. (1) by v(0) to perform an ensemble average. Since $\langle v(0)\xi(t)\rangle = 0$, and using (3) we obtain

$$\dot{C}_{v}(t) + \int_{0}^{t} dt' \gamma(t - t') C_{v}(t') = 0.$$
(4)

Now, we assume that the memory kernel $\gamma(t)$ satisfies the Langevin equation,

$$\dot{\gamma}(t) + \int_0^t dt' \eta(t - t') \gamma(t') = 0,$$
 (5)

where the function $\eta(t)$ is called second-order memory [33,34]. In the Laplace domain, Eqs. (4) and (5) can be written as

$$\widehat{C}_{v}(s) = \frac{1}{s + \widehat{\gamma}(s)},\tag{6}$$

and

$$\widehat{\gamma}(s) = \frac{\gamma(0)}{s + \widehat{\eta}(s)},\tag{7}$$

inserting Eq. (7) in Eq. (6), we have

$$\widehat{C}_{v}(s) = \frac{s + \widehat{\eta}(s)}{s^{2} + s\,\widehat{\eta}(s) + \omega^{2}},\tag{8}$$

where we have defined $\omega^2 = \gamma(0)$. Taking the inverse of Laplace transform of (8) and considering the initial conditions

 $C_v(0) = 1$ and $\dot{C}_v(0) = 0$, the equation for $C_v(t)$ in the time domain can be written as

$$\ddot{C}_{v}(t) + \int_{0}^{t} dt' \eta(t-t') \dot{C}_{v}(t') + \omega^{2} C_{v}(t) = 0.$$
(9)

As pointed out by Bonn and Yip in [33], this last equation is quite suggestive because it reminds us of a restoring force in the medium with a characteristic frequency proportional to ω , while the integral term represents a time-dependent frictional force which is specified through $\eta(t)$. Following [33], the presence of these two kinds of forces means that the behavior of $C_v(t)$ is influenced by both, and depending on the competition between them, $C_v(t)$ will appear more solidlike or more fluidlike.

On the other hand, Eq. (8) for $\widehat{C}_{v}(s)$ can be written as

$$\widehat{C}_{v}(s) = \frac{1}{s} \frac{(s^{2} + s\widehat{\eta}(s) + \omega^{2} - \omega^{2})}{(s^{2} + s\widehat{\eta}(s) + \omega^{2})} = \frac{1}{s} - \frac{\omega^{2}s^{-1}}{s^{2} + s\widehat{\eta}(s) + \omega^{2}}.$$
 (10)

Then, the Laplace inversion produce,

$$C_v(t) = 1 - \omega^2 I(t),$$
 (11)

where I(t) is the Laplace inversion of

$$\widehat{I}(s) = \frac{s^{-1}}{s^2 + \widehat{\eta}(s)s + \omega^2}.$$
(12)

III. MITTAG-LEFFLER NOISE

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 directly obtained [35]. However, in a complex or viscoelastic environment one must take into account the memory effects through a long-time tail noise to describe the effect of the environment on the particle. The non-Markovian dynamics is involved in these physical processes.

In recent years a Mittag-Leffler noise was introduced [25],

$$C(t) = \frac{C}{\tau^{\lambda}} E_{\lambda}(-(|t|/\tau)^{\lambda}), \qquad (13)$$

where τ acts as a characteristic memory time, and C is a coefficient of proportionality independent of time. The exponent λ can be taken as $0 < \lambda < 2$, which is determined by the dynamical mechanism of the physical process considered. The $E_{\alpha}(y)$ function denotes the Mittag-Leffler function [36] defined through the following series:

$$E_{\alpha}(y) = \sum_{j=0}^{\infty} \frac{y^j}{\Gamma(\alpha j+1)}, \quad \alpha > 0.$$
(14)

Using the asymptotic behaviors of the Mittag-Leffler function [37] one can easily deduce that for $\lambda \neq 1$, the correlation function (13) behaves as a stretched exponential for short times and as an inverse power law in the long-time regime [37,38]. Setting $\lambda = 1$, the correlation function (13) is reduced to an exponential form,

$$C(t) = \frac{C}{\tau} e^{-|t|/\tau},$$
(15)

which describes a standard Ornstein-Uhlenbeck process [35]. Moreover, in the limit $\tau \to 0$ and from the limit representation of the Dirac delta [39], we get that $C(t) = 2 C \delta(t)$ corresponding to a white noise, nonretarded friction, and standard Brownian motion [35]. On the other hand, for $\lambda \neq 1$ the limit $\tau \to 0$ of the proposed correlation function (13) reproduces the power-law correlation function,

$$C(t) = C \frac{|t|^{-\lambda}}{\Gamma(1-\lambda)}.$$
(16)

This last result is obtained introducing in expression (13) the asymptotic behavior at large y of the Mittag-Leffler function [37],

$$E_{\alpha}(-y) \sim [y \Gamma(1-\alpha)]^{-1}, \quad y > 0.$$
 (17)

It is worth pointing out that the Mittag-Leffler correlation function (13) is a well-defined and nonsingular function. Its value at t = 0 is $C(0) = C/\tau^{\lambda}$, while for the power-law correlation (16) C(0) diverges. Then, the introduction of the characteristic time τ enables us to avoid the singularity of the power law at the origin.

