Analytical results for long-time behavior in anomalous diffusion

R. M. S. Ferreira,[1] M. V. S. Santos,[2] C. C. Donato,[2] J. S. Andrade, Jr.,[1] and F. A. Oliveira[2]

[1]*Departamento de Física,Universidade Federal do Ceará, Caixa Postal 6030, 60455-900 Fortaleza, Ceará, Brazil**

[2]*Instituto de Física e Centro Internacional de Física da Matéria Condensada, Universidade de Brasília, Caixa Postal 04513,*

70919-970 Brasília, Distrito Federal, Brazil

We investigate through a generalized Langevin formalism the phenomenon of anomalous diffusion for asymptotic times, and we generalized the concept of the diffusion exponent. A method is proposed to obtain the diffusion coefficient analytically through the introduction of a time scaling factor λ. We obtain as well an exact expression for λ for all kinds of diffusion. Moreover, we show that λ is a universal parameter determined by the diffusion exponent. The results are then compared with numerical calculations and very good agreement is observed. The method is general and may be applied to many types of stochastic problem.

I. INTRODUCTION

The study of systems with long range memory reveals some physical phenomena that are still not well understood, especially in systems which are outside the state of equilibrium or those in which the existence of anomalous diffusion is verified [1–8]. Here we show a simple analytical method which describes the behavior of the diffusion for large and intermediate times. In order to do that, we first generalize the concept of the diffusion exponent. Then we present a conjecture to obtain, through the introduction of a time scaling factor λ, an analytical asymptotic result for the diffusion coefficient for long times. We obtain the scaling factor exactly and we show as well its universal behavior. We derive a numerical method to obtain the correlation function of velocities for an ensemble of particles from any given memory. We compare both methods and we obtain excellent agreement. The method has general application in the study of stochastic processes and it could be applied to several situations of physical interest.

II. GENERALIZED LANGEVIN EQUATION AND DIFFUSION

The generalized Langevin equation (GLE) is a stochastic differential equation which can be used to model systems driven by colored random forces. For the velocity operator $v(t)$ this equation can be written as

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

where $\Gamma(t)$ is the retarded friction kernel of the system, or the memory function. Here, $\xi(t)$ is a stochastic noise subject to the conditions $\langle\xi(t)\rangle = 0$, $\langle\xi(t)v(0)\rangle = 0$, and

$$C_\xi(t) = \langle\xi(t)\xi(0)\rangle = m^2\langle v^2(t)\rangle\Gamma(t), \qquad (2)$$

where $C_\xi(t)$ is the correlation function for $\xi(t)$, and the angular brackets denote an average over the ensemble of particles. Equation (2) is Kubo's fluctuation dissipation theorem (FDT) [9,10]. 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 correlation between the various stages of dynamic evolution. This property is what we call memory, and it makes remote events of the past important to dynamic events in the present time.

Using the GLE it is possible to study the asymptotic behavior of the second moment of the particle movement,

$$\lim_{t\to\infty}\langle x^2(t)\rangle = 2D(t)t \sim t^\alpha, \qquad (3)$$

which characterizes the type of diffusion presented by the system. Here, $D(t)$ is the diffusion coefficient as a function of time.

Moreover, for an asymptotic behavior of the form

$$\lim_{t\to\infty}\langle x^2(t)\rangle \sim t^\alpha[\ln(t)]^{\pm 1}, \qquad (4)$$

we shall define respectively an $\alpha^\pm$ diffusive behavior. Here the exponent $\alpha = \alpha^\pm$ arises in analogy with the critical exponents in a phase transition. For example, in the two-dimensional Ising model the critical exponent for the specific heat is $\alpha = 0^+$ because it does not have a power law behavior; rather it has $\ln|T - T_c|$ behavior for temperatures T close to the transition temperature T_c. This generalized nomenclature is pertinent here since there are quite a large number of possibilities of combinations for logarithmic and power law behaviors.

