From generalized Langevin stochastic dynamics to anomalous diffusion

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Scaling methods are fundamental in all branches of physics. In stochastic process, we usually try to describe the long time behavior of a given time correlation function. In this work we investigate a scaling method for anomalous diffusion in systems with memory that produces good results for long and intermediate times. We will initially present a generalization of the diffusion exponent. Then, we present an asymptotic method to obtain an analytical expression for the diffusion coefficient by introducing a time scale factor $\lambda(t)$. We found an exact expression for the function $\lambda(t)$, which allows us to describe the diffusive process. For large times, $\lambda(t)$ becomes a universal parameter determined by the diffusion exponent. In turn, the analytical results are then compared to the numerical results, with a good matching. Then, we'll show the practical effects of scaling. An important first result is that $\lambda(t)$ quickly converges to a constant. Another very important point was the classification of new forms of diffusion due to the generalized exponent. In previous works, we verified the existence of ergodic ballistic diffusion with diffusion exponent $\alpha = 2^-$. Here, we verify the existence of the nonergodic ballistic diffusion type with the obtainment of the diffusion coefficient $\alpha = 2$. Finally, we show that the scaling works. This method is general and can be applied to various types of stochastic problems.

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I. INTRODUCTION

The Generalized Langevin Equation (GLE) is a stochastic differential equation that can be used to model systems with friction kernels driven by colored random forces, and therefore describes a non-Markovian stochastic process [1–3]. In the absence of an external potential, the GLE for a particle of mass m is given by

$$m\frac{dv(t)}{dt} = -m\int_0^t \Gamma(t-t')v(t')dt' + \xi(t), \tag{1}$$

where $\Gamma(t)$ is the friction memory kernel, which acts as generalized friction that depends on events in earlier times, and satisfies $\lim_{t\to\infty}\Gamma(t) = 0$. The presence of the memory kernel in the friction term gives the influence of the complex environment on the particle movement. In 1926 Lewis Fry Richardson analyzed an exception to the linear time dependence of the mean square displacement of Brownian motion. For the relative diffusion of two tracer particles in a turbulent flow he observed strongly non-Brownian behavior [4]. Today anomalous diffusion typically refers to the power-law form, which may result in a behavior of the particle of form [5–8]

$$\left\langle x^2(t \gg \tau)\right\rangle \simeq t^\alpha, \tag{2}$$

i.e., power-law dependence of mean square displacement on time for times larger than a given characteristic time τ. Here the angular brackets $\langle\rangle$ denote an average over the ensemble of particles. The exponent α is associated with the memory of the system [9] and determines the type of diffusion regime as follows

$$\begin{array}{ll} 0<\alpha<1 & \text{, Subdiffusion} \\ \alpha = 1 & \text{, Normal Diffusion} \\ \alpha > 1 & \text{, Superdiffusion} \end{array} \tag{3}$$

The Brownian particle motion occurs due to fluctuations in the thermal equilibrium bath with a noise $\xi(t)$, where the presence of the memory function $\Gamma(t)$ plays the role of generalized friction. The noise $\xi(t)$ is a random colored stochastic force that satisfies the following conditions:

(i) The noise has a zero average

$$\langle\xi(t)\rangle = 0. \tag{4}$$

(ii) At $t \geqslant 0$ the noise is not correlated with the set of particles' initial velocities

$$\langle\xi(t)v(0)\rangle = 0. \tag{5}$$

(iii) The noise at a given time t is correlated with the noise at another time t' by

$$C_\xi(t) = \langle\xi(t)\xi(t')\rangle = mk_BT\Gamma(t-t'), \tag{6}$$

where $C_\xi(t)$ is the correlation function for a noise $\xi(t)$, and T is the absolute temperature. It represents a useful tool for modeling diffusion in complex systems. Equation (6) is known as the generalized fluctuation-dissipation theorem and predicts how the energy balance occurs in thermal equilibrium. Equation (6) was proposed by Kubo [10], which is a non-Markovian version of the fluctuation dissipation theorem (FDT), or the Kubo FDT. The presence of the kernel $\Gamma(t)$ allows us to study a large number of correlated processes. In the real world, the vast majority of problems are non-Markovian, i.e., there is a correlation between the various stages of dynamic evolution.

A major quantity to be obtained is the normalized velocity-velocity correlation function defined as [11]:

$$R(t) = \frac{C_v(t)}{C_v(0)} = \frac{\langle v(t)v(0)\rangle}{\langle v^2(0)\rangle}, \tag{7}$$

from which is possible to obtain the Kubo formula

$$D = C_v(0)\int_0^\infty R(t)dt. \tag{8}$$

For a white Gaussian noise $\xi(t)$, the correlation function is $C_\xi(t) = 2m\gamma k_B T\delta(t)$, $\delta(t)$ is Dirac delta, and the generalized Langevin equation yields as a special case of the classical Langevin equation for a Brownian particle [11] with $R(t) = e^{-\gamma t}$. Thus, for the canonical Brownian motion, the mean square displacement is given by

$$\langle x^2(t)\rangle = 2Dt, \tag{9}$$

with a diffusion coefficient $D = k_B T/m\gamma$.