IV. ANALYTICAL VACF FOR FREE PARTICLE DRIVEN BY A MITTAG-LEFFLER NOISE

From relation (2), the memory kernel $\gamma(t)$ corresponding to the Mittag-Leffler noise (13) can be written as

$$\gamma(t) = \frac{\gamma}{\tau^{\lambda}} E_{\lambda}(-(|t|/\tau)^{\lambda}), \qquad (18)$$

where $\gamma = C/k_BT$. The Laplace transform of the memory kernel reads [37]

$$\widehat{\gamma}(s) = \frac{\gamma s^{\lambda - 1}}{1 + s^{\lambda} \tau^{\lambda}} = \frac{\gamma(0)}{s + s^{1 - \lambda} \tau^{-\lambda}},$$
(19)

where $\gamma(0) = \frac{\gamma}{\tau^{\lambda}}$. Comparing Eqs. (19) and (7) as [34] we can deduce that

$$\widehat{\eta}(s) = s^{1-\lambda} \tau^{-\lambda}.$$
(20)

Therefore, from Eq. (12) the relaxation function I(t) can be written as the Laplace inversion of

$$\widehat{I}(s) = \frac{s^{-1}}{s^2 + \tau^{-\lambda}s^{2-\lambda} + \omega^2}.$$
(21)

Following the approach given in Ref. [40] we have

$$I(t) = \sum_{n=0}^{\infty} \frac{(-\omega^2 t^2)^n}{n!} t^2 E_{\lambda,3+(2-\lambda)n}^{(n)}(-(t/\tau)^{\lambda}), \quad (22)$$

where $E_{\alpha,\beta}(y)$ is the generalized Mittag-Leffler function [37] defined by the series expansion,

$$E_{\alpha,\beta}(y) = \sum_{j=0}^{\infty} \frac{y^j}{\Gamma(\alpha j + \beta)}, \quad \alpha > 0, \quad \beta > 0, \quad (23)$$

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

$$E_{\alpha,\beta}^{(k)}(y) = \frac{d^k}{dy^k} E_{\alpha,\beta}(y) = \sum_{j=0}^{\infty} \frac{(j+k)! \, y^j}{j! \, \Gamma(\alpha(j+k)+\beta)}.$$
 (24)

Then, from (22) and (11) we obtain

$$C_{v}(t) = 1 + \sum_{n=0}^{\infty} \frac{\left(-\omega^{2} t^{2}\right)^{n+1}}{n!} E_{\lambda,3+(2-\lambda)n}^{(n)}(-(t/\tau)^{\lambda}).$$
(25)

As a direct consequence of this approach, we get for the VACF an analytical expression as a single series, instead of the expression as sum of two series obtained in [25] for the same relaxation function derived by Laplace inversion. Moreover, in Appendixes A and B we show that for $\lambda = 1$ and rational λ , respectively, Eq. (25) can be written as a simple sum of functions instead a series. Although the expression (25) obtained for $C_v(t)$ is valid for all $0 < \lambda < 2$, the corresponding expression for rational λ showed in the appendixes is much more convenient for numerical computations.

V. TEMPORAL LIMITS BEHAVIOR OF THE VACF

The behavior of the VACF in the short-time limit can be obtained replacing the series (23) and (24) and taking $t \rightarrow 0$ in Eq. (25), we have

$$C_{\nu}(t) \approx 1 - \omega^2 \frac{t^2}{2}, \qquad (26)$$

which is the expected expression for a free particle driven by an internal noise with a finite correlation at the origin [12,13]. From (26), clearly the VACF of a free particle driven by a Mittag-Leffler noise has derivative zero at the origin, which is a property required according to [41]. In contrast the respective derivative for the power-law model diverges in the superdiffusive range [24], violating the recognized condition that the VACF must have zero initial slope [42]. In the following we will see more qualitative differences between both noise models. On the other hand, introducing in (25) the asymptotic behaviors of the generalized Mittag-Leffler function [40],

$$E_{\alpha,\beta}(-y) \sim \frac{1}{y \,\Gamma(\beta - \alpha)}, \quad y > 0,$$
 (27)

and its derivative,

$$E_{\alpha,\beta}^{(n)}(-y) \sim \frac{n!}{y^{n+1}} \frac{1}{\Gamma(\beta - \alpha)},\tag{28}$$

we obtain the behavior of the VACF $C_v(t)$ for times bigger than the noise characteristic time τ , i.e., $t \gg \tau$,

$$C_{\nu}(t) \approx E_{2-\lambda}(-\gamma t^{2-\lambda}).$$
⁽²⁹⁾

The VACF given by (29) has the same expression of that obtained for a pure power-law model [23,24].

