GENERAL SCALING RELATIONS IN ANOMALOUS DIFFUSION*

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Diffusion regimes most frequently found in nature are described in terms of asymptotic behaviors. In this work, we use a generalization of the final-value theorem for Laplace transform in order to investigate the anomalous diffusion phenomenon for asymptotic times. We generalize the concept of the diffusion exponent, including a wide variety of asymptotic behaviors than the power law. 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, which makes possible to describe all diffusive regimes featuring a universal parameter determined by the diffusion exponent. We show the existence of two kinds of ballistic diffusion, ergodic and non-ergodic. The method is general and may be applied to many types of stochastic problem.

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1. Introduction

The study of systems with long-range memory-friction kernel reveals some physical phenomena that are still not well understood, especially whether they are outside of equilibrium or in anomalous diffusive regime [1–26]. In this context, studies on correlation functions have contributed to new insights and methodologies of wide application influencing many

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fields, such as the dynamics of polymeric chains [27–35], metallic liquids [36], Lennard–Jones liquids [37], ratchet devices [38, 39], reaction rates [29–31], diffusion of spin waves in disordered systems [40], Heisenberg ferromagnets and dense fluids [41], biological systems [42–46], to cite just a few examples. The vast majority of these problems are non-Markovian since there is correlation between the various stages of dynamic evolution; this property is the so-called memory-friction, which makes remote events of the past important to dynamic events in the present time. In a recent work, Ferreira *et al.* [1] have been discussing a scaling method to obtain asymptotic results for long time behavior in anomalous diffusion. We revisit this work to call attention to connection between this approach and other stochastic phenomena in which memory-friction is present. Although the method can be applied to several situations, we focus our attention on the analysis of diffusion.

Here, we show a simple analytical method which describes the diffusion behavior for large and intermediate times. First, we generalize the understanding of the diffusion exponent. In order to obtain an analytical asymptotic result for the diffusion coefficient, a conjecture is presented from introducing a time scaling factor λ; as we shall doubtless see, the scaling factor assumes an exact value beyond expressing a universal behavior. We derive a numerical method to obtain the velocity autocorrelation function for an ensemble of particles from any given memory-friction kernel; the results are in close agreement. The method has general application in the study of stochastic processes and it could be applied to several situations of physical interest.

2. Memory-friction kernel and anomalous diffusion

The generalized Langevin equation (GLE) is a stochastic differential equation which can be used to model systems driven by colored random forces; the stochastic force is not anymore delta-correlated. For the velocity $v(t)$, this equation can be written as

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

where $\Gamma(t)$ is the retarded memory-friction kernel of the system, or merely the memory function. Here, $\xi(t)$ is a stochastic force (noise), which is fully characterized by the ensemble averages $\langle\xi(t)\rangle = 0$, $\langle\xi(t)v(0)\rangle = 0$, and

$$C_\xi(t) = \langle\xi(t)\xi(0)\rangle = m^2\left\langle v^2(t)\right\rangle\Gamma(t)\,, \tag{2}$$

where $C_\xi(t)$ is the noise autocorrelation function. Equation (2) is Kubo's fluctuation dissipation theorem (FDT) [47, 48]. The presence of the kernel $\Gamma(t)$ allows us to study a large number of correlated processes.

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

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

which characterizes the type of diffusion exhibit by the system; as a generalization of Einstein's relation for the mean square displacement of an ensemble of particles. Here, $D(t)$ is the diffusion coefficient as a function of time. As usual, the system is in a normal diffusive regime for $\alpha = 1$, likewise $\lim_{t\to\infty} D(t) =$ constant; a subdiffusive regime if $0 < \alpha < 1$, similarly $\lim_{t\to\infty} D(t) = 0$; a superdiffusive regime if $2 \geq \alpha > 1$, similarly $\lim_{t\to\infty} D(t) = \infty$. Moreover, for an asymptotic behavior of the form

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

we shall define respectively, an $\alpha^\pm$ diffusive behavior [1]. 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 $\ln|T - T_\mathrm{c}|$ 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