Anomalous diffusion in the presence or absence of an external velocity or force field has been modeled in numerous ways. The GLE is widely used in different areas of science from physics, chemistry, and biology to financial markets to implement memory effects in the behavior of stochastic systems [8,9,12–16]. Scaling methods have also had a large application in physics, in particular, in Statistical mechanics. Here we show a simple analytical method that describes the behavior of the diffusion for large and intermediate times. First, the Kubo formula (8) cannot be used when Eq. (9) refers to a time t, usually large but finite, while in Eq. (8) the integration goes to infinity, i.e., a time t_0 in the range $t < t_0 < \infty$ is a time that have not existed as yet, and it cannot contribute to the integral. Thus it should be defined as

$$D(t) = \int_0^t C_v(t')dt'. \tag{10}$$

Note that for normal diffusion Eq. (8) is correct because Eq. (10) converges to a constant. For anomalous diffusion however, the time dependence can not be omitted. Second, we presented a conjecture to obtain, through the introduction of a time scaling factor λ, an analytical asymptotic result for the diffusion coefficient for intermediate and long times. We obtained the scaling factor exactly for all kinds of diffusion and we showed its universal behavior as well. We also derived a numerical method to obtain the correlation function of velocities for an ensemble of particles from any given memory. We compared both methods and we obtained an excellent match. The method has a general application in the study of stochastic processes and it could be applied to several situations of physics interest.

This paper is organized as follows. In Sec. II we presented the GLE that allows us to study the asymptotic behavior of diffusive processes with memory. In Sec. III we analytically obtained the function $\lambda(t)$ and showed that its behavior for large times leads to a universal value; in other words, we showed the universality of the scaling practical effects. In Sec. IV, using the Khinchin theorem, we presented the connection between the types of diffusive regimes and the system ergodicity. In Sec. V we showed applications for the scale theory in some types of diffusion. We verified the existence of ballistic diffusion with $\alpha = 2$, this being not ergodic. We obtained another type of diffusive regime, beyond those known from the literature, this being the weak superdiffusion with $\alpha = 1^+$.

II. GENERALIZATION OF THE DIFFUSION EXPONENT

Using the GLE it is possible to study the asymptotic behavior of the second moment of the particle movement for large t as

$$\langle x^2(t)\rangle \sim 2D(t)t \sim t^\alpha. \tag{11}$$

Here, $D(t)$ is the diffusion coefficient as a function of time as defined in Eq. (10). Note as well that not only power law arises from; another possibility is the combination of power law and logarithmic behavior, see for example [8] in the form namely

$$\langle x^2(t)\rangle \sim t^\alpha[\ln(t)]^\epsilon \equiv t^{\alpha_\epsilon}, \tag{12}$$

where α_ϵ is related with α as follows:

$$\epsilon = \begin{cases} 1, & \alpha_\epsilon = \alpha^+ \\ 0, & \alpha_\epsilon = \alpha \\ -1, & \alpha_\epsilon = \alpha^- \end{cases}. \tag{13}$$

This generalization allows the classification of new forms of diffusion.

Now supposing the existence of the Laplace transform of $D(t)$ and using the final value theorem [17] in Eq. (10), we have

$$\lim_{t\to\infty} D(t) = \lim_{z\to 0}[z\tilde{D}(z)] = C_v(0)\lim_{z\to 0}\widetilde{R}(z), \tag{14}$$

where tilde stands for the Laplace transform and $R(t) = C_v(t)/C_v(0)$. The Laplace transform of the integral gives $\widetilde{D}(z) = R(z)/z$ and we end up with the equation above.

Multiplying Eq. (1) by $v(0)$ and taking the average over the ensemble and using Eq. (5), we obtain a self-consistent equation to $R(t)$

$$\frac{dR(t)}{dt} = -\int_0^t \Gamma(t-t')R(t')dt'. \tag{15}$$

The Laplace transform of Eq. (15) yields

$$\tilde{R}(z) = \frac{1}{z+\tilde{\Gamma}(z)}. \tag{16}$$

Time correlation functions play a central role in nonequilibrium statistical mechanics in many areas such as the dynamics of polymeric chains [18], spin waves [19], and microbead rheology [20]. Consequently, to invert this transformed or a similar one is crucial. Unfortunately, in most cases, it is not an easy task. In those situations, the use of numerical methods is an alternative to overcome this problem. Our main objective here is to show a process to obtain the asymptotic behavior analytically. Although the method can be applied to several situations, we concentrate here on the analysis of ballistic diffusion in the case of systems where ergodicity is broken.