The strict asymptotic behavior of the VACF $C_v(t)$ can be obtained introducing the asymptotic behavior (17) of the Mittag-Leffler function in Eq. (29). Then, for $\gamma t^{2-\lambda} \gg 1$, with $\lambda \neq 1$, the velocity autocorrelation can be written as

$$C_{\nu}(t) \approx \frac{1}{\gamma \Gamma(\lambda - 1)} t^{\lambda - 2}.$$
 (30)

As expected, the VACF (30) behaves as a power law in the long-time limit. These results are in agreement with those obtained in Refs. [23–25].

From Eq. (30), one realizes that the VACF 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 VACF decays with a long negative tail. This negative correlation is called the whip-back effect [1,23,43], which 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).

VI. TEMPORAL BEHAVIOR OF THE VACF IN THE SUPERDIFFUSIVE CASE

In this section we study in more detail the temporal behavior of the VACF for $1 < \lambda < 2$ (superdiffusive case).

The second-order memory kernel $\eta(t)$ is the Laplace inversion of the Eq. (20) and therefore,

$$\eta(t) = \frac{t^{\lambda - 2} \tau^{-\lambda}}{\Gamma(\lambda - 1)}, \qquad t \ge 0.$$
(31)

By replacing (31) in Eq. (9) we obtain

$$\ddot{C}_{v}(t) + \frac{1}{\tau^{\lambda}} \int_{0}^{t} dt' \frac{(t-t')^{\lambda-2}}{\Gamma(\lambda-1)} \, \dot{C}_{v}(t') + \omega^{2} C_{v}(t) = 0, \quad (32)$$

where $\omega^2 = \gamma / \tau^{\lambda}$. This last equation can be written as a fractional Langevin equation (FLE),

$$\ddot{C}_{v}(t) + \frac{1}{\tau^{\lambda}} \frac{d^{2-\lambda}}{dt^{2-\lambda}} (C_{v}(t)) + \omega^{2} C_{v}(t) = 0, \qquad (33)$$

where the fractional derivative is defined in the Caputo sense [44],

$$\frac{d^{\alpha}f(t)}{dt^{\alpha}} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \left(t-t'\right)^{-\alpha} \frac{df(t')}{dt'} dt', \quad (34)$$

with $0 < \alpha < 1$. Using $\eta = \frac{1}{\tau^{\lambda}}$, and calling $\alpha = 2 - \lambda$, we rewrite (33) as

$$\ddot{C}_{v}(t) + \eta \frac{d^{\alpha} C_{v}(t)}{dt^{\alpha}} + \omega^{2} C_{v}(t) = 0.$$
(35)

The FLE for the VACF $C_v(t)$ given by Eq. (35) is formally the same as that corresponding to the position autocorrelation function $C_x(t)$ obtained by Burov and Barkai for a harmonically bound particle [see Eq. (8) in Ref [32]]. In other words, the VACF for a free particle driven by a Mittag-Leffler noise in the superdiffusive case has an equivalent analytical expression to the position correlation function of the harmonic oscillator with frequency ω driven by a power-law noise in the subdiffusive case.

From Eq. (35) we can identify two contributions affecting the movement of the particle due to the medium: a frictional term (second term), which through η depends on τ and λ , and a term (third term) from which we can infer that the medium induces oscillations. This last one depends on all noise parameters (γ , τ , and λ). The behavior of the VACF will depend highly on the competition of these two always present terms.