In this way the behavior of $D(t)$ can be determined using

$$\lim_{t\to\infty}D(t) = \lim_{t\to\infty}\lim_{z\to 0}\int_0^t C_v(t')\exp(-zt')dt' = \lim_{z\to 0}\widetilde{R}(z),$$
$$(5)$$

where $R(t) = C_v(t)/C_v(0)$, with $C_v(0) = 1$, and $\widetilde{R}(z)$ is the Laplace transform of $R(t)$. For $t \to \infty$ and normal diffusion this is the Kubo formula [10]. The limits can be justified using the final value theorem (FVT) for a Laplace transform [11], i.e., for any function $g(t)$ with Laplace transform $\widetilde{g}(z)$ then $\lim_{t\to\infty}g(t) = \lim_{z\to 0}z\widetilde{g}(z)$. Now a Laplace transform of the integral gives $\widetilde{D}(z) = \widetilde{R}(z)/z$, and we end up with the equation above.

Now we multiply Eq. (1) by $v(0)$ and take the average over the ensemble, with $\langle\xi(t)v(0)\rangle = 0$, to obtain a self-consistent

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*rogelma@fisica.ufc.br

equation for $R(t)$ in the form

$$\dot{R}(t) = -\int_0^t \Gamma(t - t')R(t')dt'. \tag{6}$$

We then Laplace transform Eq. (6) to get

$$\widetilde{R}(z) = \frac{1}{z + \widetilde{\Gamma}(z)}. \tag{7}$$

Time correlation functions play a central role in nonequilibrium statistical mechanics in many areas, such as the dynamics of polymeric chains [12], metallic liquids [13], Lennard-Jones liquids [14], ratchet devices [15,16], spin waves [17], Heisenberg ferromagnets, and dense fluids [18]. Consequently to invert this transform, 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 diffusion.

III. THE CONJECTURE

We claim that after a "transient time" τ, i.e., for $t > \tau$, the leading term for $D(t)$ will fulfill Eq. (5) within a given approximation. In this context $t \to \infty$ is equivalent to $t \gg \tau$. Now we imposed the scaling

$$z \to \lambda/t. \tag{8}$$

In order to determine λ we rewrite Eq. (5) as

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \widetilde{R}(z = \lambda/t) = \lim_{t\to\infty} \frac{t}{f(t)}, \tag{9}$$

where

$$f(t) = \lambda + t\widetilde{\Gamma}(\lambda/t). \tag{10}$$

The derivative of Eq. (9) yields

$$\lim_{t\to\infty} R_1(t) = \lim_{t\to\infty} \frac{d}{dt}D(t) = \lim_{t\to\infty} \left[1 - t\frac{d}{dt}\ln[f(t)]\right] \bigg/ f(t), \tag{11}$$

while from the FVT we have

$$\lim_{t\to\infty} R_2(t) = \lim_{z\to 0} z\widetilde{R}(z) = \lim_{t\to\infty} \frac{\lambda}{f(t)}. \tag{12}$$

The relative difference

$$\Delta R(t) = \frac{R_2 - R_1}{R_2} = \left[\lambda - 1 + t\frac{d}{dt}\ln[f(t)]\right] \bigg/ \lambda \tag{13}$$

should evolve to zero as $t \to \infty$. For $\lambda \neq 0$ this yields the exact value

$$\lambda = 1 - \lim_{t\to\infty} t\frac{d}{dt}\ln[f(t)]. \tag{14}$$

The scaling works as long as the GLE, Eq. (7), works. To obtain λ we need more information about $\widetilde{\Gamma}(z)$, which may be different for every system. However, since our interest is in the asymptotic behavior, we can expand $\widetilde{\Gamma}(z)$, in Taylor or Laurent series around $z = 0$, in the form