Equation (15) also imposes some requirements on $R(t)$. First, its derivative must be null at the origin, i.e., the integral in the right hand side must be null at $t = 0$. This is true except for nonanalytical memories, such as δ functions. In fact, to analyze the derivative at the origin we need to do an analytic extension to include negative times. That is an answer of the form $R(t) = \exp(-\gamma|t|)$, which has a discontinuous derivative at the origin [7]. Second, in Eq. (1), for a bath of harmonic oscillators the noise can be obtained as [7]

$$\xi(t) = \int \sqrt{2k_BT\rho(\omega)}\cos[\omega t + \phi(\omega)]d\omega, \tag{17}$$

where $0 < \phi(\omega) < 2\pi$ are random phases and $\rho(\omega)$ is the noise spectral density. The FDT given by Eq. (6) yields

$$\Gamma(t) = \int \rho(\omega)\cos(\omega t)d\omega. \tag{18}$$

Thus all description of the stochastic process can be done if we know the spectral density. This shows as well that the memory is an even function of t. An analytical extension of $\tilde{\Gamma}(z)$ in the whole complex plane has the property $\tilde{\Gamma}(-z) = -\tilde{\Gamma}(z)$. Consequently, from Eq. (16), $\tilde{R}(-z) = -\tilde{R}(z)$, or $R(-t) = R(t)$. In short, it requires well-behaved functions and derivatives. Even functions have zero derivatives at the origin, as required before [7].

III. A SCALE THEORY FOR DIFFUSION

We know from the final value theorem that $t \to \infty$ is equivalent to $z \to 0$ in the corresponding Laplace transform Eq. (14). Now we want to investigate what happens not for infinite, but for intermediate times, where the leading term for $D(t)$ will fulfill Eq. (14) within a given approximation. Thus we imposed that

$$D(t) = \tilde{R}\left(z = \frac{\lambda(t)}{t}\right), \tag{19}$$

with the scaling

$$z \to \frac{\lambda(t)}{t}, \tag{20}$$

where $\lambda(t)$ is a function to be determined. Note that the Tauberians theorem demands that as $t \to \infty$, $z \to 0$ in such way that in the Laplace transform $\exp(-zt)$ has the same weight, $z = 1/t$, in these limits. However, it does not say anything for intermediate times. In order to fill this gap, we introduced the scaling above and work now to make it true. For large t, we rewrite Eq. (19) as

$$D(t) = \tilde{R}\left(\frac{\lambda(t)}{t}\right) = \frac{t}{f(t)}. \tag{21}$$

Now, we can obtain the $R(t)$ in two ways:

(1) Deriving Eq. (21)

$$R_1(t) = \frac{d}{dt}D(t) = \left[1 - t\frac{d}{dt}\ln[f(t)]\right]/f(t). \tag{22}$$

(2) Through the final value theorem

$$R_2(t) = z\tilde{R}(z) = \frac{\lambda(t)}{f(t)}. \tag{23}$$

Now let's consider that Eqs. (22) and (23) are valid for a finite time t. Take the relative difference,

$$\Delta R(t) = \frac{R_2 - R_1}{R_2} = \left[\lambda(t) - 1 + t\frac{d}{dt}\ln[f(t)]\right]/\lambda(t), \tag{24}$$

and making $\Delta R(t) = 0$, with $\lambda \neq 0$ we get

$$\lambda(t) = 1 - t\frac{d}{dt}\ln[f(t)] \tag{25}$$

and

$$f(t) = \lambda(t) + t\tilde{\Gamma}\left(\frac{\lambda}{t}\right). \tag{26}$$

We solve these equations self consistently. This relation forces the two functional relations for $R(t)$ to quickly converge on each other making the result approximate the exact value. We'll show as well that $\lambda(t)$ quickly converges to a constant λ and its value is universal, i.e., the limit

$$\lambda = \lim_{t\to\infty}\lambda(t) = 1 - \lim_{t\to\infty} t\frac{d}{dt}\ln[f(t)], \tag{27}$$

is a universal constant.