In Ref. [31], the exact solution $C_x(t)$ of the FLE exhibits depending on the parameters α and ω , exponent of the frictional kernel and harmonic frequency, respectively—three



FIG. 1. The VACF $C_v(t)$ as a function of the time t for $\lambda = 1.5$ and $\tau = 1$. Three types of behaviors are exhibited: (a) monotonical decay for $\gamma = 0.09$, (b) nonmonotonical decay limit without zero crossings at critical value $\gamma = 1.1088$, and (c) nonmonotical decay with zero crossings for $\gamma = 9$.

different dynamical behaviors: monotonic decay, nonmonotonic decay with no zero crossings $C_x(t) \ge 0$, and nonmonotonic decay with zero crossings. From the aforementioned mathematical analogy, it is clear that the VACF displays the same three dynamical behaviors. In Fig. 1 we illustrate the analytical solution for the VACF obtained from Eq. (25). Three typical types of behavior are shown: (a) positive monotonic decay of $C_v(t)$; (b) nonmonotonic decay in the non-negative half of the plane $C_v(t) \ge 0$; and (c) oscillations where $C_v(t)$ also takes negative values depicting transitions between positive velocity correlations and velocity anticorrelations.

Some important result in [31] are the phase diagram of the fractional oscillator and the existence of a critical exponent $\alpha_c \approx 0.402$ that marks a transition to a nonmonotonic underdamped phase. In a similar way, we obtain an analogous diagram and a critical value of the exponent λ_c for the dynamics of the free particle driven by a Mittag-Leffler noise. Investigating the exact analytical expression of $C_v(t)$ Eq. (25) for fixed time relaxation $\tau = 1$, and different values of friction γ and exponent λ , we get critical curves $\eta_u(\lambda)$ and $\eta_l(\lambda)$ that depict the phase diagram of the Fig. 2. By numerical inspection of the VACF, we found that the critical value of the exponent parameter is $\lambda_c \approx 1.6$. It is consistent with the expected value $\lambda_c = 2 - \alpha_c \approx 1.598$ that we can infer from the oscillator



FIG. 2. (Color online) Regions in the (γ, λ) parameter plane with different dynamical behavior of the VACF for $\tau = 1$. The upper solid line with diamonds separates the region with oscillations and zero crossings regarding the region with oscillations without zero crossings. The lower solid line with circles separates the region of oscillations regarding the region with monotonic decay. Upper and lower lines converge at $\gamma_c = 0.25$ for $\lambda = 1$. Note that for $\lambda > \lambda_c \simeq 1.598$, monotonic decay does not exist.

problem [31]. For $1 < \lambda < \lambda_c$ we have the three dynamical behaviors outlined in Fig. 1. In contrast, for $\lambda > \lambda_c$ only two dynamical behaviors are possible. As in [31], a remarkable result emerges: The VACF never decay monotonically in that range. Thus, for $\lambda > \lambda_c$ an oscillatory behavior is always found for any γ value (except the case with no sense of $\gamma = 0$). The discussion on a physical explanation of this result is at the end of this section. Figure 2 shows that the critical curves converge to $\gamma_c = 1/4$ when $\lambda \to 1$. The specifical case $\lambda = 1$ for any value of τ and γ is solved analytically in Appendix A. We found that in this case exist only two dynamical regions: one where the VACF has a monotonic decay and another with oscillations with zero crossings. The critical case that separates the regions is given for the relation $\gamma \tau = 1/4$. In particular for $\tau = 1$, the critical coefficient γ_c is exactly 1/4. When the λ parameter crosses from $\lambda = 1$ to the range $1 < \lambda < \lambda_c$, the VACF goes from two to three dynamical regions. We point out that for $\lambda = 1$ and $\gamma > 1/4$ the VACF has damped oscillations by an exponentially decreasing amplitude, exhibiting an indefinite number of zeros. On the other side, when $1 < \lambda < 2$, the VACF decays as a positive power law at long time [see Eq. (30)] and for above of $\eta_u(\lambda)$ it exhibits oscillations with an even finite number of zeros [45]. The phase diagram showed in Fig. 2 can be generalized to other scales. From dimensional analysis,

$$\gamma_u = \eta_u(\lambda)\tau^{\lambda-2} \qquad \gamma_l = \eta_l(\lambda)\tau^{\lambda-2}, \tag{36}$$

where $\eta_u(\lambda) \ge \eta_l(\lambda)$ are functions depending on λ that represent the critical curves previously mentioned. It is worth noting that $\eta_l(\lambda) \propto (\lambda - \lambda_c)$ for λ near to λ_c . We can see that below $\eta_u(\lambda)$ the motion is persistent, i.e., $C_v(t) > 0$.

We now turn the attention to the evaluation of $C_v(t)$ for different values of the time relaxation τ and fixed γ . We evaluate (25) as before and again we find three types of dynamical behaviors. Figure 3 illustrates our results: (a) positive monotonic decay, (b) nonmonotonic decay in the



FIG. 3. The VACF $C_v(t)$ as a function of the time t for $\lambda = 1.2$ and $\gamma = 1$. Three types of behaviors are exhibited: (a) monotonical decay for $\tau = 0.4$, (b) nonmonotonical decay limit without zero crossings at critical value $\tau = 0.835$, and (c) nonmonotonical decay with zero crossings for $\tau = 3$.

non-negative half of the plane $C_v(t) \ge 0$, and (c) oscillations of the VACF where $C_v(t)$ also takes negative values, denoting transitions between positive velocity correlations and velocity anti-correlations.