$$\widetilde{\Gamma}(z) \sim z^\nu[a - b\ln(z) - c/\ln(z)], \tag{15}$$

where a, b, and c are positive constants. Note that we give especial attention to $\ln(z)$, since it will give us the behavior pointed out in Eq. (4). For $b = 0$ this gives a diffusion with exponent α; for $b \neq 0$ this gives an α^-, and for $a = b = 0$ and $c \neq 0$ we get an α^+ diffusion. If $\widetilde{\Gamma}(z)$ 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. (15) for small z. Now we introduce Eq. (15) into Eq. (14) to obtain $\lambda = \nu$ for $\nu < 1$ and $\lambda = 1$ for $\nu \geqslant 1$. Notice that it does not depend on a, b, or c, which suggests a universal behavior.

In our conjecture some points deserve attention: First, we are considering integrals, of the form Eq. (5), where the function $R(t)$ is well behaved, and limited to $-1 < R(t) < 1$, since $C_v(t) \leqslant C_v(0)$. $R(t)$ is such that it always has a well-defined behavior for finite t, even when the integral diverges as $t \to \infty$, as in superdifusion. Second, $D(t)$ must have a leading term as $t \to \infty$, which determines the diffusion. For example, the inverse Laplace transform of $\widetilde{R}(z)$ is

$$R(t) = \frac{1}{2\pi i}\int_{-i\infty+\eta}^{+i\infty+\eta} \widetilde{R}(z)\exp(zt)dz. \tag{16}$$

Here the real number η is such that all the singularities lie at the left of the line joining the limits. Consider now Eq. (15) with $b = c = 0$ and $\nu \leqslant 1$; then $\lim_{z\to 0}\widetilde{R}(z) \sim z^{-\nu}$, and

$$\lim_{t\to\infty} R(t) \propto t^{\nu-1}\int_{-i\infty+\eta'}^{+i\infty+\eta'} s^{-\nu}\exp(s)ds \propto t^{\nu-1}, \tag{17}$$

where we have done the transformations $s = zt$ and $\eta' = \eta/t$. For $\nu > 0$ the only pole is at $s = 0$, and the condition in η' will be automatically satisfied. Now by direct integration on Eq. (5) we obtain $D(t) \propto t^\nu$. From the scaling we get the equivalent result

$$\lim_{t\to\infty} D(t) = \lim_{z\to 0} \widetilde{R}(z = \lambda/t) \sim \lim_{t\to\infty} \widetilde{R}(\lambda/t) \sim t^\nu. \tag{18}$$

Note that the above exact result is not only for power laws, but for any function behaving as a power law for large t. We confirm as well the relation $\alpha = \nu + 1$, obtained by Morgado *et al.* [1]. Our results can be readily expressed as

$$\lambda = \alpha - 1 = \alpha^\pm - 1 = \begin{cases} \nu, & -1 < \nu < 1, \\ 1, & \nu \geqslant 1 \end{cases} \tag{19}$$

The factor λ depends only on the diffusion exponent α; consequently it is universal. Moreover it will be the same for α or $\alpha^\pm$. For normal diffusion $\alpha = 1$, or for $\alpha = 1^\pm$, $\lambda = 0$. However, we still can obtain the final value. Consider as example the Langevin equation without memory; for that we have $R(t) = \exp(-\gamma t)$ and $\widetilde{R}(z) = (\gamma + z)^{-1}$. From Eq. (9) we get

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \widetilde{R}(\lambda/t) = \frac{t}{\gamma t + \lambda} = \gamma^{-1}, \tag{20}$$

while direct integration gives

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \int_0^t R(t')dt' = \gamma^{-1}. \tag{21}$$

In this case the scaling yields correctly the wanted final value.