To obtain $\lambda(t)$ we need to know $\tilde{\Gamma}(z)$. However, once our interest is on the asymptotic behavior, we can expand $\tilde{\Gamma}(z)$ in Taylor or Laurent series around $z = 0$. A considerable general form to $\tilde{\Gamma}(z)$ is given by

$$\tilde{\Gamma}(z) \sim z^{\nu}[a - b\ln(z) - c/\ln(z)], \tag{28}$$

where a, b, and c are positive constants. In this expansion, we preserve $ln(z)$ that can't be expanded around $z = 0$. Consider now the following cases: if $b = 0$, the dominant term is $\Gamma(z) \sim z^{\nu}$, and we have diffusion with the exponent α. To $b \neq 0$, the diffusion is type α^-, and for $a = b = 0$ and $c \neq 0$, we have diffusion type α^+. If $\tilde{\Gamma}(z)$ has another contribution, besides $\ln(z)$, that cannot be expanded at the origin we keep it and expand the other parts. However, most of the memories in the literature can be cast in the form Eq. (28) for small z. Now we introduce Eq. (28) into Eq. (25) to obtain $\lambda = \nu$ for $\nu < 1$ and $\lambda = 1$ for $\geqslant 1$. Notice that it does not depend on a, b, or c, which suggests a universal behavior.

In this conjecture, some points deserve our attention. First, we are considering integrals from the form of Eq. (14), where the function $R(t)$ is well behaved and limited in $-1 < R(t) < 1$, since $C_v(t) \leqslant C_v(0)$. Second, $D(t)$ must have a main term when $t \to \infty$, which determines the diffusion. For example, the inverse of the Laplace Transform of $R(z)$ is

$$R(t) = \frac{1}{2\pi i}\int_{-i\infty+\eta}^{+i\infty+\eta}\tilde{R}(z)\exp(zt)dz, \tag{29}$$

where the real number η is such that all $\tilde{R}(z)$ singularities are from the left side of the line $Re(z) = \eta$ on the complex plan. Consider now Eq. (28) with $b = c = 0$ and $\nu \leqslant 1$. Then

$$\lim \tilde{R}(z) \sim z^{-\nu}, \tag{30}$$

and Eq. (29) becomes

$$\lim_{t\to\infty} R(t) \propto t^{\nu-1}\int_{-i\infty+\eta'}^{+i\infty+\eta'} s^{-\nu}\exp(s)ds \propto t^{\nu-1}, \tag{31}$$

where the transformation $s = zt$ and $\eta' = \eta/t$ was made, and the new integral is a constant. For $\nu > 0$ we have a single pole in $s = 0$, and the condition in $\eta' = \eta/t$ will be automatically satisfied. Still, using Eq. (10) or Eq. (14) we get $D(t) \sim t^{\nu}$ and using the scaling we obtain

$$\lim_{t\to\infty} D(t) = \lim_{z\to 0} \tilde{R}(z = \lambda/t) \sim \lim_{t\to\infty} \tilde{R}(\lambda/t) \sim t^{\nu}, \tag{32}$$

i.e., the same result.

We must note that the result above is not only valid to power laws, but to any function that behaves like power law for small z. In addition, we confirmed the relation $\alpha = \nu + 1$ obtained by Morgado [9]. Therefore, taking the limit Eq. (27) we get

$$\lambda = \alpha - 1 = \alpha^{\pm} - 1 = \begin{cases} \nu & -1 < \nu < 1, \\ 1 & \nu \geqslant 1. \end{cases} \tag{33}$$

In this way, the factor λ depends only on the diffusion exponent α, and moreover, λ is the same for α or $\alpha^{\pm}$. Consequently, it presents an universal behavior.

Diffusive regime, Ergodicity and the FDT

Once the diffusion type has been determined from the memory functions, we may go a step further and analyze the ergodicity in the diffusive process.

The connection with the ergotic proprieties is given by the theorem of Khinchin [21,22], which states that: If the mixing condition

$$\lim_{t\to\infty} R(t) = 0, \tag{34}$$

holds, than ergodicity holds. From Eq. (34), and using the final limit theorem, we define the nonergodic factor

$$\kappa = \lim_{t\to\infty} R(t) = \lim_{z\to 0} z\tilde{R}(z). \tag{35}$$

Then, ergodicity holds only if $\kappa = 0$. Otherwise we have an ergodicity breaking.

The mixing condition $\kappa = 0$ tells us that after some time $t \gg \tau$, the system reaches the thermodynamic balance, i.e., $R(t)$ does not remember its initial condition $R(0)$. In this way the Khinchin theorem establishes that irreversibility is a necessary and sufficient condition to the ergodicity. The FDT holds only if ergodicity holds. The FDT is a weak theorem and it fails in many situations such as in structural glass [23–26], in proteins [27], in mesoscopic radiative heat transfer [28,29], and as well in ballistic diffusion [22,30–32]. For growth phenomena such as those described by the Kadar-Parisi-Zhang equation [33], different formulations of the FDT have been proposed [34–36]. Recently, Anjos *et al* [37] proposed that the growth dynamics builds up an interface with a fractal dimension d_f, which modified the FDT, and allowed a possible solution for the KPZ exponents [38,39].