Regarding the negative correlation of the VACF we do the following digression. The analytical expression of the VACF for a free particle driven by a power-law noise [24] is

$$C_{\nu}(t) = E_{2-\lambda}(-\gamma t^{2-\lambda}), \qquad (37)$$

which is expressed as a one-parameter Mittag-Leffler function. This function is completely monotone and positive, tending to zero from above when $t \to \hat{\infty}$ for $1 < \lambda < 2$ [37]. As a consequence, the corresponding expression $C_v(t)$ for a free particle driven by a power-law noise does not provide negative correlations (neither oscillations) in the superdiffusive range whereas a Mittag-Leffler noise does it. We note that using the asymptotic behaviors of the generalized Mittag-leffler function, Eqs. (27) and (28), the limit $\tau \to 0$ of $C_v(t)$ given by (25) is reduced to the VACF of a free particle driven by a power-law noise Eq. (37). As a consequence, we obtain a monotonic behavior of the VACF for $\tau = 0$.

Using the same numerical procedures, we investigate the VACF for $\gamma = 1$ and different values of the parameters τ and λ . From our results, we obtain critical curves $\kappa_u(\lambda)$ and $\kappa_l(\lambda)$ performing the phase diagram showed in Fig. 4.



FIG. 4. (Color online) Regions in the (τ, λ) parameter plane with different dynamical behavior of the VACF for $\gamma = 1$. The upper solid line with diamonds separates the region with oscillations and zero crossings regarding the region with oscillations without zero crossings. The lower solid line with circles separates the region of oscillations regarding the region with monotonic decay. Upper and lower lines converge at $\tau_c = 0.25$ for $\lambda = 1$. Note that for $\lambda > \lambda_c \simeq 1.598$, monotonic decay does not exist.

There, the exponent value $\lambda = \lambda_c \approx 1.598$ is also a critical value of the exponent parameter that marks the transition in the behaviors of the VACF. For $\lambda > \lambda_c$, the VACF never decays monotonically. We note that $\kappa_l(\lambda)$ depicts the boundary between the monotonic and nonmonotonic phases, and for λ near to λ_c we have $\kappa_l(\lambda) \propto (\lambda - \lambda_c)^2$. We also note here that below $\kappa_u(\lambda)$ we have persistent motion $(C_v(t) > 0)$. From dimensional analysis we get

$$\tau_{u} = \kappa_{u}(\lambda)\gamma^{\frac{1}{(\lambda-2)}} \quad \tau_{l} = \kappa_{l}(\lambda)\gamma^{\frac{1}{(\lambda-2)}}, \quad (38)$$

where $\kappa_u(\lambda)$ and $\kappa_l(\lambda)$ are functions of λ .

As Fig. 4 illustrates, we can see that for $\lambda > \lambda_c$ the VACF never decays monotonically. These results are consistent with theoretical statements expressed by Eq. (35). The dynamical behavior of the VACF is determined by the competition given by the frictional and oscillatory terms in the FLE. To illustrate these phenomena, we explicitly work out two limit cases. First, let us take the limit $\alpha \rightarrow 0$ ($\lambda \rightarrow 2$) the FLE Eq. (35) yields

$$\ddot{C}_{v}(t) + \eta (C_{v}(t) - C_{v}(0)) + \omega^{2} C_{v}(t) = 0.$$
(39)

This shows that the existence of a purely oscillating behavior is expected in this limit, even for small values of ω . In our context, a plausible physical explanation is that, in this limit, the medium is similar to a solid in which the particle is compelled to move back and forth in a cage formed by the surrounding particles in the environment. It is worth noting that $\omega = 0$ has no physical sense because in this case that would imply absence of medium (and noise). Taking now the opposite limit of $\alpha \rightarrow 1$ ($\lambda \rightarrow 1$) we get

$$\ddot{C}_{v}(t) + \eta \dot{C}_{v}(t) + \omega^{2} C_{v}(t) = 0, \qquad (40)$$

which is the equation of a standard damped oscillator. In this limit, the medium operates as a viscous fluid where the particle moves.