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

where $R(t) = C_v(t)/C_v(0)$, with $R(0) = 1$, and $\widetilde{R}(z)$ is the Laplace transform of $R(t)$; this is the Kubo's formula [48] for $t \to \infty$ and normal diffusion. The limits can be justified using the final-value theorem (FVT) for a Laplace transform [49], *i.e.* for any function $g(t)$ with a 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 $\widetilde{D}(z) = \widetilde{R}(z)/z$, ending up with the equation above. From this, it is straightforward to derive a self-consistent equation for $R(t)$ in the form

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

In such a situation, applying the Laplace transform, one gets

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

In order to describe the time-correlation function, it is crucial to invert this transform, or a similar one. 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.

3. The λ-scaling method

We consider now the FVT for $D(t)$

$$\lim_{t\to\infty} D(t) = \lim_{z\to 0} z\widetilde{D}(z) = \lim_{z\to 0} \widetilde{R}(z) \,. \tag{8}$$

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

$$z \to \frac{\lambda}{t} \,. \tag{9}$$

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

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \widetilde{R}(z = \lambda/t) = \lim_{t\to\infty} \frac{t}{f(t)} \,, \tag{10}$$

where

$$f(t) = \lambda + t\widetilde{\Gamma}(\lambda/t) \,. \tag{11}$$

The derivative of Eq. (10) yields

$$\lim_{t\to\infty} R_1(t) = \lim_{t\to\infty} \frac{d}{dt} D(t) = \lim_{t\to\infty} \frac{1 - t\dfrac{d}{dt}\ln\left[f(t)\right]}{f(t)} \,, \tag{12}$$

while from the FVT for $R(t)$, we get

$$\lim_{t\to\infty} R_2(t) = \lim_{z\to 0} z\widetilde{R}(z) = \lim_{t\to\infty} \frac{\lambda}{f(t)} \,. \tag{13}$$

The relative difference

$$\Delta R(t) = \frac{R_2 - R_1}{R_2} = \frac{\lambda - 1 + t\dfrac{d}{dt}\ln\left[f(t)\right]}{\lambda} \tag{14}$$

should evolve to zero as $t \to \infty$. The exact value is obtained for $\lambda \neq 0$, which yields

$$\lambda = 1 - \lim_{t\to\infty} t\frac{d}{dt}\ln\left[f(t)\right]. \tag{15}$$

The scaling works as long as the GLE holds. It is, generally, possible to derive a GLE for the Markovian systems by eliminating variables in which effects are incorporated in the memory-friction kernel and in the colored noise [50]. In particular, the absence of a coupling to a thermal bath (explicit in the GLE) and consequently, the lack of a detailed balance relation or FDT may require a specific analysis of each case. However, since it is possible to give a kinetic description of the Hamiltonian dynamics by means of a fractional Fokker–Planck–Kolmogorov equation [51], it is expected that the treatment of anomalous diffusion in such systems should also be possible by the GLE formalism.

In order to obtain λ, we need to make progress on $\widetilde{\Gamma}(z)$, which may be different in each system. However, we can expand $\widetilde{\Gamma}(z)$ in Taylor or Laurent series around $z = 0$ since we are interested in the asymptotic behavior. Based on this, one obtains

$$\widetilde{\Gamma}(z) \sim z^{\nu}[a - b\ln(z) - c/\ln(z)], \tag{16}$$

where a, b, and c are positive constants. Note that we pay special attention to $\ln(z)$; it will give us the behavior pointed out in Eq. (4). For $b = 0$, it furnishes a diffusion with exponent α; for $b \neq 0$, an α^{-}; for $a = b = 0$ and $c \neq 0$, an α^{+}. If $\widetilde{\Gamma}(z)$ has another contribution besides $\ln(z)$, it cannot be expanded at the origin as we kept it but does in other points. Nevertheless, for small z, most of the memories in the literature can be cast in the form of Eq. (16). Inserting Eq. (16) into Eq. (15), we obtain $\lambda = \nu$ for $\nu < 1$, and $\lambda = 1$ for $\nu \geq 1$. 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 $-1 < R(t) < 1$, whereas $C_v(t) \leq C_v(0)$ [10]. The function $R(t)$ 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, the function $D(t)$ must have a leading term as $t \to \infty$, which drives the diffusive motion. For instance, the inverse Laplace transform of $\widetilde{R}(z)$ is