IV. BALLISTIC DIFFUSION

Ballistic diffusion is extremely important in condensed systems. Perhaps the best-known examples are superconductivity and superfluidity [40,41]. However, ballistic diffusion appears in a large number of situations, such as spin waves in the disordered Heisenberg chain [42,43] and in many diffusive systems. Although the method can be applied to several situations, we concentrate here on the analysis of diffusion. In previous works, we considered the case of ergodic ballistic diffusion with the obtainment of diffusion of the type $\alpha = 2^{-}$ [44]. The slow ballistic motion $\alpha = 2^{-}$ has properties that differ markedly from the ballistic. Now, in this paper, we concentrate here on the analysis of ballistic diffusion in the case of systems where there isn't ergodicity.

Let us consider the spectral density

$$\rho(\omega) = \begin{cases} \frac{A}{w_2 - w_1}, & \omega_1 < \omega < \omega_2, \\ 0, & \text{out of the interval.} \end{cases} \tag{36}$$

where A is a constant. For $w_1 = 0$ and $w_2 \to \infty$ we have a white noise and a memoryless Langevin's equation. For $w_1 = 0$ and w_2 finite, we have normal diffusion [9] and it applies to many systems, such as the free electron gas [45]. For $w_1 > 0$, the absence of the lower modes in the spectra makes the relaxation very slow and a full equilibrium is not reached. We shall see that it originates a nonergodic ballistic motion. For introducing $\rho(\omega)$ in Eq (18), we'll find the following memory function

$$\Gamma(t) = \frac{A}{w_1 - w_2}\left(\frac{\sin(\omega_1 t)}{t} - \frac{\sin(\omega_2 t)}{t}\right). \tag{37}$$

Using the Laplace transform from Eq. (37), we have

$$\widetilde{\Gamma}(z) = \frac{A}{w_1 - w_2}\left[\arctan\left(\frac{\omega_1}{z}\right) - \arctan\left(\frac{\omega_2}{z}\right)\right]. \tag{38}$$

For small values of x $\arctan(1/x) \sim \pi/2 - x$, so

$$\widetilde{\Gamma}(z) = \frac{A}{w_1 - w_2}\left(\frac{1}{w_2} - \frac{1}{w_1}\right)z = \frac{A}{w_1 w_2}z, \tag{39}$$

and we obtain the nonergodic factor

$$\kappa = \lim_{t\to\infty} R(t) = \lim_{z\to 0} z\widetilde{R}(z) = \frac{w_1 w_2}{w_1 w_2 + A}, \tag{40}$$

where we have used Eq. (16). According to the Khinchin Theorem, this diffusive system is not ergodic. In simple terms, this system doesn't simply forget the past completely, even after a long time, such as what happens within ballistic diffusion. Additionally, see that $\lambda = \lim_{t\to\infty} \lambda(t) = \nu = 1$ e $\alpha = \nu + 1 = 2$.

A. Temporal behavior of $\lambda(t)$ function

In Fig. 1 we show $\lambda(t)$ as a function of time t. We used the Laplace transform of the memory function, Eq. (38) and the relations in Eqs. (26) and (25). For curve (a) $\omega_1 = 2.5$, $\omega_2 = 3.5$; for curve (b) $\omega_1 = 1.5$, $\omega_2 = 2.5$. Note that both curves rapidly converge to $\lim_{t\to\infty} \lambda(t) = 1$. This fast convergence is a warranty that the scaling approximates the exact value. Again, the constant value of $\lambda(t \to \infty)$ shows that the simple form of scaling $z \propto 1/t$ works for $t \to \infty$.

B. Temporal behavior of correlation function - Numerical and asymptotics results

Now, we compare the analytical asymptotic solution with the numerical solution of Eq. (15). To do this, we rewrite this equation in a discrete form, and then we expand it up to terms

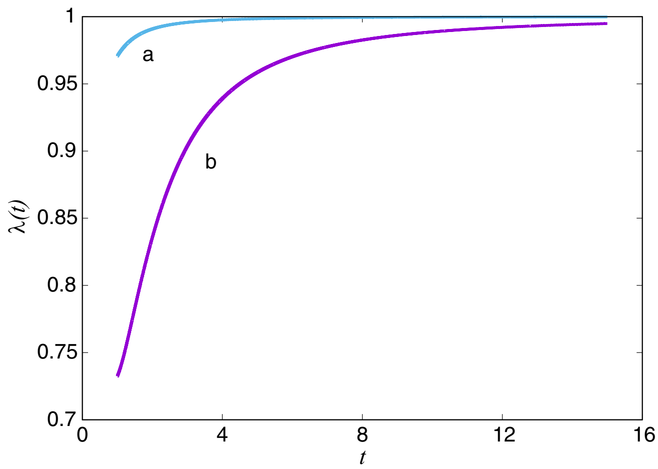

FIG. 1. $\lambda(t)$ as a function of time t. The curves are obtained using Eqs. (26), (25), and Eq. (38) with $A = 1$. On curve (a), $\omega_1 = 2.5$ and $\omega_2 = 3.5$. On curve (b), $\omega_1 = 1.5$ and $\omega_2 = 2.5$. For longer times both curves converge to 1.