VII. SUMMARY AND CONCLUSION

In this paper, we studied the dynamics of an anomalously diffusing free particle driven by a Mittag-Leffler noise, which motion is described by a generalized Langevin equation. Our main goal has been to describe the dynamical behaviors of the system through the VACF-an experimentally measurable quantity-posing a hierarchical relationship of memory kernels as the method. In this way, we show that a memory kernel $\gamma(t)$ described by a Mittag-Lefler function, satisfies a generalized Langevin equation which has a power-law function as the second-order memory kernel. Based on this fact, we get a tractable general expression of the VACF for a free particle driven by a Mittag-Leffler noise as a single series for all real $0 < \lambda < 2$. Moreover, we show that for rational λ this VACF may be expressed as a simple sum of functions, which is even more convenient for numerical computations.

We found three different dynamical behaviors of the VACF in the superdiffusive range. Depending on the noise parameters (and ultimately from the properties of the environment where the particle moves) we obtained three regions of distinct dynamical regimes defined by two critical curves as is summarized in Figs. 2 and 4. We observed the existence of a critical value for the exponent $\lambda = \lambda_c \approx 1.598$, where for $\lambda > \lambda_c$, the monotonic decay of the VACF is not already possible and it only displays some type of nonmonotonic decay.

The formalism of hierarchical memory kernels used allowed us to establish a correspondence between the oscillator driven by a power-law noise problem and that of a free particle driven by a Mittag-Leffler noise. Specifically, we found that the FLE of the VACF for a free particle driven by a Mittag-Leffler noise in the superdiffusive range is formally identical to the FLE for the normalized position autocorrelation function of a harmonically bounded particle driven by a power-law noise in the subdiffusive range. From a qualitative analysis of the FLE, we may infer properties of the system and a physical explanation of the dynamical behaviors. By taking the limit $\lambda \rightarrow 1$ in the FLE, we observe that the frictional term of the FLE has an interplay with the oscillatory term and the particle moves in an environment assimilable to viscous fluid. On the other hand, if $\lambda \rightarrow 2$, the FLE is reduced to an equation of an oscillator and the particle has a rattling motion in the cage formed by the surrounding particles, and the environment is assimilable to a solid.

Another remarkable result is the dynamical difference between the case $\lambda = 1$ corresponding to a free particle driven by an exponential noise regarding the case $\lambda \rightarrow 1^+$ for which the particle is driven by a Mittag-Leffler noise. As we showed, when $\lambda \rightarrow 1^+$ the three dynamical regions in which the VACF decays as a power law, collapses to two dynamical regions with exponential decay at $\lambda = 1$.

We point out some relevant differences between powerlaw and Mittag-Leffler models for a free particle in the superdiffusive range. While the VACF always takes positive values for a memory kernel power law, the VACF may take positive and negative values for a Mittag-Leffler noise with the appropriate parameter values. As a consequence, the power-law model does not provide oscillations nor negative To our knowledge, the behaviors of the VACF at intermediate times—as the oscillatory regime—has not been observed in any natural system. In this way, the results presented in this work require experimental validation.

Finally, in view of the utility provided by the formalism of hierarchical memory kernels in our study, it deserves a more detailed analysis in connection with its potential use as a theoretical instrument.

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APPENDIX A: ANALYTICAL EXPRESSION OF THE VACF FOR $\lambda = 1$

Inserting Eq. (20) in Eq. (8) we obtain the Laplace expression for $C_v(t)$ of a free particle driven by a Mittag-Leffler noise, which reads

$$\widehat{C}_{v}(s) = \frac{s + s^{1-\lambda}\tau^{-\lambda}}{s^{2} + s^{2-\lambda}\tau^{-\lambda} + \gamma\tau^{-\lambda}}.$$
(A1)

In particular, for $\lambda = 1$ (corresponding to the free particle driven by an exponential noise), we have

$$\widehat{C_{v}}(s) = \frac{s + \tau^{-1}}{s^{2} + s\tau^{-1} + \gamma\tau^{-1}}.$$
(A2)

The Laplace inversion of Eq. (A2) [46] produces the following three cases.

(1) For $\gamma \tau > \frac{1}{4}$, we obtain the underdamped case,

$$C_{v}(t) = e^{-t/2\tau} \bigg(\cos(\Omega t) + \frac{1}{2\Omega\tau} \sin(\Omega t) \bigg), \qquad (A3)$$

where

$$\Omega = \frac{1}{\tau} \sqrt{\gamma \tau - \frac{1}{4}}.$$

(2) For $\gamma \tau < \frac{1}{4}$, we have the overdamped case,

$$C_{v}(t) = e^{-t/2\tau} \left(\cosh(\Omega t) + \frac{1}{2\Omega\tau} \sinh(\Omega t) \right), \quad (A4)$$

where

$$\Omega = \frac{1}{\tau} \sqrt{\frac{1}{4} - \gamma \tau}.$$

(3) Finally, for $\gamma \tau = \frac{1}{4}$, we get the critical case,

$$C_v(t) = e^{-t/2\tau} (1 + t/2\tau).$$
 (A5)

We note that for $\tau = 1$, we obtain $\gamma_c = 1/4$, and for $\gamma = 1$, we obtain $\tau_c = 1/4$.