$$R(t) = \frac{1}{2\pi i}\int_{-i\infty+\eta}^{+i\infty+\eta} \widetilde{R}(z)\exp(zt)dz. \tag{17}$$

Here, the real number η is such that all the singularities lie at the left of the line joining the limits. Consider now Eq. (16) with $b = c = 0$, and $\nu \leq 1$. Thus $\lim_{z\to 0} \widetilde{R}(z) \sim z^{-\nu}$ and

$$\lim_{t\to\infty} R(t) \propto t^{\nu-1} \int_{-i\infty+\eta'}^{+i\infty+\eta'} s^{-\nu} \exp(s) ds \propto t^{\nu-1}\,, \tag{18}$$

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, one obtains the equivalent result

$$\lim_{t\to\infty} D(t) = \lim_{z\to 0} \widetilde{R}(z = \lambda/t) \sim \lim_{t\to\infty} \widetilde{R}(\lambda/t) \sim t^{\nu}\,. \tag{19}$$

Note that the above exact result is not only for power laws, but also for any function performing as a power law for large t. We verify as well the relation $\alpha = \nu + 1$, obtained by Morgado *et al.* [2]. Our results can be readily expressed as

$$\lambda = \alpha - 1 = \alpha^{\pm} - 1 = \begin{cases} \nu, & -1 < \nu < 1 \\ 1, & \nu \geq 1 \end{cases}\,. \tag{20}$$

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. (10), one gets

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \widetilde{R}(\lambda/t) = \frac{t}{\gamma t + \lambda} = \gamma^{-1}\,, \tag{21}$$

while direct integration gives

$$\lim_{t\to\infty} D(t) = \lim_{t\to\infty} \int_0^t R\left(t'\right) dt' = \gamma^{-1}\,. \tag{22}$$

In this case, the scaling yields correctly the expected 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 correct except for non-analytical 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 [52, 53]. Second, in Eq. (1), for a bath of harmonic oscillators the noise can be obtained as [52]

$$\xi(t) = \int \sqrt{2k_{\mathrm{B}}Tg(\omega)}\cos[\omega t + \phi(\omega)]d\omega\,, \tag{23}$$

where $0 < \phi(\omega) < 2\pi$ are random phases and $g(\omega)$ is the noise spectral density. From the FDT, one obtains

$$\Gamma(t) = \int g(\omega)\cos(\omega t)d\omega\,. \tag{24}$$

This shows that the memory is an even function of t; even functions have zero derivatives at the origin as required before. 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. For finite times, we shall pay attention that one can obtain values of $\lambda(t)$ using Eq. (15) as a map in the form

$$\lambda_{n+1}(t) = F_l(\lambda_n(t), t) \tag{25}$$

with

$$F_l = 1 - t\frac{d}{dt}\ln[f(t)] = t\frac{d}{dt}\ln\left[\widetilde{R}(\lambda_n/t)\right]. \tag{26}$$

For a given memory function, this map converges readily for a final value of $\lambda(t)$ after few iterations.