of the order of Δt^{2n} to obtain

$$R(t + \Delta t) = R(t - \Delta t) + 2\sum_{k=0}^{n} R^{(2k-1)}(t)\frac{(\Delta t)^{2k-1}}{(2k-1)!}, \quad (41)$$

where $R^{(n)}(t)$ is the time derivative of $R(t)$ of the order of n. Note that this expression eliminates all the even derivatives. Now, we can all $R(t + \Delta t)$ from the sequence of the previous value of $R(t)$, starting from $R(0) = 1$. From these values, it is possible to get the diffusion coefficient through direct integration of Eq. (14). In the Appendix we show the numeric solution of the correlation function $R(t)$ with more details.

In Figs. 2 and 3 we show $R(t)$ as a function of time t. On curve (a) we numerically solve Eq. (15). Curve (b) is obtained

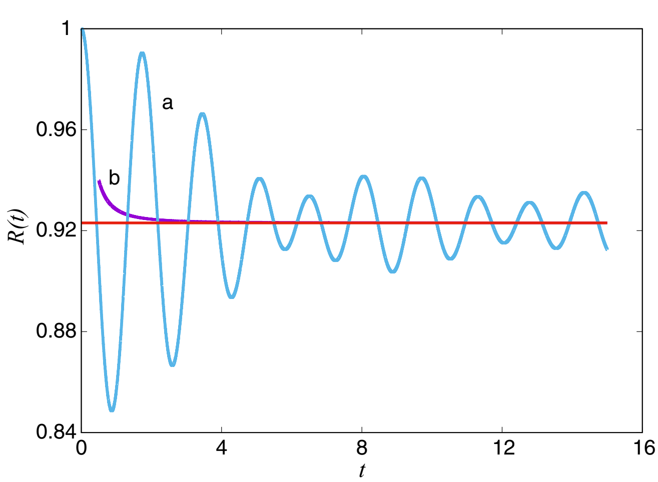

FIG. 2. The normalized correlation $R(t)$ as a function of time t. In both cases, $\omega_1 = 3.0$, $\omega_2 = 4.0$, and $A = 1$. The curve (a) corresponds to the numerical integration of Eq. (15), while curve (b) corresponds to the scaling. The horizontal line is the expected limit value $\kappa = R(t \to \infty)$.

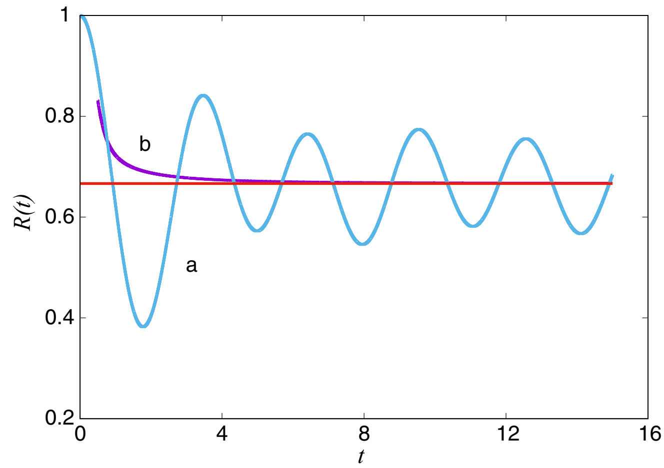

FIG. 3. The normalized correlation $R(t)$ as a function of time t. In both cases, $\omega_1 = 1.0$, $\omega_2 = 2.0$, and $A = 1$. The curve (a) corresponds to the numerical integration of Eq. (15), while curve (b) corresponds to the scaling. The horizontal line is the expected limit value.

using the scaling

$$R(t) = z\tilde{R}(z)|_{z=\lambda/t}, \quad (42)$$

and Eq. (38) with $\lambda(t)$ shown in Fig. 1. For curve (a) $\omega_1 = 1.0$, $\omega_2 = 2.0$, and $A = 1$; for curve (b) $\omega_1 = 3.0$, $\omega_2 = 4.0$, and $A = 1$. The horizontal line on curves (a) and (b) is the expected value of the correlation function $R(t)$ obtained in Eq. (37). Note that curve (b) is an average value of $R(t)$ and rapidly converges to the expected value give by the nonergodic factor $\kappa = R(t \to \infty)$, while the numeric result oscillates around this value.