APPENDIX B: ANALYTICAL EXPRESSION OF THE VACF FOR RATIONAL λ

In this appendix, following [47] we derive an analytical expression of the VACF for all rational λ (with $0 < \lambda < 2$) as

a simple summatory of Mittag-Leffler functions. This provides an advantageous expression for it from a numerical perspective. In this way, we introduce a function G(t) defined as

$$G(t) = \frac{dI(t)}{dt},\tag{B1}$$

where I(t) is given by the Laplace inversion of Eq. (21). From Eqs. (B1) and (21), the Laplace transform of G(t) yields

$$\widehat{G}(s) = s \,\widehat{I}(s) = \frac{1}{s^2 + s^{2-\lambda}\tau^{-\lambda} + \gamma \tau^{-\lambda}},\tag{B2}$$

which can be written as

$$\widehat{G}(s) = \frac{\tau^2}{s^2 \tau^2 + s^{2-\lambda} \tau^{2-\lambda} + \gamma \tau^{2-\lambda}}.$$
(B3)

We rewrite (B3) as

$$\frac{\tau^2}{\widehat{G}(s)} = (s\tau)^2 + (s\tau)^{\alpha} + \gamma \tau^{\alpha}, \tag{B4}$$

where $\alpha = 2 - \lambda$. Assuming rational $\alpha = p/q$, where p and q are positive integers and $p \neq q$, we introduce the variable $z = (s\tau)^{1/q}$, leading (B4) to a polynomial in z of degree 2q,

$$\frac{\tau^2}{\widehat{G}(s)} \equiv P(z) = z^{2q} + z^p + \gamma \tau^{\alpha}.$$
 (B5)

The polynomial P(z) has 2q complex roots z_j . Assuming that all roots are different, we write

$$\frac{1}{P(z)} = \prod_{j=1}^{2q} \frac{1}{z - z_j} = \sum_{j=1}^{2q} \frac{A_j}{z - z_j},$$
 (B6)

where the coefficients A_i are

$$A_j = \frac{1}{[P'(z)]_{z=z_j}} = \prod_{k\neq j}^{2q} \frac{1}{z_j - z_k}.$$
 (B7)

Now, we consider the following Laplace transform:

$$\int_0^\infty e^{-st} t^{\beta-1} E_{\alpha,\beta}(ct^\alpha) dt = \frac{1}{s^{\beta-\alpha}(s^\alpha - c)}, \qquad (B8)$$

where $E_{\alpha,\beta}(y)$ is the generalized Mittag-Lefler function defined by Eq. (23).

Introducing $z = (s\tau)^{1/q}$ in Eq. (B6) and making use of Eq. (B8) we obtain

$$G(t) = \tau \sum_{j=1}^{2q} A_j(t/\tau)^{\frac{1}{q}-1} E_{\frac{1}{q},\frac{1}{q}} \Big[z_j(t/\tau)^{\frac{1}{q}} \Big].$$
(B9)

Using the identity,

$$\frac{\partial}{\partial t} [t^{\beta-1} E_{\alpha,\beta}(ct^{\alpha})] = t^{\beta-2} E_{\alpha,\beta-1}(ct^{\alpha}), \qquad (B10)$$

and according to Eq. (B1), we get

$$I(t) = \tau^2 \sum_{j=1}^{2q} A_j(t/\tau)^{\frac{1}{q}} E_{\frac{1}{q},\frac{1}{q}+1} \Big[z_j(t/\tau)^{\frac{1}{q}} \Big].$$
(B11)

Replacing (B11) in Eq. (11) we obtain

$$C_{v}(t) = 1 - (\omega\tau)^{2} \sum_{j=1}^{2q} A_{j}(t/\tau)^{\frac{1}{q}} E_{\frac{1}{q},\frac{1}{q}+1} \Big[z_{j}(t/\tau)^{\frac{1}{q}} \Big].$$
(B12)