4. The ballistic diffusion

Let us consider the spectral density

$$g(\omega) = \begin{cases} b\omega_s^{1-\beta}\omega^{\beta}, & \omega \le \omega_s \\ 0, & \omega > \omega_s \end{cases}\,. \tag{27}$$

The above equation acts as a generalization of the Debye density of states. Here $b > 0$ is a dimensionless constant and ω_s is a cutoff frequency. Notice that, for $\beta \neq 0$, one obtains anomalous diffusion. In particular, for $\beta = 1$, by inserting Eq. (27) into Eq. (24), it yields

$$\Gamma(t) = b\omega_s^2\left[\frac{\sin(\omega_s t)}{\omega_s t} + \frac{\cos(\omega_s t) - 1}{(\omega_s t)^2}\right], \tag{28}$$

with the Laplace transform

$$\widetilde{\Gamma}(z) = \frac{bz}{2}\ln\left[1 + \left(\frac{\omega_s}{z}\right)^2\right]. \tag{29}$$

First, we have the analytical function $D(t) = \widetilde{R}(z = \lambda/t)$; second, from Eq. (15), we have $\lim_{t\to\infty} \lambda = 1$, exactly. This corresponds to the ballistic diffusion in the form of $\alpha = 2^-$.

In Fig. 1, we have shown $\lambda(t)$ by using Eq. (25) and the Laplace transform of the memory-friction, Eq. (29). After 50 iterations the difference $|\lambda_{n+1} - \lambda_n|$ becomes less than 10^{-12}, thus reaching the numerical convergence; the convergence is faster as the ratio ω_s/b increases. For both curves, the plot has displayed the evolution of $\lambda(t)$ towards 1. The convergence is faster as the ratio ω_s/b increases. In addition, a comparison between the analytical asymptotic result and the numerical solution of Eq. (6) shall be provided. In this sense, we rewrite Eq. (6) in a discrete form and expand it up to terms of the order of Δt^{2n}, obtaining

$$R(t + \Delta t) = R(t - \Delta t) + 2\sum_{k=0}^{n} R^{(2k-1)}(t)\frac{(\Delta t)^{2k-1}}{(2k-1)!}, \tag{30}$$

where $R^{(n)}(t)$ is the time derivative of $R(t)$ of the order of n. Note that this expansion eliminates all the even derivatives. Thus, 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).

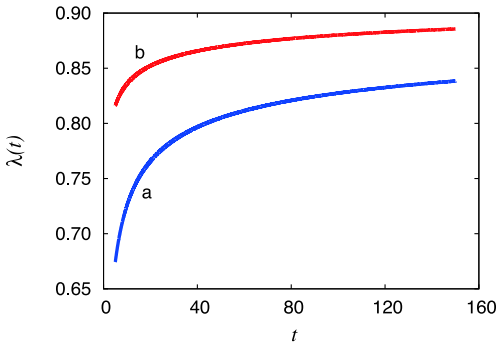


Fig. 1. The λ-scaling parameter as a function of time t. We have used the map (25) and the memory-friction kernel (29). The convergence has been reached over 50 rounds of iterations. The line 'a' (blue), we have used $\omega_s = 1$ and $b = 1$; the curve 'b' (red), we have used $\omega_s = 5$, and $b = 1/2$.

In Fig. 2, we have plotted the normalized correlation $R(t)$. The curves correspond to the numerical solution and are calculated by using Eq. (30) and Eq. (28) with $\Delta t = 10^{-5}$. The oscillations exhibited in Fig. 2 emphasize all dynamical contributions due to the response for the coupling between the system plus reservoir [15, 47, 48]. In this case, the system's dynamics

assuming different parameters impose non-Markovian evolutions in dissimilar transient regimes of the order of memory-friction time. This will reflect on the diffusion coefficient $D(t)$, Fig. 3.

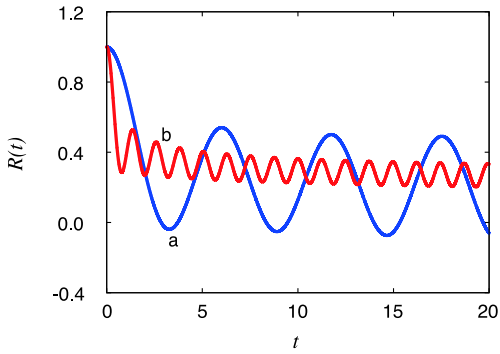


Fig. 2. The normalized velocity autocorrelation R as a function of time t. We have used the map (25) and the memory-friction kernel (29). The line 'a' (blue), we have used $\omega_s = 1$ and $b = 1$; the line 'b' (red), we have used $\omega_s = 5$ and $b = 1/2$.