C. Temporal behavior of diffusion - Numerical and asymptotics results

In Fig. 4 we show $D(t)$ as a function of time t. The curve with large oscillations is obtained by the numerical integration of $R(t)$. Here $a = 1$. For curve (a) $\omega_1 = 3.0$ and $\omega_2 = 4.0$; for curve (b) $\omega_1 = 1.0$ and $\omega_2 = 2.0$. The more stretched line is obtained using the scaling theory Eq. (21). The result is excellent for curve (b) and almost identical for (a). Note again that the faster convergence for $D(t)$ occurs in the case where $\lambda(t)$ reaches the limit faster.

We highlight that the diffusion $\alpha = 2^+$ doesn't exist, once, introducing $\tilde{\Gamma}(z) \sim -bz/lnz$ in the $\tilde{R}(z)$, denominator, the dominant term of $\tilde{R}(z) = 1/(z + \tilde{\Gamma}(z))$ to $z \to 0$ will be $\tilde{R}(z) \sim 1/z$. That way, $\alpha = 2$ stays as the higher diffusive exponent possible. Exponents $\alpha > 2$ are possible only with external force, but never due to the thermal bath.

To normal diffusion, $\alpha = 1$, or $\alpha = 1^{\pm}$, it has $\lambda = 0$. Therefore, the scaling in Eq. (20) is apparently inapplicable. In really it is its lowest limit. Thus, we still can obtain the limit value. Consider, as an example, the memoryless Langevin equation. For this, we have $R(t) = e^{-\gamma t}$ and $\tilde{R}(z) = (\gamma + z)^{-1}$. Using $D(t) = \widetilde{R}(\lambda(t)/t) = t/f(t)$, in units of $k_B T/m$,

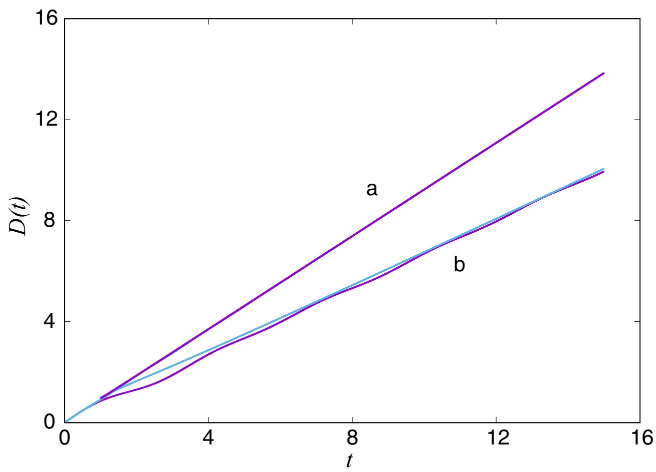

FIG. 4. The diffusion coefficient $D(t)$ as a function of time. In both cases $A = 1$. In curve (a), $\omega_1 = 3.0$ and $\omega_2 = 4.0$. In curve (b), $\omega_1 = 1.0$ and $\omega_2 = 2.0$. In (b) the curve with little oscillations is the result obtained by the numerical integration of $R(t)$. The less sinuous line corresponds to the scaling, Eq. (19). In (a) the two curves overlap.

we have

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \widetilde{R}(\lambda/t) = \frac{t}{\gamma t + \lambda} = \gamma^{-1}, \tag{43}$$

and for direct integration we obtain,

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \int_0^t R(t')dt' = \gamma^{-1}. \tag{44}$$

In this case, the scaling obtains exactly the desired limit value. On the other hand, note that a diffusion of the types $\langle x^2(t \gg \tau)\rangle \sim t\ln(t)$ possess diffusion exponent $\alpha = 1^+$. This type of diffusion can be classified as weak superdiffusion, once only the term $\ln(t)$ makes it superdiffusive.

V. SUMMARY AND CONCLUSIONS

In this work we study how generalized Langevin's stochastic dynamics can be used to investigate anomalous diffusion. Next, we presented an asymptotic method to obtain an analytical expression for the diffusion coefficient through the introduction of a time scale factor $\lambda(t)$. We found an exact expression for $\lambda(t)$, and we showed that for large times, $\lambda(t)$ becomes a universal parameter determined by the diffusion exponent α, i.e., $\lambda(t\to\infty) = \lambda = \alpha - 1$. The analytical results agree with the numerical ones. Next, we showed the practical effects of scaling. The first observation was that $\lambda(t)$ rapidly converges to a constant. Another very important point was the classification of new forms of diffusion due to the generalized exponent. We verified as well the existence of the nonballistic diffusion type, with $\alpha = 2$ with the obtainment of the diffusion coefficient and we showed that the scaling works. This method is general and can be applied to various types of stochastic problems. The dynamics of relaxation mechanisms have attracted great attention in recent decades. Correlation functions with nonexponential relaxation [46–48] appear constantly in the literature; some examples can be found in supercooled colloidal systems [49], diffusion in ratchet potentials [50,51], glass and granular materials [52,53], hydrated proteins [54,55], growing interface [56], plasma [57,58], and disordered vortex networks in superconductors [59,60]. These systems have characteristics similar to those presented by systems with anomalous diffusion. Thus, there are great perspectives on the use of scaling, such as used in this work, in different stochastic processes.