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- [1] K. G. Wang and C. W. Lung, Phys. Lett. A 151, 119 (1990).
- [2] K. G. Wang, Phys. Rev. A 45, 833 (1992).
- [3] R. Metzler and J. Klafter, Phys. Rep. 339, 1 (2000); J. Phys. A: Math. Gen. 37, R161 (2004).
- [4] A. Bunde, S. Havlin, J. Klafter, G. Graff, and A. Shehter, Phys. Rev. Lett. 78, 3338 (1997).
- [5] E. Barkai and R. J. Silbey, J. Phys. Chem. B 104, 3866 (2000).
- [6] E. Barkai, Phys. Rev. E 63, 046118 (2001).
- [7] P. Dieterich, R. Klages, R. Preuss, and A. Schwab, Proc. Natl. Acad. Sci. USA 105, 459 (2008).
- [8] B. Yilmaz, S. Ayik, Y. Abe, and D. Boilley, Phys. Rev. E 77, 011121 (2008).
- [9] A. A. Dubkov, B. Spagnolo, and V. V. Uchaikin, Int. J. Bifurcation Chaos 18, 2649 (2008).
- [10] H. Mori, Prog. Theor. Phys. 33, 423 (1965).
- [11] J. M. Porra, K. G. Wang, and J. Masoliver, Phys. Rev. E 53, 5872 (1996).
- [12] K. G. Wang and J. Masoliver, Physica A 231, 615 (1996).
- [13] K. G. Wang and M. Tokuyama, Physica A 265, 341 (1999).
- [14] S. Chaudhury, D. Chatterjee, and B. J. Cherayil, J. Chem. Phys. 129, 075104 (2008).
- [15] S. Chaudhury, S. C. Kou, and B. J. Cherayil, J. Phys. Chem. B 111, 2377 (2007).
- [16] S. C. Kou and X. S. Xie, Phys. Rev. Lett. 93, 180603 (2004).
- [17] K. S. Fa, Phys. Rev. E **73**, 061104 (2006).
- [18] K. S. Fa, Eur. Phys. J. B 65, 265 (2008).
- [19] A. A. Dubkov and B. Spagnolo, Fluct. Noise Lett. 5, L267 (2005).
- [20] A. D. Viñales and M. A. Despósito, Phys. Rev. E 73, 016111 (2006).
- [21] R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957).
- [22] R. Zwanzig, *Nonequilibrium Statistical Mechanics* (Oxford University Press, New York, 2001).
- [23] E. Lutz, Europhys. Lett. 54, 293 (2001).
- [24] N. Pottier, Physica A **317**, 371 (2003).
- [25] A. D. Viñales and M. A. Despósito, Phys. Rev. E 75, 042102 (2007).

- [26] B. Uma et al., J. Chem. Phys. 135, 114104 (2011).
- [27] R. Mankin, K. Laas, and A. Sauga, Phys. Rev. E 83, 061131 (2011).
- [28] A. D. Viñales, K. G. Wang, and M. A. Despósito, Phys. Rev. E 80, 011101 (2009).
- [29] M. A. Despósito and A. D. Viñales, Phys. Rev. E 80, 021111 (2009).
- [30] R. Morgado, F. A. Oliveira, G. G. Batrouni, and A. Hansen, Phys. Rev. Lett. 89, 100601 (2002).
- [31] S. Burov and E. Barkai, Phys. Rev. Lett. 100, 070601 (2008).
- [32] S. Burov and E. Barkai, Phys. Rev. E 78, 031112 (2008).
- [33] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (Dover Publication, New York, 1991).
- [34] N. Pottier, Physica A **390**, 2863 (2011).
- [35] H. Risken, *The Fokker-Plank Equation* (Springer-Verlag, Berlin, 1989).
- [36] A. Erdelyi *et al.*, *Higher Transcendental Functions*, Vol. 3 (Krieger, Malabar, 1981).
- [37] F. Mainardi and R. Gorenflo, J. Comput. Appl. Math. 118, 283 (2000).
- [38] R. Granek and J. Klafter, Europhys. Lett. 56, 15 (2001).
- [39] C. Cohen-Tannoudji *et al.*, *Quantum Mechanics*, Vol. 2 (Hermann, Paris, 1977).
- [40] I. Podlubny, Fractional Differential Equations (Academic Press, London, 1999).
- [41] M. Howard Lee, Phys. Rev. Lett. 51, 1227 (1983).
- [42] W. Marshall and S. W. Lovesey, *Theory of Thermal Neutron Scattering* (Oxford University Press, London, 1970).
- [43] R. Muralidhar et al., Physica A 167, 539 (1990).
- [44] K. S. Miller and B. Ross, An Introduction to the Fractional Differential Equations (Wiley, New York, 1993).
- [45] R. Gorenflo and F. Mainardi, *Fractal and Fractional Calculus in Continuum Mechanics* (Springer Verlag, Wien/New York, 1997).
- [46] M. R. Spiguel, *Theory and Problems of Laplace Transform* (McGraw-Hill, New York, 1965).
- [47] D. S. Grebenkov and M. Vahabi, Phys. Rev. E 89, 012130 (2014).