In Fig. 3, the oscillatory (blue) lines correspond to the numerical solution and have been calculated from the data of Fig. 1. The lines without oscillations (red) correspond to the analytical asymptotic limit, Eq. (10), with memory function as Eq. (29). Here, we see that the asymptotic (red) lines are mean values of the oscillatory ones. In this range, the fit yields $\lambda = 0.928 \pm 0.002$, for line 'a', and $\lambda = 0.94822 \pm 0.00001$, for line 'b'. We

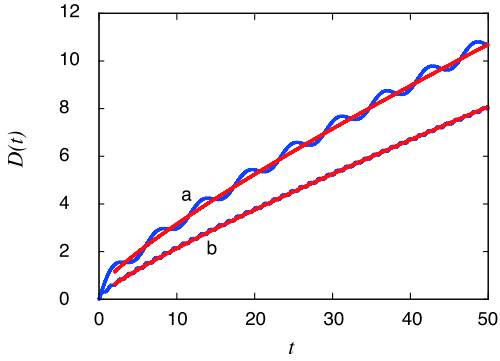


Fig. 3. The diffusion coefficient D as a function of time t. Lines 'a', we have used $\omega_s = 1$ and $b = 1$; lines 'b', we have used $\omega_s = 5$ and $b = 0.5$. The oscillatory (blue) lines are the numerical result. The (red) lines, without oscillations, are the analytical asymptotic limit. We see in lines 'b' that the two curves collapse onto a single one.

see in lines 'b' that the two curves collapse onto a single one. Here, the transient time τ to which we refer before, Eq. (10), 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, lines 'a', the asymptotic curve gives us an average value that can be used to understand the main characteristics of the process.

Consider now $\widetilde{\Gamma}(z) = az$, where a is a constant. It is straightforward to show that $\widetilde{R}(z) = [(1+a)z]^{-1}$, or $R(t) = [1+a]^{-1}$, and, by direct integration, $D(t) = t/(1+a)$, exactly. This covers ballistic diffusion with $\alpha = 2$. By applying Eq. (10), we obtain the same result with $\lambda = 1$. Since from the relations (16) and (20) the value of λ does not depend on $\ln(z)$, this result is exactly what we get from Eq. (29). There are important differences between the $\alpha = 2^-$ diffusion, which according to the Khinchin theorem [15, 54] 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.

5. Conclusion and perspectives

In this work, we have generalized the concept of the diffusion exponent by proposing a conjecture to investigate the asymptotic limits of anomalous diffusion. We have obtained an exact time scaling factor λ and also we have shown that it is universal, depending only on the diffusion exponent. We have analyzed the ballistic diffusions in two different regimes: $\alpha = 2^-$ and $\alpha = 2$; both analytically and numerically. Our method can be useful as well to analyze large amounts of data in stochastic processes [9] and in different fields of science, where is necessary to inverse a Laplace transform of the form of Eq. (7).

The diffusion phenomenon also poses challenges in the understanding of fundamental concepts in statistical physics, such as entropy [10] and general properties as correlation functions [52], ergodicity [15, 17, 54–59], Khinchin theorem [15, 54], FDT [11, 60], and so on. In biological systems, where motion [42] and pattern formation [61–63] are tangled, diffusion has still important contributions to be done. A very broad and growing area is that of synchronization [14, 64–66], in which one expects the scaling may produce more analytical results. In nonlinear phenomena, such as growth and etching [67–69], analytical results are rather difficult to obtain. For example, the KPZ equation has exact solution for one-dimension. However, solutions for higher dimensions have been not found; as in many other areas of nonequilibrium physics, where even not exact solutions can be considered major results. In this way, we hope that this work may inspire research into similar asymptotic limits.

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