Equation (6) imposes as well 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. Indeed, we do not expect exponential behavior of the form $R(t) = \exp(-\gamma|t|)$ with a discontinuous derivative at the origin [19,20]. Second, in Eq. (1), for a bath of harmonic oscillators the noise can be obtained as [19]

$$\xi(t) = \int \sqrt{2k_B T g(\omega)} \cos[\omega t + \phi(\omega)] d\omega, \qquad (22)$$

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

$$\Gamma(t) = \int g(\omega) \cos(\omega t) d\omega. \qquad (23)$$

This shows that the memory is an even function of t. An analytical extension of $\widetilde{\Gamma}(z)$ in the whole complex plane has the property $\widetilde{\Gamma}(-z) = -\widetilde{\Gamma}(z)$. Consequently, from Eq. (7), $\widetilde{R}(-z) = -\widetilde{R}(z)$, 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.

IV. BALLISTIC DIFFUSION

Let us consider the spectral density

$$g(\omega) = \begin{cases} b\omega_s^{1-\beta}\omega^\beta, & \omega \leqslant \omega_s, \\ 0, & \omega > \omega_s. \end{cases} \qquad (24)$$

This is a generalization of the Debye density of states. Here $b > 0$ is a dimensionless constant, and ω_s is a cutoff frequency. For $\beta \neq 0$ we get anomalous diffusion. In particular, for $\beta = 1$ we introduce Eq. (24) into Eq. (23) to obtain

$$\Gamma(t) = b\omega_s^2 \left(\frac{\sin(\omega_s t)}{\omega_s t} + \frac{\cos(\omega_s t) - 1}{(\omega_s t)^2} \right), \qquad (25)$$

with the Laplace transform

$$\widetilde{\Gamma}(z) = \frac{bz}{2} \ln\left[1 + \left(\frac{\omega_s}{z} \right)^2 \right]. \qquad (26)$$

First, we have the analytical function $D(t) = \widetilde{R}(z = \lambda/t)$; second, from Eq. (14) we obtain $\lim_{t\to\infty} \lambda = 1$ exactly. This is ballistic diffusion of the form $\alpha = 2^-$.

Now we compare the analytical asymptotic with a numerical solution of Eq. (6). To do this, we rewrite this equation in a discrete form, and then we expand it up to terms of order Δt^{2n} to obtain

$$R(t + \Delta t) = R(t - \Delta t) + 2 \sum_{k=0}^{n} R^{(2k-1)}(t) \frac{(\Delta t)^{2k-1}}{(2k-1)!}, \qquad (27)$$

where $R^{(n)}(t)$ is the time derivative of $R(t)$ of order n. Note that this expansion eliminates all the even derivatives. Now we can obtain all $R(t + \Delta t)$ from the sequence of the previous value of $R(t)$, starting from $R(0) = 1$. From these values, its possible to get the diffusion coefficient through direct integration of Eq. (5).

In Fig. 1 we plot the correlation function $R(t)$ as a function of time t. The curves correspond to the numerical solution and are calculated using Eq. (27), and Eq. (25) with $\Delta t = 10^{-5}$. For curve a, $\omega_s = 1$ and $b = 1$; for curve b, $\omega_s = 5$ and $b = 1/2$.
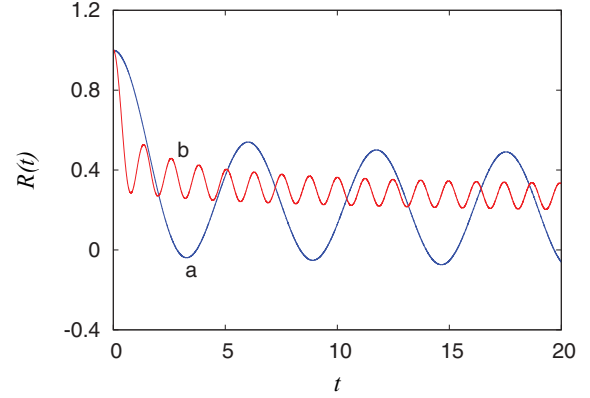

FIG. 1. (Color online) Correlation function $R(t)$ as a function of time t. We use the memory (25) and numerical integration. Curve a, $\omega_s = 1$ and $b = 1$; curve b, $\omega_s = 5$, and $b = 1/2$.