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APPENDIX: CORRELATION FUNCTION NUMERICAL RESOLUTION

In this section we show how to obtain the correlation functions numerically. Expanding Eq. (39) to the fifth order, we have

$$R(t+\Delta t) - R(t-\Delta t) = 2\Delta t\left[\frac{dR(t)}{dt}\Delta t + \frac{1}{3!}\frac{d^3R(t)}{dt^3}(\Delta t)^3 + \frac{1}{5!}\frac{d^5R(t)}{dt^5}(\Delta t)^5\right]. \tag{A1}$$

Here we will use the notation $R^{(n)}$ and $\Gamma^{(n)}$ for the derivative of order n concerning the time. Remembering that

$$R^{(1)} = \frac{dR(t)}{dt} = -\int \Gamma(t-t')R(t')dt', \tag{A2}$$

and that all the odd-order derivatives $R^{(2n+1)}(t)$ and $\Gamma^{(2n+1)}(t)$ are equal to zero at the origin because they are even functions. It follows that

$$R^{(2)} = -\Gamma(0)R(t) - \int \Gamma^{(1)}(t-t')R(t')dt', \tag{A3}$$

$$R^{(3)} = -\Gamma(0)R^{(1)}(t) - \int \Gamma^{(2)}(t-t')R(t')dt', \tag{A4}$$

or for the n order

$$R^{(n)} = -\Gamma(0)R^{(n-2)}(t) - \int \Gamma^{(n-1)}(t-t')R(t')dt'. \tag{A5}$$

We define the effective memory $\Gamma_n(t)$, that is, the order n approximation that is placed in Eq. (39) allows the obtainment of $R(t+\Delta(t))$ making only one integral so that

$$R(t+\Delta t) = R(t-\Delta) + 2\Delta t\int_0^t \Gamma_n(t-t')R(t')dt'. \tag{A6}$$

For the first order, we have $\Gamma_1(t) = \Gamma(t)$. For third order

$$R(t+\Delta t) = R(t-\Delta t) + 2\Delta t\left[R^{(1)}(t)\Delta t + \frac{1}{3!}R^{(3)}(t)\Delta t^3\right]. \tag{A7}$$

Replacing the Eqs. (A2) and (A4) in Eq. (A7), we get third order effective memory

$$\Gamma_3(t) = \left[1 - \frac{\Gamma(0)\Delta t^2}{3!}\right]\Gamma(t) + \frac{\Delta t^2}{3!}\Gamma_2(t). \tag{A8}$$

For the fifth order

$$R(t+\Delta t) = R(t-\Delta t) + 2\Delta t \times \left[R^{(1)}(t)\Delta t + \frac{1}{3!}R^{(3)}(t)\Delta t^3 + \frac{1}{5!}R^{(5)}(t)\Delta t^5\right]; \tag{A9}$$

in this way we obtain the effective fifth order memory function

$$\Gamma_5(t) = \left[1 - \frac{\Gamma(0)\Delta t^2}{3!} + \frac{\Gamma(0)^2\Delta t^4}{5!}\right]\Gamma(t) + \left[\frac{\Delta t^2}{3!} - \frac{\Gamma(0)\Delta t^4}{5!}\right]\Gamma_2(t) + \frac{\Delta t^4}{5!}\Gamma_4(t), \tag{A10}$$

and so on. For example, considering a very small integration interval in Eq. (A2), such that $\Gamma(t-t') \sim \Gamma(0)$ and

$$\frac{dR(t)}{dt} = -\Gamma(0)\int_0^t R(t')dt'. \tag{A11}$$

Deriving Eq. (A11)

$$\frac{d^2R(t)}{dt} = -\Gamma(0)R(t). \tag{A12}$$

This way we can write

$$R(t) = \cos(\omega_0 t), \tag{A13}$$

where $\omega_0^2 = \Gamma(0)$. Equation (A13) satisfies $R(0) = 1$ and $R^{(2k+1)}(0) = 0$. Let's now rewrite $\Gamma_n(t)$ in the form

$$\Gamma_n(t) = \sum_{k=0}^{n} A_{n,k}\Gamma^{(k)}(t), \tag{A14}$$

since $\Gamma(t)$ is even $A_{n,2k+1} = 0$ and

$$A_{n,2k} = \frac{(-1)^k}{(\omega_0)^{2k}}\sum_{j=k}^{(n-1)/2}\frac{(-1)^j(\omega_0\Delta t)^{2j}}{(2j+1)!}. \tag{A15}$$

In practice, $n = 5$ already produces excellent results.

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