In Fig. 2 we plot the diffusion coefficient $D(t)$ as a function of time t. The oscillatory curves corresponds to the numerical solution and are calculated from the data of Fig. 1. The curves without oscillations correspond to the analytical asymptotic limit, Eq. (9), with memory Eq. (26). Here we see that the asymptotic curves are mean values of the oscillatory ones. In this range the fit yields for curve a, $\lambda = 0.928 \pm 0.002$, and for curve b, $\lambda = 0.948\,22 \pm 0.000\,01$. We see in curve b that the two curves collapse onto a single one. Here the transient time τ to which we refer before Eq. (9) is a decreasing function of b/ω_s. The value of λ approaches the exact value 1 as the ratio b/ω_s decreases, or as time increases. This shows the efficiency of the scaling; even before convergence is fully established, curve a, the asymptotic curve gives us an average value that can be used to understand the main characteristics of the process.

Consider now $\widetilde{\Gamma}(z) = az$, exactly. That means $\widetilde{R}(z) = [(1 + a)z]^{-1}$ or $R(t) = [1 + a]^{-1}$, and by direct integration we get $D(t) = t/(1 + a)$ exactly. This is ballistic $\alpha = 2$ diffusion. If we apply Eq. (9) we obtain the same result with $\lambda = 1$. Since from the relations (15) and (19) the value of λ does not depend on $\ln(z)$, this result is exactly what we get from Eq. (26).
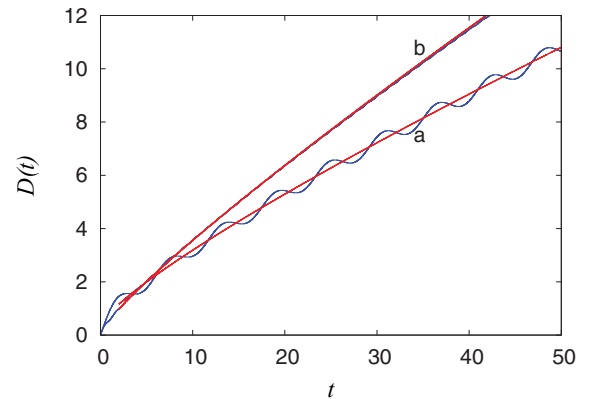

FIG. 2. (Color online) Diffusion coefficient $D(t)$ as a function of time t. Curve a, $\omega_s = 1$ and $b = 1$; curve b, $\omega_s = 5$ and $b = 1/2$. The oscillatory curves are the numerical result. The curves without oscillations are the analytical asymptotic limit. We see in curve b that the two curves collapse onto a single one.

There are important differences between the $\alpha = 2^-$ diffusion, which according to the Khinchin theorem [6,21] is ergodic, and the $\alpha = 2$ diffusion, which does violate ergodicity. This distinction was not possible before the generalization of the diffusion exponent we present here.

V. CONCLUSION

In this work we generalize the concept of the diffusion exponent, and we propose a conjecture to investigate the asymptotic limits of anomalous diffusion, through the introduction of a time scaling factor λ. We obtain the scaling parameter exactly and we show that it is universal and depends only on the diffusion exponent. We analyze the ballistic diffusions $\alpha = 2^-$ and $\alpha = 2$, both analytically and numerically. The method can be useful as well to analyze large amounts of data in stochastic processes [5], and in different fields of science where is necessary to inverse a Laplace transform of the form of Eq. (7). The phenomenon of diffusion also poses challenges in the understanding of fundamental concepts in statistical physics, such general properties as the correlation function [19], ergodicity [6,8,21–23], and the Khinchin theorem [6,21]. In nonlinear phenomena, such as growth and etching [24], analytical results are rather difficult to obtain. In this way we hope that this work may inspire research into similar asymptotic limits.

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